The density of highly localized states in disordered systems

N. M. Storonskii and B. I. Fuks

Institute of Radio Engineering and Electronics, Academy of Sciences of the USSR, Moscow
(Submitted 20 December 1990; revised 7 August 1991)
Zh. Eksp. Teor. Fiz. **100**, 1873–1892 (December 1991)

An asymptotically exact expression is derived for the density $\rho(\varepsilon)$ of localized states of a particle in a d-dimensional random field. It is shown that in the continuum approximation the pre-exponential factor in the expression for $\rho(\varepsilon)$ is the inverse of the product of the root-mean-square variations of the potential energy and the volume corresponding to concentration fluctuations close to the optimum, is fairly large, and is especially important in the Poisson section of the localized-state spectrum, where the exponent in $\rho(\varepsilon)$ increases fairly slowly with the binding energy ε. Allowing for the discreteness of the centers in deriving an asymptotically exact expression for $\rho(\varepsilon)$ causes (a) an increase in the binding energy by a second-order correction that appears when one allows for the potential of individual scatterers and (b) an increase in $\rho(\varepsilon)$. If the particle space is three-dimensional and the scatterers are weak, allowing for the discreteness of the latter results in a significant renormalization of the boundary of the localized-state spectrum. ρ vs. ε dependence in the random three-dimensional field of centers with an attractive potential $u(\mathbf{r}) \propto r^{-1} \exp(-Qr)$ is also calculated. Comparison of the results with those of the extensively cited research of Halperin and Lax based on the use of the Gaussian and continuum approximations defines the applicability range for these approximations. It is revealed that for such a potential the Gaussian approximation is applicable only for extremely small ε. In heavily doped semiconductors the approximation almost always strongly underestimates $\rho(\varepsilon)$ in the "tails" of the density of states, especially for large ε. On the other hand, the effect of the discreteness of the centers proves important in the region of small ε.

1. INTRODUCTION

This paper is devoted to finding the density $\rho(\varepsilon)$ of strongly localized states in the field of randomly distributed scattering centers. We are speaking of states with a binding energy ε so high that the overwhelming contribution to $\rho(\varepsilon)$ is provided by the ground states of particles localized on large, and therefore infrequent, center fluctuations. The characteristic scale over which the wave function of these states decreases is much smaller than the distance between the fluctuations, which means that the states can be considered independent. In studies of the "tails" of the density of states this problem has been solved in a number of papers, among which the basic ones are Refs. 1–4 (see also Refs. 5 and 6). At their base lies the so-called optimal-fluctuation method. The most general account of this method is given in Ref. 4, where it is used in the continuum approximation to derive expressions that define for an arbitrary random field the expontentially small density of states $\rho(\varepsilon)$ with logarithmic accuracy (without the pre-exponential factor). The latter was found in the three-dimensional case numerically in Ref. 1 only for Gaussian fluctuations of centers with the potential $u(\mathbf{r}) \propto (1/r)e^{-Qr}$.

To find $\rho(\varepsilon)$ with absolute accuracy one must go beyond the framework of the optimal-fluctuation equation, which describes states created by the continuum fluctuations of the scatterer concentration, and allow for the discreteness of these scatterers. Approaches to this problem have been developed in Refs. 2 and 3 only for Gaussian fluctuations. Development of the approach suggested in Ref. 2, applicable only for a random field of the "white noise" type, which is generated by the Gaussian fluctuations of point scatterers, $u(\mathbf{r}) \propto \delta(\mathbf{r})$, made it possible to obtain an expression for $\rho(\varepsilon)$ in the two- and three-dimensional cases that is exact in the limit of high binding energies.[7–9] The approach suggested in Ref. 3 can be applied to centers with a potential of a fairly arbitrary shape, but it provides only an approximate description of $\rho(\varepsilon)$ with unknown accuracy. In this paper we derive an asymptotically exact (as in Refs. 2 and 8) expression for $\rho(\varepsilon)$ for uncorrelated fluctuations without resorting to such abstractions as a point potential of a center or the Gaussian nature of fluctuations, abstractions that strongly distort the physics of the process in real situations (see Sec. 4 of Ref. 10) and in some cases are totally inappropriate.[9] In Sec. 2 the density of states $\rho(\varepsilon)$ is calculated in the continuum approximation and the pre-exponential factor in $\rho(\varepsilon)$ is shown to be fairly large, increasing with the binding energy and the number of dimensions of the scatterer space. In Sec. 3 we derive the final asymptotically exact expression for $\rho(\varepsilon)$, which surpasses the result obtained in the continuum approximation more, the smaller the overlap of the potentials of the centers and the smaller the characteristic radii of the potentials as compared to the radius of the wave function. Finally, in Sec. 4 we show how greatly the results of the numerical calculation with $u(\mathbf{r}) \propto r^{-1} \exp(-Qr)$ of Ref. 1 are modified owing to rejection of the Gaussian approximation and allowance for the discreteness of the centers.

2. THE DENSITY OF STATES IN THE CONTINUUM APPROXIMATION

Consider the localization of a particle in a field of randomly distributed scatterers such that the particle's potential energy at point $\mathbf{r}$ of the space R caused by the presence of a center at point $\mathbf{l}$ of space L is equal to $u(\mathbf{r}-\mathbf{l})$. The particle space R and the scatterer space L do not necessarily coincide (say, in heterostructures of different types) and may even be of different dimensions.[11] Calculations of $\rho(\varepsilon)$ are simplified by employing the method of successive approximations.

 0038-5646/91/121036-10$03.00

We use this method to find the probability density of states $P(\varepsilon)$ equal to[4]

$$P(\varepsilon)=\langle\delta[\varepsilon-\varepsilon_0(\mathbf{l}_j)]\rangle. \tag{1}$$

Here $\mathbf{l}_j$ stands for the coordinates of the centers, the angle brackets designate averaging over all the $\mathbf{l}_j$'s, and $\varepsilon_0(\mathbf{l}_j)$ is the energy of the ground state described by the Schrödinger equation

$$-\frac{\hbar^2}{2m}\Delta\psi(\mathbf{r})+\left[\sum_j u(\mathbf{r}-\mathbf{l}_j)-\bar{\varepsilon}\right]\psi(\mathbf{r})=\varepsilon_0(\mathbf{l}_j)\psi(\mathbf{r}) \tag{2}$$

with $\bar{\varepsilon}=N\int d\,\mathbf{l}u(\mathbf{r}-\mathbf{l})$, and N the average center concentration (i.e., the energy is reckoned from the average-potential level). We select the initial continuum fluctuation $\xi_{i\varepsilon}(\mathbf{l})$ generating the potential $V_{i\varepsilon}(\mathbf{r})=\int d\,\mathbf{l}\xi_{i\varepsilon}(\mathbf{l})u(\mathbf{r}-\mathbf{l})$ in such a manner that the ground-state energy of a particle of mass m is ε:

$$-\frac{\hbar^2}{2m}\Delta\psi_{i\varepsilon}(\mathbf{r})+V_{i\varepsilon}(\mathbf{r})\psi_{i\varepsilon}(\mathbf{r})=\varepsilon\psi_{i\varepsilon}(\mathbf{r}). \tag{3}$$

Equations (2) and (3) imply that in first-order perturbation theory

$$\varepsilon_0(\mathbf{l}_j)=\varepsilon+\int d\mathbf{r}\psi_{i\varepsilon}^2(\mathbf{r})\left[\sum_j u(\mathbf{r}-\mathbf{l}_j)-\bar{\varepsilon}-V_{i\varepsilon}(\mathbf{r})\right].$$

Substituting this into (1), we arrive at the following expression for the uncorrelated distributions of centers after averaging over all the $\mathbf{l}_j$'s:

$$P_1(\varepsilon)=\int_{-\infty}^{\infty}\frac{d\lambda}{2\pi}\exp\left\{i\lambda\int d\mathbf{l}g_{i\varepsilon}(\mathbf{l})[\xi_{i\varepsilon}(\mathbf{l})+N]+N\times\int d\mathbf{l}[\exp[-i\lambda g_{i\varepsilon}(\mathbf{l})]-1]\right\} \tag{4}$$

with $g_{i\varepsilon}(\mathbf{l})=\int d\mathbf{r}\psi_{i\varepsilon}^2(\mathbf{r})u(\mathbf{r}-\mathbf{l})$. The points of maxima and minima of the integrand in (4), λ_m, are solutions of the following equation:

$$\int d\mathbf{l}g_{i\varepsilon}(\mathbf{l})[\xi_{i\varepsilon}(\mathbf{l})+N]=N\int d\mathbf{l}[\exp[-i\lambda_m g_{i\varepsilon}(\mathbf{l})]-1].$$

When $u(\mathbf{r})$ does not change sign and, hence, $g_{i\varepsilon}(\mathbf{l})$ does not either, among the λ_m there is always a unique imaginary point $\lambda_0=-i\alpha$ corresponding to a maximum, in view of the condition that $\xi_{i\varepsilon}(\mathbf{l})+N>0$. For ε negative, when $\int d\,\mathbf{l}g_{i\varepsilon}(\mathbf{l})\xi_{i\varepsilon}(\mathbf{l})<0$ is negative, α is always positive. For many-particle fluctuations (for greater details see below), the neighborhood of point λ_0 provides the main contribution to the integral in (4). Evaluating this integral by the method of steepest descents, we find that

$$P_1(\varepsilon)=\left[2\pi N\int d\mathbf{l}\exp[-\alpha g_{i\varepsilon}(\mathbf{l})]g_{i\varepsilon}^2(\mathbf{l})\right]^{-1/2}\times\exp\left\{\alpha\int d\mathbf{l}g_{i\varepsilon}(\mathbf{l})[\xi_{i\varepsilon}(\mathbf{l})+N]+N\int d\mathbf{l}[\exp[-\alpha g_{i\varepsilon}(\mathbf{l})]-1]\right\}. \tag{5}$$

When states with high binding energies are involved, $P_1(\varepsilon)$ is determined primarily by the value of the expression within the braces on the right-hand side of (5). Denoting this expression by $S(\varepsilon,\xi)$, introducing the notation $\xi_{f\varepsilon}\equiv N(e^{-\alpha g_{i\varepsilon}(\mathbf{l})}-1)$ and $\delta\xi_\varepsilon\equiv\xi_{f\varepsilon}-\xi_{i\varepsilon}$, and writing the equation for α in the form

$$\int d\mathbf{l}\ln\left(1+\frac{\xi_{f\varepsilon}}{N}\right)\delta\xi_\varepsilon=0,$$

we can use (5) to find the following two expressions for $S(\varepsilon,\xi)$:

$$S(\varepsilon,\xi)=\int d\mathbf{l}\left[(\xi_{i\varepsilon}+N)\ln\left(1+\frac{\xi_{f\varepsilon}}{N}\right)-\xi_{f\varepsilon}\right]$$

$$=\int d\mathbf{l}\left[(\xi_{f\varepsilon}+N)\ln\left(1+\frac{\xi_{f\varepsilon}}{N}\right)-\xi_{f\varepsilon}\right]$$

$$S(\varepsilon,\xi)=\int d\mathbf{l}\left\{\left[(\xi_{i\varepsilon}+N)\ln\left(1+\frac{\xi_{i\varepsilon}}{N}\right)-\xi_{i\varepsilon}\right]+\left[(\xi_{i\varepsilon}+N)\ln\left(1+\frac{\delta\xi_\varepsilon}{\xi_{i\varepsilon}+N}\right)-\delta\xi_\varepsilon\right]\right\}.$$

The first expression reveals that $S(\varepsilon,\xi)$ is the increase in entropy caused by the continuum fluctuation $\xi_{f\varepsilon}(\mathbf{l})$, while the second expression combined with the fact that $\xi_\varepsilon+N$ is positive and $\ln(1+x)-x$ is negative for $-1<x<\infty$ implies that $S(\varepsilon,\xi)$ is smaller than the increase in entropy caused by the fluctuation $\xi_{i\varepsilon}(\mathbf{l})$, that is, the probability of a fluctuation $\xi_{f\varepsilon}(\mathbf{l})$ forming is always higher than that of any initial fluctuation $\xi_{i\varepsilon}(\mathbf{l})$ if $\delta\xi_\varepsilon(\mathbf{l})\not\equiv 0$.

