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THEORY OF FLUCTUATION LEVELS IN DISORDERED SYSTEMS

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The energy spectrum of a particle in the field of a disordered system of scattering centers is investigated. A classification of such spectra based on the "intensity" of a single scattering center is presented and the structure of the spectrum in some limiting cases is elucidated. It is shown that for low "intensity" centers the energy levels located at the left of the renormalized spectrum boundary (defined by the mean potential acting on the particle) outside its narrow smearing region are of a fluctuation nature and due to macroscopic fluctuations of the scatterer density. A complete and consistent theory of such fluctuation levels is developed which is based on a statistical description of the scatterer system. The spectral density $\nu(E)$, the form of the wave functions for the fluctuation levels E, and the shape of the density fluctuations at which the levels originate, are found. It is shown that for sufficiently low scatterer concentrations, c, the spectral density $\nu(E, c)$ has a singularity line located near the renormalized spectrum boundary in the (E, c) plane. This line separates states created by weak "long-wave" concentration fluctuations from states corresponding to high-concentration local fluctuations.

1. INTRODUCTION

THE problem of the structure of the energy spectrum and of the quantum states of a disordered system has been attracting more and more attention. The lack of simple systematics for the states in such systems and of a general method for their investigation makes it very important to be able to obtain a qualitative and all the more a quantitative solution of this problem within the framework of any sufficiently realistic model. In an earlier paper[1] we discussed different physical situations which make it possible to reduce the problem of the spectrum of elementary excitations in a disordered system to the model of the wave equation of a particle in a field of random potentials. Principal attention was paid in that article to the case of low concentration of the scattering centers, and also to the structure of the spectrum in the vicinity of the singular points of the spectral density, where a re-arrangement takes place in the systematics of the quantum states. In the present paper we shall analyze another important class of cases which admit of an exact asymptotic solution of the problem in a broad region of the spectrum.

In accordance with the foregoing, we start from the equation ($\hbar^2/2m = 1$)

$$\Delta\psi + (E - U)\psi = 0, \quad U = \sum_j v_j, \quad v_j = v(\mathbf{x} - \mathbf{x}_j) \tag{1.1}$$

with boundary condition $\psi|_\Omega = 0$ on the boundary Ω of the region occupied by the system. Here $v(\mathbf{x} - \mathbf{x}_j)$ is the field of an individual scattering center located at the point $\mathbf{x}_j$; ($\int |v|\, d^3x < \infty$). The points $\mathbf{x}_j$ are assumed to be random, and the probability of the configurations $(\mathbf{x}_1, \ldots, \mathbf{x}_j, \ldots)$ is specified by the distribution function $\rho(\Gamma)\, d\Gamma$ in configuration space $\Gamma = (\ldots, \mathbf{x}_j, \ldots)$. The density of the scattering centers ("impurities") is $n = N/V$, where V is the volume of the system; it is assumed that the average density n is constant in all the limiting transitions $V \to \infty$. By spectral density $\nu(E)dE$ is meant the number of levels, normalized to unit volume, in the energy interval dE:

$$\nu(E)\, dE = \lim_{V\to\infty} \frac{dN_V(E)}{V}. \tag{1.2}$$

The sought spectral density $\nu(E)$ is a macroscopic ("self-averaging") characteristic of the system and should be expressed in terms of the scattering potential $v(\mathbf{x})$ and of the distribution function of the scattering center $\rho(\Gamma)$. Of course, no effective solution exists for this problem in such a general formulation, but in a number of important limiting cases it is possible to carry through to conclusion not only a qualitative investigation, but also a quantitative solution.

For a classification of these cases, we start with certain estimates connected with the characteristic of the scattering potential $v(\mathbf{x})$. We assume that $v(\mathbf{x})$ corresponds to a potential well ($v < 0$) or a potential barrier ($v > 0$) localized in some small region of the volume $\sim a^3$ (a—interaction radius), the potential in this region being of the order of $|v_0| = k_0^2$. One of the most important characteristics of the potential $v(\mathbf{x})$ is the dimensionless quantity $J = (ak_0)^3$. In the case of attraction forces ($v < 0$) the discrete level appears in the potential well at $J > J_{cr} \sim 1$. When $(ak_0)^3 \gg 1$ this quantity coincides, apart from a factor ~ 1, with the number of levels in an individual potential well. Thus, when $J \gg 1$ each well is "classical." To the contrary, when $J = (ak_0)^3 \ll 1$, the individual well is too small for the appearance of a local level, and only an accumulation of a sufficiently large number of scattering centers ensures its occurrence.1)

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1)In the one-dimensional and two-dimensional cases, one level in the well exists even when $ak_0 \ll 1$, but it is "pressed" against the very boundary of the continuous spectrum; in the one-dimensional case $|E_0|/k_0^2 \sim (ak_0)^2$; in the two-dimensional case $\ln |E_0|/k_0^2 \sim -1/(ak_0)^2$. To obtain levels comparable with the depth of the well $|E| \sim k_0^2$ it is necessary, as before, to accumulate a large number of centers.