For the Schrödinger equation (3) with a potential $V_{f\varepsilon}$ generated by fluctuation $\xi_{f\varepsilon}$ instead of $\xi_{i\varepsilon}$, the ground-state binding energy exceeds $|\varepsilon|$, that is, the energy ε corresponds to $V_{f\varepsilon}$ for $\psi_{i\varepsilon}(\mathbf{r})$, while the exact wave functions yields the greatest binding energy. The binding energy $|\varepsilon|$ is generated by a fluctuation smaller than $\xi_{f\varepsilon}(\mathbf{l})$, say $N(e^{-\alpha_1 g_{i\varepsilon}(\mathbf{l})}-1)$, with $\alpha>\alpha_1>0$ (the value of α_1 is found from the solution of the Schrödinger equation), a binding energy corresponding to a probability density greater than $P_1(\varepsilon)$. Using this fluctuation instead of $\xi_{i\varepsilon}(\mathbf{l})$, we can again derive (5) and obtain a higher value of the probability density, say $P_2(\varepsilon)$ and an expression for the fluctuation that realizes $P_2(\varepsilon)$. Each time this procedure is repeated, the value of $P_n(\varepsilon)$ increases. Its limit in the class of continuum fluctuations, $\tilde{P}(\varepsilon)$, is attained at an initial fluctuation $\tilde{\xi}_\varepsilon(\mathbf{l})$ such that $\delta\tilde{\xi}_\varepsilon(\mathbf{l})=0$. This implies that

$$\tilde{\xi}_\varepsilon(\mathbf{l})=N\{\exp[-\tilde{\alpha}\tilde{g}_\varepsilon(\mathbf{l})]-1\}, \tag{6}$$

$$-\frac{\hbar^2}{2m}\Delta\tilde{\psi}_\varepsilon(\mathbf{r})+\left[\int d\mathbf{l}\tilde{\xi}_\varepsilon(\mathbf{l})u(\mathbf{r}-\mathbf{l})-\varepsilon\right]\tilde{\psi}_\varepsilon(\mathbf{r})=0, \tag{7}$$

$$\tilde{g}_\varepsilon(\mathbf{l})=\int d\mathbf{r}\tilde{\psi}_\varepsilon^2(\mathbf{r})u(\mathbf{r}-\mathbf{l}), \tag{8}$$

where $\tilde{\alpha}$ is a parameter determined as a result of solving the system of equations (6)–(8). The value of $\tilde{P}(\varepsilon)$ is then given by the following equation:

$$P(\varepsilon)=\left[2\pi N\int d\mathbf{l}\exp[-\tilde{\alpha}\tilde{g}_\varepsilon(\mathbf{l})]\tilde{g}_\varepsilon^2(\mathbf{l})\right]^{-1/2}\times\exp\left\{\tilde{\alpha}\int d\mathbf{l}\tilde{g}_\varepsilon(\mathbf{l})N\times\exp[-\tilde{\alpha}\tilde{g}_\varepsilon(\mathbf{l})]+N\int d\mathbf{l}[\exp[-\tilde{\alpha}\tilde{g}_\varepsilon(\mathbf{l})]-1]\right\}. \tag{9}$$

The system of equations (6)–(8) can be written as follows:

$$-\frac{\hbar^2}{2m}\Delta\tilde{\psi}_\varepsilon(\mathbf{r})+\left\{N\int d\mathbf{l}\left[\exp\left(-\tilde{\alpha}\int d\mathbf{r}_1\tilde{\psi}_\varepsilon^2(\mathbf{r}_1)u(\mathbf{r}_1-\mathbf{l})\right)-1\right]u(\mathbf{r}-\mathbf{l})-\varepsilon\right\}\times\tilde{\psi}_\varepsilon(\mathbf{r})=0. \tag{10}$$

This is the equation of an optimal fluctuation (an optimal wave function) derived in Ref. 4. Equations (9) and (10) are valid if the fluctuation is of a many-particle origin, or

$$\bar{n}_\varepsilon + Z_\varepsilon \gg 1 \tag{11}$$

and if it is relatively infrequent, or

$$(\bar{n}_\varepsilon + Z_\varepsilon) \ln (1 + Z_\varepsilon/\bar{n}_\varepsilon) - Z_\varepsilon \gg 1. \tag{12}$$

Here $\bar{n}_\varepsilon \propto N l_\xi^d$, $Z_\varepsilon = \int d\mathbf{l}\, \xi_\varepsilon(\mathbf{l})$, l_ξ is the characteristic size of the optimal fluctuation, and d the number of dimensions of space L.

Deriving Eqs. (9) and (10) by the method of successive approximations reveals that the continuum approach is equivalent to allowing for the contribution of discrete scatterers to the binding energy in the first-order perturbation theory setting. This makes it possible to simplify the calculation of $\rho(\varepsilon)$ considerably:

$$\rho(\varepsilon) = V_L^{-1} \left\langle \sum \delta[\varepsilon - \varepsilon_s(\mathbf{l}_j)] \right\rangle \tag{13}$$

with $\varepsilon_s(\mathbf{l}_j)$ the energy eigenvalues of the single-particle Schrödinger equation corresponding to the set of quantum numbers s, and V_L the volume of the L-space. As before, we allow only for the ground-state contribution. As a quantum number we take $\mathbf{L}_s$, the centroid of the fluctuation localizing the particle (the definition of $\mathbf{L}_s$ is given below). Hence $\varepsilon_s(\mathbf{l}_j) = \varepsilon_0(\mathbf{L}_s, \mathbf{l}_j)$ in (13). Below, in calculating $\rho(\varepsilon)$ in the continuum approximation we use the wave functions $\tilde{\psi}_\varepsilon(\mathbf{r} - \mathbf{L}_s)$ corresponding to the optimal fluctuation $\tilde{\xi}_\varepsilon(\mathbf{l} - \mathbf{L}_s)$ and allow for the contribution of centers to $\varepsilon_s(\mathbf{l}_j)$ in first-order perturbation theory. Since for a translation-invariant space L the integral $\int d\mathbf{l} \tilde{\xi}_\varepsilon(\mathbf{l} - \mathbf{L}_s) \tilde{g}_\varepsilon(\mathbf{l} - \mathbf{L}_s)$ is independent of $\mathbf{L}_s$, we have

$$\varepsilon_0(\mathbf{L}_s, \mathbf{l}_j) = \varepsilon + \sum_j \tilde{g}_\varepsilon(\mathbf{l}_j - \mathbf{L}_s) - \bar{\varepsilon} - \int d\mathbf{l} \tilde{\xi}_\varepsilon(\mathbf{l}) \tilde{g}_\varepsilon(\mathbf{l})$$

and Eq. (13) assumes the form

$$\tilde{\rho}(\varepsilon) = V_L^{-1} \left\langle \sum_s \delta \left[\int d\mathbf{l} (\tilde{\xi}_\varepsilon(\mathbf{l}) + N) \tilde{g}_\varepsilon(\mathbf{l}) - \sum_j \tilde{g}_\varepsilon(\mathbf{l}_j - \mathbf{L}_s) \right] \right\rangle. \tag{14}$$

The values of $\mathbf{L}_s$ are found by minimizing $\varepsilon_0(\mathbf{L}_s, \mathbf{l}_j)$ for given $\mathbf{l}_j$. Below, as in Ref. 1, they are found from the condition

$$\frac{\partial}{\partial \mathbf{L}} \sum_j \tilde{g}_\varepsilon(\mathbf{l}_j - \mathbf{L}) \Big|_{\mathbf{L} = \mathbf{L}_s} = 0.$$

Of course, with such a definition of $\mathbf{L}_s$ the contribution to $\tilde{\rho}(\varepsilon)$ from (14) is provided not only by the optimal-fluctuation centering points, which correspond to the absolute maxima in the binding energy generated by the centers in the given fluctuation, but also by the "superfluous" centering points corresponding to "saddles" and local maxima in the binding energy. However, the contribution of the second type of points to $\tilde{\rho}(\varepsilon)$ is exponentially small, since at the superfluous points only excessively localized fluctuations generate a state with energy ε.

Using the definition of $\mathbf{L}_s$, we can simplify Eq. (14):

$$\tilde{\rho}(\varepsilon) = \left\langle \delta \left[\int d\mathbf{l} (\tilde{\xi}_\varepsilon(\mathbf{l}) + N) \tilde{g}_\varepsilon(\mathbf{l}) - \sum_j \tilde{g}_\varepsilon(\mathbf{l}_j) \right] \times \delta \left[\sum_j \frac{\partial}{\partial \mathbf{l}_j} \tilde{g}_\varepsilon(\mathbf{l}_j) \right] \det \sum_j \nabla_{\mathbf{l}_j} \nabla_{\mathbf{l}_j} \tilde{g}_\varepsilon(\mathbf{l}_j) \right\rangle. \tag{15}$$

Then, expanding the delta function in Fourier integrals in λ and $\mathbf{k}$ and averaging over all the l_j's, we find

$$\tilde{\rho}(\varepsilon) = \int \frac{d\lambda}{2\pi} \int \frac{d\mathbf{k}}{(2\pi)^d} \exp \left\{ \int d\mathbf{l} (\tilde{\xi}_\varepsilon + N) \tilde{g}_\varepsilon + N \int d\mathbf{l} \left[\exp \left(-i\lambda \tilde{g}_\varepsilon - i\mathbf{k} \frac{\partial g_\varepsilon}{\partial \mathbf{l}} \right) - 1 \right] \right\} \times \det N \int d\mathbf{l} \exp \left(-i\lambda \tilde{g}_\varepsilon - i\mathbf{k} \frac{\partial g_\varepsilon}{\partial \mathbf{l}} \right) \nabla_{\mathbf{l}} \nabla_{\mathbf{l}} \tilde{g}_\varepsilon(\mathbf{l}), \tag{16}$$

where we have retained only the leading terms that emerge as a result of averaging the determinant. The other terms are small in view of the multiparticle nature of $\tilde{\xi}_\varepsilon(\mathbf{l})$ [see condition (11)] and, hence, the weak correlation of the co-factors in each term of the expansion of the determinant. In further calculations we allow for the fact that under condition (11) the main contribution to the integral is provided by small values of k and therefore retain in the exponent only terms of the lowest (second) order in k. The integral with respect to λ in (16) can easily be evaluated, since the weak (algebraic) dependence on λ of the pre-exponential factor in the integrand and condition (11) suggest that the principal saddle point differs little from $-i\alpha$ [see the discussion related to the derivation of Eq. (5)]. Going over to the major axes in the space L, in terms of which the quadratic form $\int d\mathbf{l} (\tilde{\xi}_\varepsilon + N)(\partial^2 \tilde{g}_\varepsilon / \partial l_i \partial l_k) \equiv \int d\mathbf{l} (\tilde{\xi}_\varepsilon + N)(\partial \tilde{g}_\varepsilon / \partial l_i)(\partial \tilde{g}_\varepsilon / \partial l_k)$ is diagonal, and integrating with respect to $\mathbf{k}$, we obtain

$$\tilde{\rho}(\varepsilon) = \rho_d(\varepsilon) \tilde{P}(\varepsilon), \tag{17}$$

where $\tilde{P}(\varepsilon)$ is defined in (9), and

$$\rho_d(\varepsilon) = \prod_{i=1}^{d} \left\{ \frac{1}{2\pi} \int d\mathbf{l} (\tilde{\xi}_\varepsilon + N) \left[\frac{\partial}{\partial l_i} \ln \left(1 + \frac{\tilde{\xi}_\varepsilon}{N} \right) \right]^2 \right\}^{1/2}. \tag{18}$$

For a spherically symmetric potential and mass this formula acquires the following form after integration with respect to the angle variables:

$$\rho_d(\varepsilon) = \left\{ \frac{\pi^{d/2-1}}{2(d/2)!} \int_0^\infty dl\, l^{d-1} (\tilde{\xi}_\varepsilon + N) \left[\frac{\partial}{\partial l} \ln \left(1 + \frac{\tilde{\xi}_\varepsilon}{N} \right) \right]^2 \right\}^{d/2}. \tag{18a}$$

Let us examine the behavior of the pre-exponential factor in $\tilde{\rho}(\varepsilon)$ (the behavior of the exponent, first derived in Ref. 4, has been studied extensively in Ref. 6). This factor is equal to the product of $\rho_d(\varepsilon)$ and the pre-exponential factor in (9), with the latter having the dimensions of inverse energy, $\propto \varepsilon_f^{-1}$. A physical estimate of ε_f yields $\varepsilon_f \sim |\bar{g}_\varepsilon| \sqrt{\bar{n}_\varepsilon + Z_\varepsilon}^{1/2}$, where $\bar{g}_\varepsilon$ is the characteristic value of $\tilde{g}_\varepsilon(\mathbf{l})$ in the optimal-fluctuation volume, which means that ε_f is the mean-square fluctuation of the potential energy in clusters of centers that are close to the optimal fluctuation and consist of approximately $\bar{n}_\varepsilon + Z_\varepsilon$ centers. Here ε_f is much lower than $|Z_\varepsilon \bar{g}_\varepsilon|$, the potential energy in the optimal

fluctuation, since for infrequent many-particle fluctuations Z_ε^2 is always much higher than $\bar{n}_\varepsilon + Z_\varepsilon$. A similar estimate of $\rho_d(\varepsilon)$ shows that $\rho_d^{-1}(\varepsilon) \sim [l_\xi(\bar{n}_\varepsilon + Z_\varepsilon)/Z_\varepsilon^2)^{1/2}]^d$, that is, the pre-exponential factor in $\tilde{\rho}(\varepsilon)$ contains not the characteristic volume of an optimal fluctuation but a far smaller mean-square fluctuation of this volume. Thus, the pre-exponential factor in $\tilde{\rho}(\varepsilon)$ can be estimated as $(l_\xi^d|Z_\varepsilon \bar{g}_\varepsilon|)^{-1}[Z_\varepsilon^2/(\bar{n}_\varepsilon + Z_\varepsilon)]^{(d+1)/2}$. In addition to the characteristic energy and volume, it contains a large factor $[Z_\varepsilon^2/(\bar{n}_\varepsilon + Z_\varepsilon)]^{(d+1)/2}$, which increases with the binding energy all the faster the higher the number of dimensions of space L.

3. ALLOWING FOR THE DISCRETENESS OF THE SCATTERING CENTERS

To find an asymptotically exact expression for $\rho(\varepsilon)$ we must go beyond the framework of the continuum approach, namely, we must allow for the contribution of second-order correction terms to the energy of the ground state in the Schrödinger equation (2) (by doing so, we take into account the effect of the potential of a separate center on the wave function of the state, i.e., the discreteness of the centers). Using the optimal fluctuation $\tilde{\xi}_{\varepsilon'}(\mathbf{l})$, which in the continuum approximation (see Sec. 2) defines a density of states with energy ε' such that the average value of the second-order correction to the energy of these states, $-\Gamma(\varepsilon')$, is equal to $\varepsilon - \varepsilon'$ [the value of $\Gamma(\varepsilon')$ is found below], the energies ε'_m and the wave functions $\tilde{\psi}_{\varepsilon' m}(\mathbf{r})$ of the time-independent states of the Schrödinger equation, whose potential generates $\tilde{\xi}_{\varepsilon'}(\mathbf{l})$ (for this reason, $\varepsilon'_0 \equiv \varepsilon'$ and $\tilde{\psi}_{\varepsilon' 0} \equiv \psi_{\varepsilon'}$), from Eq. (2) we obtain

$$\varepsilon_0(\mathbf{l}_j) = \varepsilon' + \int d\mathbf{r} \tilde{\psi}_{\varepsilon'}^2 \Big[\sum_j u(\mathbf{r}-\mathbf{l}_j) - \bar{\varepsilon} - \bar{V}_{\varepsilon'} \Big] + \sum_{m=1}^{\infty} \Big| \int d\mathbf{r} \tilde{\psi}_{\varepsilon'} \tilde{\psi}_{\varepsilon' m}^{*} \Big[\sum_j u(\mathbf{r}-\mathbf{l}_j) - \bar{\varepsilon} - \bar{V}_{\varepsilon'} \Big] \Big|^2 \frac{1}{\varepsilon' - \varepsilon_m'}. \tag{19}$$

The contribution of the second-order correction to (19), which depends on $\mathbf{l}_j$ is always small when condition (12) is met (see below). However, the relatively small variations of the large exponent in $\rho(\varepsilon)$, which emerge after (19) is substituted into (13), increase $\rho(\varepsilon)$ significantly.

Combining this with (19), we can write Eq. (15) as follows:

$$\rho(\varepsilon) = \Big\langle \delta\Big[\varepsilon - \varepsilon' + \int d\mathbf{l}(\tilde{\xi}_{\varepsilon'} + N)\tilde{g}_{\varepsilon'} - \sum_j \tilde{g}_{\varepsilon'}(\mathbf{l}_j) - \sum_{m=1}^{\infty} \Big| \int d\mathbf{l}(\tilde{\xi}_{\varepsilon'} + N)\tilde{g}_{\varepsilon' m} - \sum_j \tilde{g}_{\varepsilon' m}(\mathbf{l}_j) \Big|^2 \frac{1}{\varepsilon' - \varepsilon_m'} \Big] \times \delta\Big[\sum_j \frac{\partial}{\partial \mathbf{l}_j} \tilde{g}_{\varepsilon'}(\mathbf{l}_j) \Big] \det \sum_j \nabla_{\mathbf{l}_j} \nabla_{\mathbf{l}_j} \tilde{g}_{\varepsilon'}(\mathbf{l}_j) \Big\rangle, \tag{20}$$

where $\tilde{g}_{\varepsilon' m} = \int d\mathbf{r} \tilde{\psi}_{\varepsilon'} \tilde{\psi}_{\varepsilon' m}^{*} u(\mathbf{r} - \mathbf{l})$. To calculate $\rho(\varepsilon)$, we generalize the method developed in Ref. 2 and expand the arguments of the delta functions in Eq. (20) in a complete system of functions orthogonal in L with a weight function $\tilde{\xi}_{\varepsilon'}(\mathbf{l}) + N$, to which end we consider the eigenfunctions $\chi_n(\mathbf{r})$ that vanish at infinity and the eigenvalues γ_n of the following integro-differential equation:

$$\Big[-\frac{\hbar^2}{2m}\Delta + \bar{V}_{\varepsilon'}(\mathbf{r}) - \varepsilon' \Big] \chi_n(\mathbf{r}) - \gamma_n 2\bar{\alpha} \times \int d\mathbf{r}_1 \psi_{\varepsilon'}(\mathbf{r}) \psi_{\varepsilon'}(\mathbf{r}_1) K(\mathbf{r}, \mathbf{r}_1) \chi_n(\mathbf{r}_1) = 0 \tag{21}$$

with $K(\mathbf{r},\mathbf{r}_1) = \int d\mathbf{l}\big[\tilde{\xi}_{\varepsilon'}(\mathbf{l}) + N\big] u(\mathbf{r} - \mathbf{l}) u(\mathbf{r}_1 - \mathbf{l})$. It can be demonstrated that the eigenfunction of the ground state, $\chi_0(\mathbf{r})$, is proportional to $\tilde{\psi}_\varepsilon(\mathbf{r})$ and that $\gamma_0 = 0$ and is nondegenerate. The remaining γ_n are real [hence, all the $\chi_n(\mathbf{r})$ can be selected real] and positive. Equation (21) has a d-fold degenerate eigenvalue $\gamma_1 = 1$. The wave function $\chi_i(\mathbf{r})$ corresponding to this eigenvalue is proportional to $\partial \tilde{\psi}_{\varepsilon'}(\mathbf{r})/\partial r_i$, where the r_i are the components of $\mathbf{r}$ parallel to the translation-invariant space L.

Let us introduce the functions $h_n(\mathbf{l}) = \int d\mathbf{r} \psi_{\varepsilon'}(\mathbf{r}) \chi_n(\mathbf{r}) u(\mathbf{r} - \mathbf{l})$. Equation (21) implies that for $\gamma_n \neq \gamma_p$ the functions h_n and h_p are mutually orthogonal with a weight function $\tilde{\xi}_{\varepsilon'} + N$. The functions $h_n(\mathbf{l})$ belonging to a degenerate eigenvalue can be orthogonalized by appropriate choice; for instance, the functions $h_i(\mathbf{l}) = \int d\mathbf{r} \psi_{\varepsilon'}(\mathbf{r}) \chi_i(\mathbf{r}) u(\mathbf{r} - \mathbf{l}) \sim \partial \tilde{g}_{\varepsilon'}(\mathbf{l})/\partial l_i$ can be mutually orthogonalized if the $\mathbf{l}_i$ are directed along the major axes introduced in deriving Eq. (17). We normalize the $\chi_n(\mathbf{r})$ in such a manner that the system of orthogonal functions $h_n(\mathbf{l})$ becomes orthonormal:

$$\int d\mathbf{l}[\tilde{\xi}_{\varepsilon'}(\mathbf{l}) + N] h_n(\mathbf{l}) h_p(\mathbf{l}) = \delta_{np}. \tag{22}$$

Equation (21) can be reduced to an integral equation by employing the Green's function $\bar{G}(\mathbf{r},\mathbf{r}_1)$ of the Schrödinger equation

$$\Big[-\frac{\hbar^2}{2m}\Delta + \bar{V}_{\varepsilon'}(r) - \varepsilon' \Big] \bar{G}(\mathbf{r}, \mathbf{r}_1) = \delta(\mathbf{r} - \mathbf{r}_1) - \psi_{\varepsilon'}(\mathbf{r}) \psi_{\varepsilon'}(\mathbf{r}_1), \tag{23}$$

which has the form

$$G(\mathbf{r}, \mathbf{r}_1) = \sum_{m=1}^{\infty} \frac{1}{\varepsilon' - \varepsilon_m'} \tilde{\psi}_{\varepsilon'}(\mathbf{r}) \tilde{\psi}_{\varepsilon' m}^{*}(\mathbf{r}_1).$$