Attention should be called to the different roles of the δ-function potential from the point of view of the criterion of its "intensity" J in the one-dimensional and three-dimensional cases. In the one-dimensional case the potential $v(x) = A\delta(x)$ corresponds to $J = 0$, and in the three-dimensional case the potential $v(x) = A\delta(x)$ corresponds to $J \to \infty$ (an infinite number of levels in the well $v(x) = -\delta(x)$).

Inasmuch as the kinetic energy E_0 of a particle localized in the volume a^3 is $1/a^2$, the condition $J \ll 1$ also has the meaning of $|v_0| \ll E_0$.

The character of the solution of the problem of the spectral density $\nu(E)$ depends essentially on the value of the parameter $J = (ak_0)^3$. The case $J \gg 1$, as already mentioned, corresponds in the limit to a purely classical problem with Hamiltonian

$$H = k^2 + U(\mathbf{x}), \quad k^2 = p^2/2m, \quad U(\mathbf{x}) = \sum_j v(\mathbf{x} - \mathbf{x}_j).$$

This means that if the summary random potential $U = \Sigma_j v_j$ has a probability density $p(U)$ which does not depend on $\mathbf{x}$,

$$p(U) = \frac{d}{dU} \int\limits_{U(\Gamma)<U} \rho(\Gamma)\, d\Gamma, \quad U(\Gamma) = \sum_j v(\mathbf{x}_j), \tag{1.3}$$

then the spectral density $\nu(E)$ is determined by the rather obvious formula[2)]

$$4\pi^2 \nu(E) = \int\limits_E^\infty \sqrt{E - U}\, p(U)\, dU = \int\limits_0^\infty \sqrt{x}\, p(E - x)\, dx. \tag{1.4}$$

The opposite case $J \ll 1$ in the limit as $J \to 0$ corresponds to a replacement of the random potential $U(\mathbf{x})$ by its mean value $\overline{U}$, that is, simply to a renormalization of the limit of the spectrum

$$4\pi^2 \nu(E) = \sqrt{E - \overline{U}} = \sqrt{E - cv_0},$$

$$\overline{U} = \frac{N \int v(\mathbf{x})\, d^3\mathbf{x}}{V} = cv_0, \quad \int v(\mathbf{x})\, d^3\mathbf{x} = v_0 a^3, \quad c = na^3, \quad |v_0| = k_0^2.$$

The dimensionless density c (the number of neutrons in the volume a^3) can be called the concentration. The limit as $J \to 0$ corresponds to the case $a^3 k_0^3 \to 0$, $na^3 = c \neq 0$ (or $cv_0 = \overline{U} \neq 0$).

Allowance for a small but nonvanishing value $J = (ak_0)^3 \ll 1$ leads to a smearing of the boundary of the spectrum $E = \overline{U}$. In the region of this smearing, there occurs a re-arrangement of the systematics and of the character of the quantum states: on the right of the smeared boundary $E_c = cv_0$ the wave function can be chosen, over sections that are not too large, in the form of weakly damped plane waves. The magnitude of this damping and the small change in the spectral density in this spectral region can be determined without difficulty from perturbation theory and are well known. To the contrary, on the left of this boundary there are located localized "fluctuation" states which result from fluctuations of the density of the scattering centers. When the quantity $J \ll 1$ is small, such fluctuations should encompass a large number ($\sim 1/J \gg 1$) centers and can be regarded as macroscopic. It is precisely this region of the spectrum which is the subject of our study.