Combining Eqs. (21) and (23) yields

$$\chi_n(\mathbf{r}) - \bar{\psi}_{\varepsilon'}(\mathbf{r}) \int d\mathbf{r}_1 \bar{\psi}_{\varepsilon'}(\mathbf{r}_1) \chi_n(\mathbf{r}_1) = \gamma_n 2\bar{\alpha} \iint d\mathbf{r}_1 \, d\mathbf{r}_2 \bar{G}(\mathbf{r}, \mathbf{r}_1) \bar{\psi}_{\varepsilon'}(\mathbf{r}_1) \bar{\psi}_{\varepsilon'}(\mathbf{r}_2) K(\mathbf{r}_1, \mathbf{r}_2) \chi_n(\mathbf{r}_2).$$

Multiplying both sides of this equation by $\psi_{\varepsilon'}(\mathbf{r}) u(\mathbf{r} - \mathbf{l})$ and integrating with respect to $\mathbf{r}$, we obtain an integral equation in the space L:

$$h_n(\mathbf{l}) - b_n h_0(\mathbf{l}) = \gamma_n 2\bar{\alpha} \int d\mathbf{l}_1 [\tilde{\xi}_{\varepsilon'}(\mathbf{l}_1) + N] \Gamma(\mathbf{l}, \mathbf{l}_1) h_n(\mathbf{l}_1), \tag{24}$$

where

$$\Gamma(\mathbf{l}_1,\mathbf{l}_1) = \iint d\mathbf{r} \, d\mathbf{r}_1 \bar{G}(\mathbf{r}, \mathbf{r}_1) \bar{\psi}_{\varepsilon'}(\mathbf{r}) \bar{\psi}_{\varepsilon'}(\mathbf{r}_1) u(\mathbf{r} - \mathbf{l}) u(\mathbf{r} - \mathbf{l}_1) = \sum_{m=1}^{\infty} \frac{\tilde{g}_{\varepsilon' m}(\mathbf{l}) \tilde{g}_{\varepsilon' m}^{*}(\mathbf{l}_1)}{\varepsilon_m' - \varepsilon'}, \tag{25}$$

and $b_n = \int d\mathbf{r} \tilde{\psi}_{\varepsilon'}^2(\mathbf{r}) \chi_n(\mathbf{r}) \chi_0(\mathbf{r})$. The symmetric kernel $\Gamma(\mathbf{l},\mathbf{l}_1)$ is positive definite in the class of functions tending to

zero at infinity [this can be proved by employing Eq. (25) and the fact that the system of functions $\tilde{\psi}_{\varepsilon' m(r)}$ is complete]. For this reason, the functions $h_n(\mathbf{l})$ with $n \geqslant 1$, which are eigenfunctions of the projection of $\Gamma(\mathbf{l},\mathbf{l}_1)$ on the subspace L' orthogonal to $h_0(\mathbf{l})$ with a weight function $\tilde{\xi}_{\varepsilon'} + N$, constitute a complete system in L'. Hence, the system of functions $h_n(\mathbf{l})$ with $n \geqslant 0$ is complete in L, and from Eqs. (22) and (24) it follows that

$$\Gamma(\mathbf{l},\mathbf{l}_1) = \frac{1}{2\tilde{\alpha}}\Big\{ c h_0(\mathbf{l}) h_0(\mathbf{l}_1) + \sum_{i=1}^{d} h_i(\mathbf{l}) h_i(\mathbf{l}_1) + \sum_{i=d+1}^{\infty} \gamma_n^{-1} [h_n(\mathbf{l}) - b_n h_0(\mathbf{l})][h_n(\mathbf{l}_1) - b_n h_0(\mathbf{l}_1)] \Big\}, \quad (26)$$

where c is a constant and we have allowed for the fact that $b_i = 0$, that is, $\int d\mathbf{r} \tilde{\psi}_{\varepsilon'} (\partial \psi_{\varepsilon'}/\partial \mathbf{r}_i) = 0$, and $b_0 = 1$.

By employing (25) and (26) the terms in (20) can be expressed in terms of the functions $h_n(\mathbf{l})$. Allowing for the fact that $\int d\mathbf{l} (\tilde{\xi}_{\varepsilon'} + N) h_i = 0$ and introducing the notation $G = [\int d\mathbf{l} (\tilde{\xi}_{\varepsilon'} + N) \tilde{g}_{\varepsilon'}^2]^{1/2}$ and $K_i = [\int d\mathbf{l} (\tilde{\xi}_{\varepsilon'} + N) (\partial \tilde{g}_{\varepsilon'}/\partial l_i)^2]^{1/2}$, we obtain

$$\rho(\varepsilon) = \prod_{n=0}^{\infty} \int ds_n \int \frac{d\lambda_n}{2\pi} \times \exp\Big\{ i\lambda_n \Big[\int d\mathbf{l} [\tilde{\xi}_{\varepsilon'} + N] h_n - s_n \Big] \Big\} \delta\Big\{ \varepsilon - \varepsilon' + G s_0 + \frac{1}{2\tilde{\alpha}} \Big[c s_0^2 + \sum_{n=d+1}^{\infty} \gamma_n^{-1} (s_n - b_n s_0)^2 \Big] \Big\} \prod_{i=1}^{d} \delta(K_i s_i) \times \Big\langle \prod_j \exp\Big[-\sum_{i=0}^{\infty} i\lambda_i h_i(\mathbf{l}_j) \Big] \det \sum_j \frac{\partial^2 \tilde{g}_{\varepsilon'}(\mathbf{l}_j)}{\partial l_{ji}\, \partial l_{jk}} \Big\rangle. \quad (27)$$

It can be demonstrated that under condition (12) the fluctuations that provide the main contribution to $\rho(\varepsilon)$ differ little from $\tilde{\xi}_{\varepsilon'}(\mathbf{l})$ and that the saddle point of the integral with respect to λ_0 is close to $-i\tilde{\alpha}G$. Replacing the variable λ_0 in (27) with $\lambda_0 - i\tilde{\alpha}G$, allowing for the above-stated and the fact that $\int d\mathbf{l} (\tilde{\xi}_{\varepsilon'} + N) (\partial^2 \tilde{g}_{\varepsilon'}/\partial l_i \partial l_k)$ is a diagonal matrix, and averaging over l_j and integrating with respect to λ_n, s_i, and s_0, we obtain

$$\rho(\varepsilon) = \frac{1}{(2\pi)^{1/2} G} \exp\Big[\tilde{\alpha} \int d\mathbf{l} (\tilde{\xi}_{\varepsilon'} + N) \tilde{g}_{\varepsilon'} + \int d\mathbf{l} \tilde{\xi}_{\varepsilon'} \Big] \prod_{i=1}^{d} \frac{\tilde{\alpha} K_i}{(2\pi)^{1/2}} \prod_{n=d+1}^{\infty} \times \exp\Big(-\frac{1}{2\gamma_n} \Big) \int \frac{ds_n}{(2\pi)^{1/2}} \exp\Big[-\frac{s_n^2}{2} \Big(1 - \frac{1}{\gamma_n} \Big) \Big] = \tilde{\rho}(\varepsilon') M_1(\varepsilon'), \quad (28)$$

where $\tilde{\rho}(\varepsilon')$ is given by (17), and

$$M_1(\varepsilon') = \prod_{n=d+1}^{\infty} \Big[\exp\Big(\frac{1}{\gamma_n} \Big) \Big(1 - \frac{1}{\gamma_n} \Big) \Big]^{-1/2} \quad (29)$$

[since $\tilde{\xi}_{\varepsilon'}(\mathbf{l})$ realizes the maximum in the probability of states with energy ε', all deviations from this maximum proportional to $h_n(\mathbf{l})$ with $n \geqslant d+1$ correspond to values of γ_n greater than unity]. From the definition of ε' given earlier it follows that ε is related to ε' through the equation

$$\varepsilon = \varepsilon' - \int d\mathbf{l} (\tilde{\xi}_{\varepsilon'}(\mathbf{l}) + N) \hat{\Gamma}(\mathbf{l},\mathbf{l}),$$

$$\text{i.e.} \quad \Gamma(\varepsilon') = \int d\mathbf{l} (\tilde{\xi}_{\varepsilon'}(\mathbf{l}) + N) \hat{\Gamma}(\mathbf{l},\mathbf{l}), \quad (30)$$

where $\hat{\Gamma}(\mathbf{l},\mathbf{l}_1)$ is the projection of kernel $\Gamma(\mathbf{l},\mathbf{l}_1)$ onto the space of functions $h_n(\mathbf{l})$ orthogonal, with the weight function $\tilde{\xi}_{\varepsilon'}(\mathbf{l}) + N$, to $h_0(\mathbf{l})$ and $h_i(\mathbf{l})$ and specified by the following equation [see Eq. (26)]:

$$\hat{\Gamma}(\mathbf{l},\mathbf{l}_1) = \frac{1}{2\tilde{\alpha}} \sum_{n=d+1}^{\infty} \gamma_n^{-1} h_n(\mathbf{l}) h_n(\mathbf{l}_1).$$

There is no way in which one can find all the γ_n in general form, but it is possible to calculate $M_1(\varepsilon')$ with a specified accuracy. To this end we introduce the coefficients

$$T_p(\varepsilon') = \sum_{n=d+1}^{\infty} \gamma_n^{-p} = (2\tilde{\alpha})^p \int d\mathbf{l} (\tilde{\xi}_{\varepsilon'}(\mathbf{l}) + N) \hat{\Gamma}_p(\mathbf{l},\mathbf{l}), \quad (31)$$

with $\hat{\Gamma}_p(\mathbf{l},\mathbf{l}_1) = \int d\mathbf{l}_2 [\tilde{\xi}_{\varepsilon'}(\mathbf{l}_2) + N] \hat{\Gamma}(\mathbf{l},\mathbf{l}_2) \hat{\Gamma}_{p-1}(\mathbf{l}_2,\mathbf{l}_1)$. Then

$$\hat{\Gamma}_p(\mathbf{l},\mathbf{l}_1) = \int d\mathbf{l}_2 (\tilde{\xi}_{\varepsilon'}(\mathbf{l}_2) + N) \hat{\Gamma}(\mathbf{l},\mathbf{l}_2) \hat{\Gamma}_{p-1}(\mathbf{l}_2,\mathbf{l}_1),$$

$$M_1(\varepsilon') = \exp\Big\{ -\frac{1}{2} \sum_{n=d+1}^{\infty} \Big[\gamma_n^{-1} + \ln\Big(1 - \frac{1}{\gamma_n} \Big) \Big] \Big\} = \exp\Big(\sum_{n=d+1}^{\infty} \sum_{p=2}^{\infty} \frac{1}{2p\gamma_n^p} \Big) = \exp\Big(\sum_{p=2}^{\infty} \frac{T_p}{2p} \Big). \quad (32)$$

Since T_p decreases as p grows (because $\gamma_n > 1$ for $n \geqslant d+1$), in concrete calculations, after evaluating several first T_p, we can provide a two-sided (upper and lower) estimate of $M_1(\varepsilon')$. Estimating by Eq. (31) the s first T_p from T_1 to T_s, whose value is smaller than unity, for T_p with $p > s$ we can provide an upper estimate: $T_p < T_s^{p/s}$ (this inequality follows from the definition of T_p), and then, since $T_s < 1$, from (32) we obtain

$$\exp\Big(\sum_{p=2}^{s} \frac{T_p}{2p} \Big) < M_1(\varepsilon') < \exp\Big(\sum_{p=2}^{s} \frac{T_p}{2p} \Big) \times (1 - T_s^{1/s})^{-1/2} \exp\Big(-\sum_{p=1}^{s} \frac{T_p^{p/s}}{2p} \Big), \quad T_s < 1. \quad (33)$$

The accuracy of the two-sided estimate of $M_1(\varepsilon')$ increases with s, since $T_{s+1}^{1/(s+1)} < T_s^{1/s}$.

It can be shown that allowing for second- and higher-order corrections to the energy of a state has little effect on $\rho(\varepsilon)$ in the case of the infrequent multicenter fluctuations [see Eqs. (11) and (12)], that is, Eq. (28) [together with (29) and (30) or (33)] is asymptotically exact.

Equations (28) and (30) suggest that the increase in $\rho(\varepsilon)$ brought on by allowing for the discreteness of the centers reflects the decrease in the absolute value of the argument in $\tilde{\rho}(\varepsilon')$ and the appearance of a factor $M_1(\varepsilon') > 1$. If $\Gamma^2(\varepsilon') |\partial^2 \ln \tilde{\rho}(\varepsilon')/\partial \varepsilon'^2| \ll 1$ (which for infrequent fluctuations is a more stringent condition than $\Gamma(\varepsilon') \ll |\varepsilon'|$), Eq. (28) simplifies since $\varepsilon \approx \varepsilon'$:

$$\rho(\varepsilon)=\tilde{\rho}(\varepsilon)M(\varepsilon),$$

$$M(\varepsilon)=\prod_{n=d+1}^{\infty}\left(1-\frac{1}{\gamma_n}\right)^{-1/2}=\exp\left(\sum_{p=1}^{\infty}\frac{T_p}{2p}\right). \tag{34}$$

To analyze $M(\varepsilon)$ we first use a simple method for deriving an expression for $\Gamma(\varepsilon')$, a method that explains the appearance in (30) of the projection of the kernel, $\hat{\Gamma}(\mathbf{l},\mathbf{l}_1)$, and enables $\Gamma(\varepsilon')$ to be represented in a form suitable for physical estimates. The average value of the second-order correction to the ground-state energy for fluctuations close to the optimal is

$$\Gamma(\varepsilon')=\iint d\mathbf{r}\,d\mathbf{r}_1\tilde{G}(\mathbf{r},\mathbf{r}_1)\tilde{\psi}_{\varepsilon'}(\mathbf{r})\tilde{\psi}_{\varepsilon'}(\mathbf{r}_1)\delta V(\mathbf{r})\delta V(\mathbf{r}_1).$$

Here $\delta V(\mathbf{r})=\int d\mathbf{l}u(\mathbf{r}-\mathbf{l})\delta\xi(\mathbf{l})$, $\tilde{G}(\mathbf{r},\mathbf{r}_1)$ has been defined earlier, and the important quantities $\delta\xi(\mathbf{l})=\Sigma_j\delta(\mathbf{l}-\mathbf{l}_j)-\tilde{\xi}_{\varepsilon'}(\mathbf{l})-N$ are the small variations of concentration $\tilde{\xi}_{\varepsilon'}(\mathbf{l})+N$ correlated by the conditions that the energy and quantum number $\mathbf{L}_s$ be constant, that is, $\int d\mathbf{l}\tilde{g}_{\varepsilon'}(\mathbf{l})\delta\xi(\mathbf{l})=0$ and $\int d\mathbf{l}\left[\partial\tilde{g}_{\varepsilon'}(\mathbf{l})/\partial l_i\right]\delta\xi(\mathbf{l})=0$. Hence,

$$\delta\xi(\mathbf{l})=\delta\xi^r(\mathbf{l})-(\tilde{\xi}_{\varepsilon'}(\mathbf{l})+N)\Big[G^{-2}\tilde{g}_{\varepsilon'}(\mathbf{l})\int d\mathbf{l}_1\tilde{g}_{\varepsilon'}(\mathbf{l}_1)\delta\xi^r(\mathbf{l}_1)+\sum_{i=1}^{d}K_i^{-2}\frac{\partial\tilde{g}_{\varepsilon'}(\mathbf{l})}{\partial l_i}\int d\mathbf{l}_1\frac{\partial\tilde{g}_{\varepsilon'}(\mathbf{l}_1)}{\partial l_{1i}}\delta\xi^r(\mathbf{l}_1)\Big],$$

with $\delta\xi^r(\mathbf{l})$ the random variations of $\tilde{\xi}_{\varepsilon'}(\mathbf{l})+N$, or $\overline{\delta\xi^r(\mathbf{l})\delta\xi^r(\mathbf{l}_1)}=\left[\tilde{\xi}_{\varepsilon'}(\mathbf{l})+N\right]\delta(\mathbf{l}-\mathbf{l}_1)$. This yields an expression for $\Gamma(\varepsilon')$ equivalent to (30):

$$\Gamma(\varepsilon')=\iint d\mathbf{r}\,d\mathbf{r}_1\tilde{G}(\mathbf{r},\mathbf{r}_1)\tilde{\psi}_{\varepsilon'}(\mathbf{r})\tilde{\psi}_{\varepsilon'}(\mathbf{r}_1)\int d\mathbf{l}(\tilde{\xi}_{\varepsilon'}(\mathbf{l})+N)\hat{u}(\mathbf{r},\mathbf{l})\hat{u}(\mathbf{r}_1,\mathbf{l}_1), \tag{35}$$

with

$$\hat{u}(\mathbf{r},\mathbf{l})=u(\mathbf{r}-\mathbf{l})-h_0(\mathbf{l})\int d\mathbf{l}_2(\tilde{\xi}_{\varepsilon'}(\mathbf{l}_2)+N)u(\mathbf{r}-\mathbf{l}_2)h_0(\mathbf{l}_2)-\sum_{i=1}^{d}h_i(\mathbf{l})\int d\mathbf{l}_2(\tilde{\xi}_{\varepsilon'}(\mathbf{l}_2)+N)u(\mathbf{r}-\mathbf{l}_2)h_i(\mathbf{l}_2). \tag{36}$$

Now let us estimate $\Gamma(\varepsilon')$ for the case where the characteristic scales of the wave function and the center potential are close (and $\varepsilon'\approx\varepsilon$).

In the Gaussian situation, that is, $N\gg\tilde{\xi}_\varepsilon(\mathbf{l})\approx-\tilde{\alpha}\tilde{g}_\varepsilon(\mathbf{l})N$, both $\tilde{\psi}_\varepsilon(\mathbf{r})$ and $\tilde{\xi}_\varepsilon(\mathbf{l})$ have the same characteristic scale, $l_\varepsilon\approx\sqrt{\hbar^2/(-2m\varepsilon)^{1/2}}$, and $\hat{u}(l_\varepsilon,l_\varepsilon)\approx u(l_\varepsilon)$. An estimate of $\tilde{\psi}_\varepsilon(r)$ from the normalization condition yields $\tilde{\psi}_\varepsilon^2\approx l_\varepsilon^{-d}$. Combining this with (23), we find that $\int\int d\mathbf{r}d\mathbf{r}_1\tilde{G}(\mathbf{r},\mathbf{r}_1)\tilde{\psi}_{\varepsilon'}(\mathbf{r})\tilde{\psi}_{\varepsilon'}(\mathbf{r}_1)\propto 2ml_\varepsilon^2/\hbar^2$. The number of centers in an optimal fluctuation can be estimated by the condition $\varepsilon\approx Z_\varepsilon u(l_\varepsilon)$. These estimated combined with Eq. (35) yield $\Gamma(\varepsilon)\approx|\varepsilon|\bar{n}_\varepsilon/Z_\varepsilon^2$, that is, $\Gamma(\varepsilon)$ is small as long as $\bar{n}_\varepsilon\ll Z_\varepsilon^2$. Allowing for $\Gamma(\varepsilon)$ results in the a state with energy ε generating a fluctuation involving $Z_\varepsilon-\Delta Z$ centers, with $\Delta Z=\beta\bar{n}_\varepsilon/Z_\varepsilon$, and β a dimensionless parameter depending on the shape of the potential of a center. From this and from the fact that $\ln P_{\bar{n}}(Z)\approx-Z^2/2\bar{n}$ we find that

$$\ln M(\varepsilon)\approx\ln P_{\bar{n}_\varepsilon}(Z_\varepsilon-\Delta Z)-\ln P_{\bar{n}_\varepsilon}(Z_\varepsilon)\approx Z_\varepsilon\Delta Z/\bar{n}_\varepsilon=\beta,$$

that is, allowing for the discreteness of the centers increases $\rho(\varepsilon)$ e^β-fold.

When the asymptotic behavior is Poisson-like ($N\ll\tilde{\xi}_\varepsilon\approx Ne^{-\tilde{\alpha}\tilde{g}_\varepsilon(\mathbf{l})}$), the characteristic radius l_ξ of $\tilde{\xi}_\varepsilon(\mathbf{l})$ is the smallest (from the expansion of $\tilde{g}_\varepsilon(\mathbf{l})$ as $l\to0$ it follows that $l_\xi\approx l_\varepsilon[-\tilde{\alpha}\tilde{g}_\varepsilon(0)]^{-1/2}\approx l_\varepsilon\ln^{-1/2}(Z_\varepsilon/\bar{n}_\varepsilon)$ and Eq. (35) simplifies:

$$\Gamma(\varepsilon)=Z_\varepsilon\int\int d\mathbf{r}\,d\mathbf{r}_1\tilde{G}(\mathbf{r},\mathbf{r}_1)\tilde{\psi}_\varepsilon(\mathbf{r})\tilde{\psi}_\varepsilon(\mathbf{r}_1)\hat{u}(\mathbf{r},0)\hat{u}(\mathbf{r}_1,0).$$

In view of the strong correlation of the fluctuations, the effective potential $\hat{u}(\mathbf{r},0)$ at $r\approx l_\varepsilon$ is small [see Eq. (36)]. An estimate yields $\hat{u}(l_\varepsilon,0)\approx(l_\xi/l_\varepsilon)^2u(l_\varepsilon)$, and hence $\Gamma(\varepsilon)\approx|\varepsilon|/[Z_\varepsilon\ln^2(Z_\varepsilon/\bar{n}_\varepsilon)]$. From this, proceeding as in the Gaussian case, we find that $\Delta Z=\beta\ln^{-2}(Z_\varepsilon/\bar{n}_\varepsilon)$, and since $\ln P_{\bar{n}}(Z)\approx-Z\ln(Z/\bar{n})$ for $Z\gg\bar{n}$, we have $\ln M(\varepsilon)\approx\Delta Z\ln(Z_\varepsilon/\bar{n}_\varepsilon)=\beta\ln^{-1}(Z_\varepsilon/\bar{n}_\varepsilon)$, that is, in the limit of large values of ε the effect of the discreteness of centers vanishes.