The intermediate case $J \sim 1$ is the most complicated one. Here individual potentials v_j can have one or several levels (true or resonant) and the scattering amplitude has in general a resonant character. However, even if the individual potential $v(\mathbf{x})$ does not possess such a level, the level can occur for two (or more) centers located close to each other and spaced $\xi \sim a(v(\mathbf{x}) + v(\mathbf{x} - \xi))$ apart. The position of the resultant level is determined here by the details of the potential $v(\mathbf{x})$, and the probability that two centers will come to within $\xi \sim a$ of each other depends essentially on the correlations between them and the interaction radius a. Therefore it is impossible to obtain any general quantitative formulas when $J \sim 1$. An exception is the case of small concentrations c, where the perturbation $U = \Sigma_j v_j$ is small "in the mean" and qualitatively again leads to a displacement and smearing of the initial boundary of the spectrum ($E_c \sim c$). However, even in this case it is possible to investigate the structure of the spectrum on the left side of the renormalized boundary and to obtain asymptotic formulas only near the singular points of the spectral density near (E, c);[1] such singular points, besides the renormalized boundary E_c itself, are the true boundary of the spectrum at $c \neq 0$ and the positions of the discrete levels as $c \to 0$.

The true boundary of the spectrum does not depend on the concentration c and is located, generally speaking, at a finite distance from the "renormalized" boundary E_c. As shown in [1], for $J \sim 1$ and arbitrary c, macroscopic fluctuations are responsible only for levels located near the true boundary of the spectrum. To the contrary, when $J \sim 1$ all the levels on the left of a narrow strip in the vicinity of the renormalized boundary E_c have a "fluctuation" origin, which makes it possible to apply fully the idea of macroscopic description of such levels,[3)] which was formulated in [1], and to develop a sufficiently simple method for their study. We now proceed to describe this method.[4)]

Unless specially stipulated, the quantity $J = (ak_0)^3$ will serve as the main small parameter, and in all the final expressions we shall be interested only in the principal nonvanishing terms with respect to this parameter. It is precisely in this sense that we shall understand the negligible smallness of the corresponding quantities where necessary. Nonetheless, most results will turn out to be qualitatively valid up to $J \sim 1$.

2. DERIVATION OF GENERAL FORMULA FOR THE DENSITY OF THE FLUCTUATION LEVELS

Let us consider a level E located sufficiently far to the left of the renormalized boundary $E_c = cv_0$; we shall see later that the term "sufficiently far" denotes that $|E - E_c|/E_c \gg (ak_0)^2$. In this case, as was already stated, the realization of such a level calls for a macroscopic fluctuation of the density of the scattering centers. By virtue of the low probability of such a fluctuation, we can always subdivide the entire system into parts of volume V which, on the one hand, are sufficiently large so that the effect of the boundaries is negligibly small, and on the other hand are sufficiently small so that the probability $W_V(E)$ that there will occur in this volume a fluctuation that leads to the appearance of levels to the left of the point E is also small. It is obvious that such a probability of the fluctuations in the volume V, which makes the level E not the first

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[2)] The natural scale for the energy is in this case the quantity $|v_0|$. Near the true boundary of the spectrum E_g, the quasiclassical description begins at $(E - E_g)/|v_0| \gg 1/J^{2/3}$.

[3)] See [1], pp. 626 – 628 and 646 – 648 [translation pp. 554 – 555 and 564 – 565].

[4)] A somewhat different method of investigating the fluctuation levels was developed in the just-published paper of Langer and Zittartz [2].

but, say, the second or third, is incomparably smaller than the probability of that "smallest" fluctuation which is sufficient for the appearance of the level E. Therefore in this case the sought-for level density $\nu(E)$ is asymptotically equal to the probability density $p_0(E)$ of a fluctuation ensuring the appearance of the first level at the point E.

The position of the ground level λ_0 of a particle in the field $U = \Sigma_j v_j$ is determined by the configuration of the scattering centers, that is, is a function of the point $\Gamma = (\ldots, \mathbf{x}_j, \ldots)$ in configuration space: $\lambda_0 = \lambda_0(\Gamma)$. We thus have

$$\nu(E) = p_0(E) = \int \rho(\Gamma)\,\delta(\lambda_0(\Gamma) - E)\,d\Gamma. \tag{2.1}$$

On the other hand, in a field corresponding to the fluctuation of the density, the wave function $\psi_0 = \psi_{0E}(\mathbf{x})$, which is a function of the ground state, varies smoothly over distances $R \gtrsim 1/\sqrt{|E - E_c|}$ subtending a large number of excess scattering centers.