For states generated by infrequent multicenter fluctuations [provided conditions (11) and (12) are met] Eq. (34) always holds true in the one-dimensional case, while for particle spaces R of higher dimensions it holds true for the random field of strong scatterers. But if the scatterers are weak, or $1\gg m|u_0|a^2/\hbar^2$, where u_0 is the characteristic potential of a center and a is the radius of the potential, for such particle spaces Eq. (34) is valid only for $|\varepsilon|\geqslant\hbar^2/ma^2$ (for $l_\varepsilon\leqslant a$), although in this case the localization of a particle at infrequent fluctuations may also occur when $|\varepsilon|\ll\hbar^2/ma^2$. The difference in the results obtained through the discrete and continuum approaches [between $\rho(\varepsilon)$ and $\tilde{\rho}(\varepsilon)$] grows as $|\varepsilon|$ decreases because of the increase in the ratio $\Gamma(\varepsilon')/|\varepsilon'|$. For instance, in the three-dimensional case, $\Gamma(\varepsilon')$ tends to the limit $\Gamma(0)$ as $\varepsilon'\to0$. This limit can easily be found from Eq. (35), allowing for the fact that $l_{\varepsilon'}\to\infty$ as $\varepsilon'\to0$ like $|\varepsilon'|^{-1/2}$, and for $|\mathbf{r}-\mathbf{r}_1|\to0$ $\tilde{G}(\mathbf{r},\mathbf{r}_1)$ tends [see Eq. (23)] to the infinitely increasing Green's function of the Laplace equation, $m(2\pi\hbar^2|\mathbf{r}-\mathbf{r}_1|)^{-1}$. For centers with a rapidly decreasing potential, $\int d\mathbf{r}u(\mathbf{r})=\omega$, and bound states, $\int d\mathbf{r}\tilde{\psi}_{\varepsilon'}^2(\mathbf{r})=1$, as $\varepsilon'\to0$ (ignoring corrections that are small as long as $|\varepsilon'|\ll|\bar{\varepsilon}|=N|\omega|$ and $\sqrt{ma^2|\varepsilon'|/\hbar^2}\ll1$), we obtain from Eq. (35) the following:

$$\Gamma(0)=\frac{mN}{2\pi\hbar^2}\int\int d\mathbf{r}\,d\mathbf{r}_1u(\mathbf{r})u(\mathbf{r}_1)|\mathbf{r}-\mathbf{r}_1|^{-1}=\frac{2mN}{(2\pi)^3\hbar^2}\int\frac{d\mathbf{p}}{p^2}|u_\mathbf{p}|^2, \tag{37}$$

where $u_\mathbf{p}=\int d\mathbf{r}u(\mathbf{r})\exp(i\mathbf{p}\mathbf{r})$. Thus, in the three-dimensional case the edge of the spectrum of localized states with $1\gg m|u_0|a^2/\hbar^2$ (i.e., in conditions corresponding to the absence of bound states on an isolated center) lies below the average level of the potential by $\Gamma(0)$, a quantity determined by the potential of a center and infinite in the "white noise" approximation[2,3,8,9] (at $a=0$). It can be demonstrated that if conditions (11) and (12) are met, $|\Gamma(\varepsilon')-\Gamma(0)|/|\varepsilon'|\ll1$. Measuring the energy from the edge of the spectrum of localized states, $\tilde{\varepsilon}=\varepsilon+\Gamma(0)$, and allowing for the closeness of ε and ε', from Eq. (30) we obtain $\varepsilon'\approx\tilde{\varepsilon}+\Gamma(\tilde{\varepsilon})-\Gamma(0)$, which together with (28)

yields

$$\rho(\bar{\varepsilon})=\bar{\rho}(\bar{\varepsilon})\exp\left\{\frac{\partial \ln \bar{\rho}(\bar{\varepsilon})}{\partial \bar{\varepsilon}}\left[\Gamma(\bar{\varepsilon})-\Gamma(0)\right]\right\}M_1(\bar{\varepsilon}). \quad (38)$$

For $1 \gg m|u_0|a^2/\hbar^2$ this formula, in contrast to (34), holds true in the entire energy range corresponding to conditions (11) and (12). (A detailed analysis of the three-dimensional situation is done in Sec. 4.) In the two-dimensional case the energy range agrees with (11) and (12) provided that not only $m|\omega|/\hbar^2 \ll 1$ but also $Na^2(m|\omega|)/\hbar^2)^2 \ll 1$. Here, too, expression (38) is asymptotically exact for all energies agreeing with conditions (11) and (12) (in the limit of point centers this leads to the results of Refs. 7 and 8) provided that $\Gamma(\varepsilon_s)$ is substituted for $\Gamma(0)$ in (38) and in renormalizing the energy, where ε_s is the energy that in the continuum approximation corresponds to the beginning of the spectrum of states generated by infrequent multicenter fluctuations. [There are two reasons why $\Gamma(0)$ cannot be used here: formally because this quantity is divergent, $\Gamma(\varepsilon) \propto \ln(\hbar^2/ma^2|\varepsilon|)$, and physically because in the two-dimensional case, in contrast to the three-dimensional, and with $m|\omega|/\hbar^2 \ll 1$, an isolated center still binds a particle, although exponentially weakly.] The reason for the higher accuracy of (38) in comparison to (34) is that $|\partial\Gamma(\varepsilon_s)/\partial\varepsilon_s| \ll 1$ even though $1 \leqslant \Gamma(\varepsilon_s)/|\varepsilon_s|$.

4. $\rho(\varepsilon)$ IN THE RANDOM FIELD OF CENTERS WITH $u(r)=(e^2/\varkappa r)e^{-\alpha r}$

A similar problem has been solved in Ref. 1 in the Gaussian and continuum approximations. Following Ref. 1, we introduce the dimensionless energy (measured in units of $E_Q = \hbar^2 Q^2/2m$) and the dimensionless length (measured in units of Q^{-1}), Then Eq. (10) for the dimensionless optimal wave function ψ, normalized by the condition $\int_0^\infty dr r^2\psi^2(r) = 1$, becomes

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\psi(r)\right) + \left\{N_1\int_0^\infty dl\,\frac{l}{r}s(r,l)\left[\exp\left(\frac{\mu g(l)}{N_1}\right)-1\right]-E\right\}\psi(r)=0, \quad (39)$$

where

$$g(l)=\int_0^\infty dl\,\frac{l}{r}s(r,l)\psi^2(r),$$

$$s(r,l)=\begin{cases} e^{-r}\operatorname{sh} l, & r \geqslant l \\ e^{-l}\operatorname{sh} r, & r<l \end{cases} \qquad \mu=\alpha e^2 Q N_1/\varkappa.$$

Equation (32) contains two dimensionless parameters, E and $N_1 = 6\bar{N}/Q^4 a_B^4$ [here $a^1{}_B = \hbar^2\varkappa^2/me^2$ and $\bar{N} = (4\pi/3)Na_B^3$], on which $\psi(r)$ and μ depend. The parameter μ is chosen in such a manner that in the Gaussian asymptotic limit (as $N_1 \to \infty$) both $\psi(r)$ and μ depend only on E. Following Ref. 1, we introduce the parameter $\zeta = N_1/Qa_B$ and represent formulas (34), (17), (18a), and (19) as

$$\rho(E)=\rho(E)M(E)=\frac{Q^3}{E_Q\zeta^2}a(E,N_1)\exp\left[-\frac{b(E,N_1)}{2\zeta}\right]M(E), \quad (40)$$

$$b(E,N_1)=N_1\int_0^\infty dll^2\left\{\exp\left(\frac{\mu g(l)}{N_1}\right)\left[\frac{\mu g(l)}{N_1}-1\right]+1\right\}, \quad (41)$$

$$a(E,N_1)=\frac{\mu^3}{4\pi^2}\left[\int_0^\infty dll^2\exp\left(\frac{\mu g(l)}{N_1}\right)\left[\frac{\partial g(l)}{\partial l}\right]^2\right]^{3/2} \times\left[\int_0^\infty dll^2\exp\left(\frac{\mu g(l)}{N_1}\right)g^2(l)\right]^{-1/2}. \quad (42)$$

For $u(\mathbf{r}) = u(r)$ the coefficients $T_p(E)$, which determine $M(E)$ [see Eqs. (33) and (34)], can be written as

$$T_p=(2\mu)^p\sum_{n=1}^\infty\frac{1}{(2n+1)^{2p-1}}\int_0^\infty dl_1 l_1^2\ldots\int_0^\infty dl_2 l_2^2 \times\exp\left\{-\frac{\mu}{N_1}\left[g(l_1)+\ldots+g(l_p)\right]\right\}F_n(l_1,l_2)\ldots F_n(l_p,l_1),$$

where

$$F_n(l,l_1)=\int_0^\infty dr\,\frac{1}{r^2 f_n^2(r)}\int_0^r d\eta\eta^2\psi(\eta)f_n(\eta)u_n(\eta,l) \times\int_0^r d\eta\eta^2\psi(\eta)f_n(\eta)u_n(\eta,l_1).$$

The functions $f_n(r)$ for $n \geqslant 1$ [$f_0(r) \equiv \psi(r)$] are solutions of the equation

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}f_n(r)\right)+\left\{N_1\int_0^\infty dl\,\frac{l}{r}s(r,l)\left[\exp\left(\frac{\mu g(l)}{N_1}\right)-1\right] -\frac{n(n+1)}{r^2}-E\right\}f_n=0,$$

that satisfy the boundary condition $f_n(0) = 0$. The coefficients $u_n(r,l)$ of the expansion of the orthogonalized potential $\hat{u}(\mathbf{r},\mathbf{l})$ in Legendre polynomials [see Eq. (36)] for $u(\mathbf{r}-\mathbf{l}) = \exp(-|\mathbf{r}-\mathbf{l}|)/|\mathbf{r}-\mathbf{l}|$ are[12]

$$u_0(r,l)=\frac{s(r,l)}{rl}-g(l)\int_0^\infty d\eta\,\frac{\eta}{r}\exp\left(\frac{\mu g(\eta)}{N_1}\right)s(r,\eta)g(\eta) \times\left[\int_0^\infty d\eta\eta^2\exp\left(\frac{\mu g(\eta)}{N_1}\right)g^2(\eta)\right]^{-1},$$

$$u_1(r,l) =-3\frac{\partial^2}{\partial r\,\partial l}\left[\frac{s(r,l)}{rl}\right]+3\frac{\partial g}{\partial l}\int_0^\infty d\eta\,\frac{\eta}{r}\exp\left(\frac{\mu g(\eta)}{N_1}\right)\left(\frac{\partial g}{\partial \eta}\right) \times\frac{\partial^2}{\partial r\,\partial\eta}\left[\frac{s(r,\eta)}{r\eta}\right]\left[\int_0^\infty d\eta\eta^2\exp\left(\frac{\mu g(\eta)}{N_1}\right)\left(\frac{\partial g}{\partial\eta}\right)^2\right]^{-1},$$

$$u_n(r,l)=(-1)^n(2n+1)(rl)^n\left(\frac{\partial}{r\,\partial r}\right)^n\left[\frac{s(r,l)}{dl}\right] \quad \text{for } n \geqslant 2.$$

4.1. The density of states in the continuum approximation

Solving Eq. (39) numerically by the method of successive approximations and substituting the obtained $\psi(r)$ and μ into (41) and (42), we find the universal functions $b(E,N_1)$ and $a(E,N_1)$ in terms of which $\rho(E)$ can be expressed via Eq. (40). The results of these calculations at $N_1 = 10^2$, 10, 1, 10^{-1}, 10^{-2} are presented in Figs. 1 and 2 (curves 2–6, respectively). For the sake of comparison we

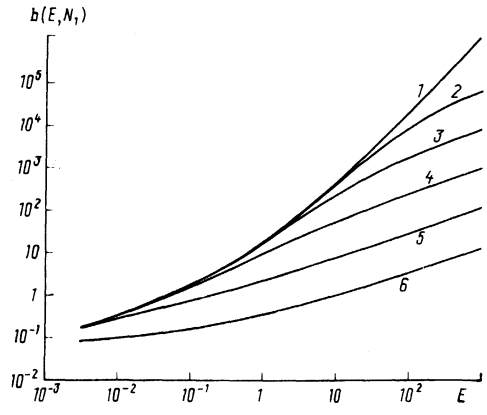

FIG. 1. The energy dependence of $b(E,N_1)$ calculated via Eq. (41) for $N_1 \to \infty$ (curve *1*), $N_1 = 10^2$ (curve *2*), 10 (curve *3*), 1 (curve *4*), 10^{-1} (curve *5*), and 10^{-2} (curve *6*).

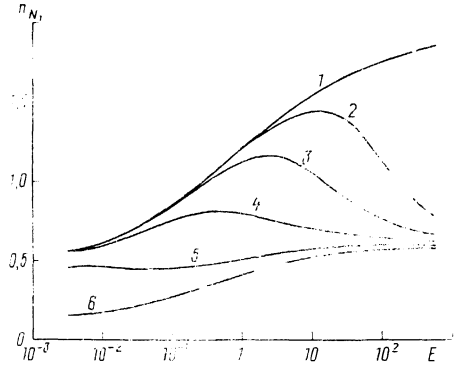

FIG. 3. The energy dependence of $n_{N_1}(E) = d \ln b(E,N_1)/d \ln E$. The values of N_1 and the numbering of the curves are the same as in Fig. 2.

also give the functions $b(E)$ and $a(E)$ (curves *1*) obtained in Ref. 1 in the Gaussian approximation [see Eqs. (41) and (42) as $N_1 \to \infty$. Figures 1 and 2 show that the Gaussian approximation provides fairly good accuracy in calculating $\rho(E)$ only when $E < 0.1N_1$. Inaccuracies increase with E, and for $E > 0.1N_1$ the Gaussian statistics strongly underestimates $\rho(E)$. The thing is that for infrequent states $b(E,N_1)/2\zeta$ is much larger than unity and, therefore, even a slight variation in $b(E,N_1)$ has a strong effect on $\rho(E)$, with Fig. 1 clearly demonstrating that $b(E)$ exceeds $b(E,N_1)$ considerably when $E > N_1$. Substantial deviations from the Gaussian pattern are clearly seen in Fig. 3, where the functions $n_{N_1}(E) = d \ln b(E,N_1)/d \ln E$ are presented for different values of N_1, including the case where $N_1 \to \infty$, which corresponds to the Gaussian curve $n(E) = d \ln b(E)/d \ln E$. (The numbering of the curves in Fig. 3 is the same as in Figs. 1 and 2.) We see that even for very large values of N_1 the values of $n_{N_1}(E)$ for all E's are considerably smaller than 2, which value corresponds to the classical localization of a particle in the field of Gaussian fluctuations. Moreover, curves *2–4* suggest that in a heavily doped semiconductor with realistic values of N_1 ($1 < N_1 < 10$ because in such a heavily doped semiconductor, according to Ref. 5, $Q = (2/a_B)(9N/4\pi^2)^{-1/6}$ and $N_1 = (\pi/4)(2\pi/3)^{1/6}\bar{N}^{1/3} \approx \bar{N}^{1/3}$) the value of $n_{N_1(E)}$ in the "tail" of the density of states [for $E > (\pi N_1/6^{1/2})^{1/6}$)] is close to unity for values of E of practical interest, which agrees with the experimental data of Ref. 3. The presence of maxima in the n_{N_1} vs E curves with $N_1 \geqslant 1$ reflects the interplay between two tendencies: on the one hand, for Gaussian fluctuations $n(E)$ grows with E (as the scale of the wave function decreases in comparison to the fluctuation scale), and, on the other, the optimal fluctuations for $E > 1$ are of the hybrid type, as in a Coulomb field.[10] To put it differently, there are small-scale Poisson clusters of centers inside large-scale Gaussian fluctuations. The contribution of Gaussian fluctuations to the binding energy decreases for large values of E, while that of Poisson clusters, for which $n(E)$ drops as E grows, increases. Hence, in the limit $E \to \infty$ ($E \gg 1, N_1$), Figs. 1 and 2 define $\rho_{\text{quantum}}(\varepsilon)$ in a random Coulomb field.

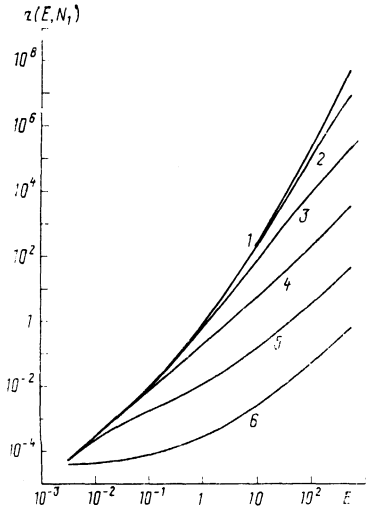

FIG. 2. The energy dependence of $a(E,N_1)$ calculated via Eq. (42). The values of N_1 and the numbering of the curves are the same as in Fig. 1.

We start by analyzing the behavior of $a(E,N_1)$ for $E > 1$, where the characteristic radius of the wave function, $l_\varepsilon \approx (\hbar^2/2m\varepsilon)^{1/2}$, is smaller than Q^{-1}. (For an analysis of the behavior of the exponent see Refs. 6 and 10.) Using the estimate of the preexponential factor in $\rho(\varepsilon)$ made in Sec. 2, for $d = 3$ we have

$$\rho_0 \approx \frac{1}{V_\xi g_\varepsilon Z_\varepsilon}\left(\frac{Z_\varepsilon^2}{Z_\varepsilon + \bar{n}_\varepsilon}\right)^2. \tag{43}$$

For $E > 1$ in the Gaussian approximation ($\bar{n}_\varepsilon \gg Z_\varepsilon$), the radius l_ε of an optimal fluctuation is approximately Q^{-1}, the volume V_ξ is $(4\pi/3)Q^{-3}$, the average number of centers $\bar{n}_\varepsilon$ in such a fluctuation is NV_ξ, the effective potential of the center, g_ε, is roughly $e^2Q/\varkappa$, and the fluctuation of the number of centers, Z_ε, is related to energy through the formula $\varepsilon \approx Z_\varepsilon g_\varepsilon$. Combining this with Eq. (43) yields $\rho_0 = (27/16\pi)(Q^3E^3\zeta^{-2}/E_Q)$, that is [see Eq. (40)], $a(E,N_1) \approx E^3/2$. In the Poisson case ($Z_\varepsilon \gg \bar{n}_\varepsilon$) we still have $\varepsilon \approx Z_\varepsilon g_\varepsilon$, but g_ε is much higher: $g_\varepsilon \approx e^2/\varkappa l_\varepsilon$. Here $l_\xi \approx l_\varepsilon \ln^{-1/2}(Z_\varepsilon/\bar{n}_\varepsilon)$ (see Sec. 2). Substituting these relations into (43), we find that $a(E,N_1) \approx (3/16\pi)N_1^2[E \ln(E^2/N_1)]^{3/2}$. The resulting expressions for $a(E,N_1)$ describe the corresponding asymptotic behavior of the curves in Fig. 2 fairly well.

To analyze the behavior of $\rho(E)$ for $E \ll 1$, when

$l_\varepsilon \gg Q^{-1}$, we examine how a random field of centers with an attractive potential of finite amplitude u_0 inside a sphere of a small radius a ($u_0 \ll (\hbar^2/2ma)^2$, since only with such a relationship between the characteristic potential and radius of a center is the condition met that the scatterers be quasipointlike, $a \ll l_\varepsilon$) and zero amplitude outside of the sphere generates states with a small binding energy $\varepsilon \ll (\hbar^2/2ma^2)$ reckoned from $\bar{\varepsilon} = 4\pi Na^3 u_0/3$. In the Gaussian case ($Z_\varepsilon \ll \bar{n}_\varepsilon$ or $\varepsilon \ll \bar{\varepsilon}$), the wave function and the optimal fluctuation are concentrated inside spheres of equal radius l_ε. Hence,

$$\psi^2 \approx [(4\pi/3) l_\varepsilon^3]^{-1} = (3/4\pi)(2m\varepsilon/\hbar^2)^{3/2},$$

$$g_\varepsilon = \int d\mathbf{r} u(\mathbf{r}) \psi^2(\mathbf{r}) \approx u_0 a^3/l_\varepsilon^3 = u_0 (2m\varepsilon a^2/\hbar^2)^{3/2},$$

$Z_\varepsilon = \varepsilon/g_\varepsilon$, and $\bar{n}_\varepsilon = 4\pi N l_\varepsilon^3/3$. To estimate the exponent in $\rho(\varepsilon)$ with logarithmic accuracy, we employ the fact that $\ln P_n(Z) = Z^2/2n$ for $Z \ll n$. Substituting Z_ε for Z and $\bar{n}_\varepsilon$ for n, we obtain $\ln P(\varepsilon) = (3/8\pi)(1/Na^3u_0^2)\sqrt{\varepsilon}(\hbar^2/2ma^2)^{3/2}$. In terms of the dimensionless variables $E = 2ma^2\varepsilon/\hbar^2$, $N_1 = 8\pi Na^5 m u_0/\hbar^2$, and $\zeta = 2N_1 ma^2 u_0/\hbar^2$ we have $\ln P(E) = -b(E)/2\zeta = -3\sqrt{E}/2\zeta$ for $E \ll N_1, 1$. The curves *1–4* in Fig. 1 yield a close value, $b(E) \approx 3\sqrt{E}$. Employing Eq. (43) and the above estimates of g_ε, Z_ε, $\bar{n}_\varepsilon$, and $V_\xi \approx 4\pi l_\varepsilon^3/3$, we find that $\rho_0(\varepsilon) = (N/u_0^4)(\hbar^2\varepsilon/2ma^2)^{3/2}(4\pi Na^3/3)^{-3}$. Now we define $a(E,N_1)$ as we did in (43), namely, $\rho_0(E) = (2m/\hbar^2 a\zeta^2) a(E,N_1)$, so $a(E,N_1) = (3/4\pi)E^{3/2}$. The curves *1–5* in Fig. 2 yield $a(E,N_1) = 0.35E^{3/2}$.

The results are the same if we put $u(\mathbf{r}) = -\omega\delta(\mathbf{r})$ in Eq. (10), with $\omega = -\int d\mathbf{r} u(\mathbf{r})$, thus transforming Eq. (10) into

$$\frac{\hbar^2}{2mr^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\psi_\varepsilon(r)\right) + \{N\omega[\exp(\alpha\omega\psi_\varepsilon^2(r)) - 1] - \varepsilon\}\psi_\varepsilon(r) = 0, \quad (44)$$

and substitute the $\psi_\varepsilon(r)$ and α found by solving Eq. (39) [with $\exp(\alpha\omega\psi_\varepsilon^2(r)) - 1$ replaced by $\alpha\omega\psi_\varepsilon^2(r)$] in the Gaussian limit, for the appropriate quantities in Eqs. (17), (19), and (18a). These simplifications reduce the random field to the "white noise" form with a potential-fluctuation correlator equal to $\gamma\delta(\mathbf{r} - \mathbf{r}_1)$, with $\gamma = N\omega^2$ (see Refs. 8 and 9).

A totally different physical pattern arises in the Poisson section of the "tail" of the density of states (for $Z_\varepsilon \gg \bar{n}_\varepsilon$ or $E \gg N_1$ or $N\omega \ll \varepsilon$). Formally this is already manifested in the fact that the solutions to Eq. (44) that retain their sign and vanish as $r \to \infty$ exist only for $\varepsilon < N\omega/18.7$, that is, deep "within" the Gaussian section. The reason for this is clarified by the method of successive approximations. It seems that when $\varepsilon > N\omega/18.7$, in the region of small values of r there appears a peak in $\psi(r)$ that becomes steeper with each successive iteration, superposed on a smooth wave function with a characteristic scale of $(\hbar^2/2m\varepsilon)^{1/2}$. This peak leads to an ever stronger and narrower peak in the center density $\xi_\varepsilon(r)$. The process can be restricted only if we assume the radius of the center's action to be small but finite. For this reason, in the three-dimensional case with $\varepsilon > N\omega/18.7$, or $E > N_1/18.7$, it is impossible to pass from quasipointlike scatterers to the limit of point scatterers [from the integrodifferential equation equation (10) to the differential equation (44)], and $\rho(\varepsilon)$ depends not only on ω but also on the shape of the potential of a center.