Therefore the position of the level λ_0 is not very sensitive to microscopic displacements of the individual centers, and should depend with sufficient accuracy only on the "macroscopic" density of the centers (or, which is the same, on the "concentration" $c(\mathbf{x}) = a^3 n(\mathbf{x})$). If c_0 is the average concentration of the system, then the macroscopic fluctuation is described by the function $\xi(\mathbf{x}) = c(\mathbf{x}) - c_0$, the radius of the decrease of which is determined by the dimensions of the fluctuation. Thus, λ_0 is a functional of $\xi(\mathbf{x})$

$$\lambda_0 = \lambda_0\{\xi\} \quad (= \lambda_0\{\xi, c_0\}). \tag{2.2}$$

As can be readily verified, we can write, with the same degree of accuracy, the wave equation (1.1) for the function ψ_0 in the form

$$\begin{gathered}\Delta\psi_0 + (E - c_0 v_0 - v_0\hat{\Theta}\xi)\psi_0 = 0.\\ \hat{\Theta}\xi = \int \Theta(\mathbf{x} - \mathbf{y})\,\xi(\mathbf{y})\,d^3\mathbf{y}, \quad \Theta(\mathbf{x}) = v(\mathbf{x}) \Big/ \int v(\mathbf{x})\,d^3x.\end{gathered} \tag{2.3}$$

The form of (2.3) serves as an interpretation of the dependence $\lambda_0 = \lambda_0\{\xi\}$ and the condition for the admissible functions $\xi(\mathbf{x})$ takes the form

$$\lambda_0\{\xi\} = E.$$

Equation (2.3) is obtained from (1.1) by replacing the random potential $U(\mathbf{x})$ at each of the macroscopically small sections of volume $\Delta^3 x$ (where $\psi(\mathbf{x})$ changes little. but $c(\mathbf{x})\Delta^3 x/a^3 \gg 1$), by its "local" mean value $\tilde{U}(\mathbf{x})$

$$\tilde{U}(\mathbf{x}) = \int c(\mathbf{x}')\,\frac{v(\mathbf{x} - \mathbf{x}')\,d^3\mathbf{x}'}{a^3}.$$

The condition $J \ll 1$ ensures the correctness of such a substitution and a transition to (2.3). By virtue of the very same condition, the appearance of the level requires a fluctuation of the "radius" $R \gg a$, provided only the potentials v_j cannot overlap strongly, that is, the maximum concentration of the scattering centers (the maximum number of such centers in the interaction sphere a^3) cannot reach a value $\sim (ak_0)^{-2} \gg 1$. The dimensions of the fluctuation are certainly large for a small overlap of the potentials, when the concentration has a maximum ~ 1. In this case (2.3) takes the simpler form

$$\Delta\psi + [E - c_0 v_0 - \xi v_0]\psi = 0. \tag{2.4}$$

We shall henceforth pay principal attention to this case.

In accordance with the foregoing, it is convenient to change over in (2.1) from integration over the configuration space $d\Gamma$ to integration over the space of the functions $\xi(\mathbf{x})$. The corresponding Jacobian of the transition, with allowance for the "weight factor" $\rho(\Gamma)$ can be written in the form $A\exp[\sigma(\xi, c_0)]$, where σ has the meaning of the entropy as a functional of ξ. Thus,

$$\nu(E) = p_0(E) = \frac{\int e^{\sigma\{\xi, c_0\}}\,\delta(\lambda_0\{\xi\} - E)\,D\xi}{\int e^{\sigma\{\xi, c_0\}}\,D\xi}. \tag{2.5}$$

The presence of a normalization factor in the denominator of (2.5) makes it possible to write out $\sigma\{\xi, c_0\}$ accurate to an additive term. Let $\sigma(c)/a^3$ be the density of the entropy of a system with a distribution function $\rho(\Gamma)$ and a homogeneous concentration c. Taking into account the additivity of the entropy[5] as well as the conservation of the total number of centers in the entire system, we have for an arbitrary macroscopic fluctuation of the concentration $\xi(\mathbf{x})$ in a system with "equilibrium" concentration c_0

$$S\{\xi\} = \sigma\{\xi, c_0\} - \sigma\{0, c_0\} = \frac{1}{a^3}\int [\sigma(c_0 + \xi) - \sigma(c_0) - \xi\sigma'(c_0)]\,d^3x. \tag{2.6}$$

The quantity $\sigma(c)$ is determined by the distribution function $\rho(\Gamma)$ and is specified by the concrete physical situation. Thus, for example, if there is no correlation at all between the centers ($\rho(\Gamma) = \text{const}$), then $\sigma(c)$ corresponds to the entropy of an ideal gas and takes the form

$$\sigma(c) = -c\ln(c/e). \tag{2.7}$$

If the scattering centers are impurity atoms in the crystal and form a "lattice gas" such that in each cell or volume a^3 there can be located not more than one impurity atom, then[6]

$$\sigma(c) = c_g\left[\frac{c}{c_g}\ln\frac{c}{c_g} + \left(1 - \frac{c}{c_g}\right)\ln\left(1 - \frac{c}{c_g}\right)\right],$$

$$c_g = \frac{b^3}{a^3}.$$

$$\sigma(c) = -c\ln c - (1 - c)\ln(1 - c). \tag{2.8}$$

Correlations of another type in the arrangement of the scattering centers reduce likewise, in final analysis, to a definite form of the $\sigma(c)$ dependence, which can be regarded as specified (or should be calculated independently).