Hence, with $E \gg N_1$ the optimal fluctuation is created by a cluster of centers lying mainly within a sphere of radius a. States with binding energies $\varepsilon \ll \hbar^2/2ma^2$ create clusters with Z_ε centers (corresponding to a potential well of depth $u \approx Z_\varepsilon u_0$), with Z_ε exceeding only slightly the value Z_c necessary for a bound state to appear. For a spherical potential well of radius a and depth u, the binding energy for $\varepsilon \ll \hbar^2/2ma^2$ depends on the depth via the law $\varepsilon = (\pi^2/4)u_c[(u/u_c)^{1/2} - 1]^2$ (see Ref. 13), with $u_c = \pi^2\hbar^2/8ma^2$. This leads to the following estimate: $Z_\varepsilon = Z_c + 4(Z_c\varepsilon/u_0)^{1/2}$, where $Z_c = u_c/u_0$. Combining this estimate and the Poisson formula $\ln P_n(Z) = -Z\ln(Z/en)$ for $Z \gg n$, allowing for the fact that $Z_\varepsilon - Z_c \ll Z_c$ and $\bar{n}_\varepsilon = 4\pi Na^3/3$, and going over to dimensionless variables, we find that $\ln P(E) = -b(E,N_1)/2\zeta = -(\pi^2/4\zeta)N_1 \ln[(1 + 8\sqrt{E}/\pi^2)/N_1]$ for $N_1 \ll E \ll 1$. The consequent expression for $b(E,N_1)$ agrees well with the curve pattern in Figs. 1 and 3 in the $N_1 \ll E \ll 1$ range. If we now substitute into Eq. (43) the above expression for Z_ε, $V_\xi = 4\pi a^3/3$, and $g_\varepsilon \approx u_0$, we find $a(E,N_1) = (3\pi/16)N_1(1 + 8\sqrt{E}/\pi^2)$, which corresponds to the pattern of curves *5* and *6* in Fig. 2 for $N_1 < E < 1$.

4.2. Allowing for discreteness

Figure 4 illustrates the behavior of the discreteness factor $M(E)$, which leads to an increase in $\rho(E)$. For $E > 1$, when because of the singularity of $u(\mathbf{r})$ as $r \to 0$ the scale of the wave function is close to the characteristic scale of the center potential, the value of $M(E)$ is moderate and decreases as E grows. This agrees with the analysis of the behavior of $M(E)$ carried out in Sec. 3 and relating to the case of $E > 1$ for the given $u(\mathbf{r})$.

The behavior of $M(E)$ for $E \ll 1$ can be explained as follows. In the case of Gaussian fluctuations of the quasipointlike centers, the effect of discreteness on $\rho(E)$ is primarily reduced to the energy scale being shifted by $\Gamma(0)$ (see Sec. 3). Hence, $\rho(E) \approx \tilde{\rho}[E - \Gamma(0)]$. For the $u(\mathbf{r})$ considered we use (37) to obtain $\Gamma(0) = 4\pi mNe^4/\hbar^2\varkappa^2 Q$, and $\rho(E) \approx \tilde{\rho}(E - \zeta)$. The expression (34) for $M(E)$ has been derived for the case of relatively small second-order correc-

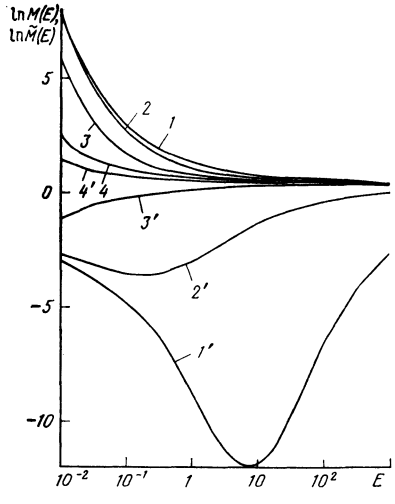

FIG. 4. The energy dependence of the discreteness factor M and the renormalized discreteness factor $\tilde{M}$ calculated for $N_1 = 10$ (curves *1* and *1a*), 1 (curves *2* and *2a*), 10^{-1} (curves *3* and *3a*), and 10^{-2} (curves *4* and *4a*).

tions, which is equivalent to E being much higher than ζ and is possible only if $\xi \ll 1$. Above we have seen that $\tilde{\rho}(E-\zeta) \approx \exp(-3\sqrt{E-\zeta}/2\zeta)$ for $E \ll 1$, N_1. Retaining in the exponent the first two terms of the series expansion in powers of ζ/E, we find that $\rho(E) \approx \tilde{\rho}(E-\zeta) \approx \tilde{\rho}(E)\exp(3/4\sqrt{E})$, and it is this behavior, $\ln M(E) \approx 3/4\sqrt{E}$, that is observed in Fig. 4 for $E \ll 1$, N_1. Hence, a description of $\rho(E)$ via Eq. (39) and Figs. 1, 2, and 4 is correct to within logarithmic accuracy for $E \gg \zeta$ and to within absolute accuracy under a more stringent condition, $E \gg \zeta^{2/3}$.

If the energy is measured from the true edge of the spectrum of localized states and Eq. (38) is used instead of Eq. (39), $\rho(E)$ can be determined with absolute accuracy starting with much lower energy values that coincide with the beginning of the infrequent-state range (i.e., for $E \gg \zeta^2$). Equation (38) in terms of dimensionless variables and with the renormalized energy $E = 2m[E-\Gamma(0)]/\hbar^2 Q^2$ assumes the form

$$\rho(E) = \tilde{\rho}(E)\tilde{M}(E),$$

$$\tilde{M}(E) = M_1(E)\exp\left\{n_{N_1}(E)b(E,N_1)\left[\frac{T_1}{\mu N_1}-1\right]\frac{1}{E}\right\}.$$

The curves illustrating the behavior of $\tilde{M}(E)$ for different values of N_1 are depicted in Fig. 4. They reflect the interplay between two factors that influence the ratio $\Gamma(E)/\Gamma(0) = T_1/\mu N_1$. A physical explanation of why the energy of a particle decreases (the appearance of a second-order correction $\Gamma(E)$) when one allows for the discreteness of the attractive centers is that each such center additionally "pulls" the wave function of the continuum approximation onto itself, with the result that the interaction of the center and the wave function becomes more effective. As $\varepsilon \to 0$, the value of $\varepsilon(E)$ tends to a limit, since an increase in the number of centers in the optimal-fluctuation volume ($\bar{n}_\varepsilon \approx N l_\varepsilon^3 \propto \varepsilon^{-3/2}$) in the zeroth approximation is completely balanced by the reduction ($\propto a^3/l_\varepsilon^3$) in the contribution of an individual center. Allowing for small corrections shows that $\Gamma(E)$ decreases as E grows but remains much smaller than N_1 or 1 [in the Gaussian limit $1-\Gamma(E)/\Gamma(0) \sim \sqrt{E}$], since in this case the correction to the wave function $\psi_E(r)$ introduced by the field of an isolated center decreases because of an increase in the "elasticity" of $\psi_E(r)$. For this reason $\ln \tilde{M}(E)$ is negative for $E \ll 1$, N_1. As $E \to 0$ the value of $\tilde{M}(E)$ tends to the limit $M(0) = e^{-1.55} = 0.21 \pm 0.01$. It can be demonstrated that this limit, in contrast to $\Gamma(0)$, is independent of the shape of the center potential. Hence, for all quasipointlike scatterers (i.e., for $2ma^2u_0/\hbar^2 \ll 1$) in the limit of infrequent Gaussian fluctuations we have

$$\rho(\varepsilon) = 0{,}21\tilde{\rho}(\varepsilon) = (17{,}0 \pm 0{,}9)\frac{\hbar^2\varepsilon^{3/2}}{\gamma^2 m^{3/2}}\exp\left(-13{,}3\frac{\varepsilon^{1/2}\hbar^3}{\gamma m^{3/2}}\right). \quad (45)$$

The expression on the right-hand side was obtained earlier in Ref. 8 for a random field with a potential-fluctuations correlator equal to $\gamma\delta(\mathbf{r}-\mathbf{r}_1)$.

On the other hand, $\Gamma(E)/\Gamma(0)$ grows with E as the concentration of centers in the optimal-fluctuation volume increases ($\propto (\bar{n}_\varepsilon + Z_\varepsilon)/\bar{n}_\varepsilon = 1 + E/N_1$). In other words, the effect of this factor is stronger the smaller the value of N_1 and the greater the value of E (see curves *1a–4a* in Fig. 4).

The quantity $M_1(E)$, which introduces a distinction between $\rho(E)$ (obtained as a result of exact averaging) and $\tilde{\rho}(E')$ (the continuum density of states with a shifted argument), that is, $\rho(E) = \tilde{\rho}(E')M_1(E')$ and $E = E' + \Gamma(E')$, enters into the coefficients $M(E)$ and $\tilde{M}(E)$ as a cofactor. Calculations show that $M_1(E)$ monotonically increases as E decreases, from the value $M_1(\infty) = 1$ to the value $M_1(0) = e^{0.45} \approx 1.57$, that is, replacing $\rho(\varepsilon)$ with $\tilde{\rho}(\varepsilon')$ reduces the density of states only slightly.

Finally, we note that in carrying out two-sided estimates of $M(E)$ and $M_1(E)$ [see Eq. (33)] we had to calculate no more than the first three coefficients $T_p(E)$. The accuracy of determining $M(E)$ and $\tilde{M}(E)$ in some cases was much higher than one percent and exceeded the accuracy of the asymptotic expression for $\rho(\varepsilon)$.

The authors are grateful to M. E. Raikh and R. A. Suris for helpful discussions.

[1] B. I. Halperin and M. Lax, Phys. Rev. **148**, 722 (1966).
[2] J. Zittarts and J. S. Langer, Phys. Rev. **148**, 741 (1966).
[3] B. I. Halperin and M. Lax, Phys. Rev. **153**, 802 (1967).
[4] I. M. Lifshits, Zh. Eksp. Teor. Fiz. **53**, 743 (1967).
[5] B. I. Shklovskii and A. L. Éfros, *Electronic Properties of Doped Semiconductors*, Springer, Berlin (1984).
[6] I. M. Lifshits, S. A. Gredeskul, and L. A. Pastur, *Introduction to the Theory of Disordered Systems*, Wiley, New York (1988).
[7] D. J. Thouless and M. E. Elzain, J. Phys. C: Solid State Phys. **11**, 3425 (1978).
[8] E. Bresin and G. Parisi, J. Stat. Phys. **19**, 269 (1978). E. Bresin and G. Parisi, J. Phys. C: Solid State Phys. **13**, L307 (1980).
[9] A. L. Éfros and M. E. Raikh, in *Modern Problems in Condensed Matter Sciences*, ed. V. M. Agranovich and A. A. Maradudin, Vol. 23, North-Holland, Amsterdam (1988), p. 133.
[10] N. M. Storonskii and B. I. Fuks, Zh. Eksp. Teor. Fiz. **96**, 1880 (1989) [Sov. Phys. JETP **69**, 1061 (1989)].
[11] V. A. Gergel' and R. A. Suris, Zh. Eksp. Teor. Fiz. **84**, 719 (1983) [Sov. Phys. JETP **57**, 415 (1983)].
[12] H. Jeffreys and B. Swirles, Methods of Mathematical Physics, Cambridge Univ. Press, London (1956).
[13] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics: Non-relativistic Theory*, Pergamon, Oxford (1977).

Translated by Eugene Yankovsky