Writing $\nu(E)$ in the form $\nu(E) = e^{F(E)}$, we have in accord with (2.5) and (2.6)

$$F(E) = \ln\nu(E) = \ln\frac{\int e^{S\{\xi\}}\,\delta[\lambda_0\{\xi\} - E]\,D\xi}{\int e^{S}\,D\xi}. \tag{2.9}$$

Taking into account the macroscopic character of $S\{\xi\}$ (with respect to the parameter $1/J$), we can easily obtain the principal term in F(E). The main contribution to the functional integrals (2.9) is made by the integration in the vicinity of the extremal points of S in

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[5] Strictly speaking, formula (2.6) holds only for sufficiently smooth functions $\xi(x)$ (which vary over distances that are large compared with the radius of the correlation of the scattering centers); however, in view of the smoothing influence of the functional $\lambda_0\,\xi$ we can confine ourselves only to such functions.

[6] If the volume of the crystal cell b^3 does not coincide with the volume of the interaction a^3, then

function space. Therefore the first term in (2.9) is determined by the maximum value of S on the hypersurface $\lambda_0\{\xi\} = E$ in function space, and the second by the absolute maximum of the same expression.

$$F_0(E) = \max S\{\xi\}\,|_{\lambda_0\{\xi\}=E} - \max S\{\xi\}.$$

The second term obviously vanishes and therefore

$$F_0(E) = \max S\{\xi\}\,|_{\lambda_0\{\xi\}=E} = S\{\tilde{\xi}\}, \tag{2.10}$$

where $\tilde{\xi}$ is the sought-for extremal.

The conditional extremum (2.10) is determined from the vanishing of the variation of the functional $S + \beta\lambda_0$:

$$\delta[S\{\xi\} + \beta\lambda_0\{\xi\}] = \tag{2.11}$$

(β is an undetermined multiplier).

The variation δS is, in accord with (2.6),

$$\delta S\{\xi\} = -\frac{1}{a^3}\int [\sigma'(c_0+\xi) - \sigma'(c_0)]\,\delta\xi d^3x. \tag{2.12}$$

To determine the variation $\delta\lambda_0$ of the first eigenvalue $\lambda_0 = \lambda_0\{\xi\}$ of the equation

$$\Delta\psi_0 + [\lambda_0 - c_0v_0 - v_0\xi(x)]\psi_0 = 0 \tag{2.13}$$

it is sufficient to note that the variation $\delta\xi$ leads to the appearance of a perturbing potential $\delta U = v_0\delta\xi$ in (2.13). Therefore, if ψ_0 is the eigenfunction of the ground state (2.13), then the variation $\delta\lambda_0$ will be

$$\delta\lambda_0 = v_0\frac{(\psi_0, \delta\xi\cdot\psi_0)}{\|\psi_0\|^2}$$
$$(f, g) = \int fg d^3x, \quad \|f\|^2 = (f, f) = \int f^2 d^3x. \tag{2.14}$$

Thus, from (2.11), (2.12), and (2.14) we have for the extremal function $\tilde{\xi}$

$$\left(\sigma'(c_0+\tilde{\xi}) - \sigma'(c_0) + \beta v_0 a^3\frac{\psi_0{}^2}{\|\psi_0\|^2}, \delta\xi\right) = 0,$$

or

$$\sigma'(c_0+\tilde{\xi}) - \sigma'(c_0) = -\beta v_0 a^3\frac{\psi_0{}^2}{\|\psi_0\|^2}. \tag{2.15}$$

On the other hand, ψ_0 itself satisfies (2.13); finally, the undetermined multiplier β is determined by the condition $\lambda_0\{\xi\} = E$.

The parameter β can be immediately excluded by introducing in lieu of $\psi_0(x)$ the quantity proportional to it:

$$z(\mathbf{x}) = \psi_0\frac{\sqrt{|\beta v_0|a^3}}{\|\psi_0\|} \tag{2.16}$$

and including the condition $\lambda_0 = E$ in (2.13).

If furthermore we go over in (2.13) to the dimensionless coordinates $\mathbf{x}' = \mathbf{x}\sqrt{|v_0|} = k_0\mathbf{x}$ (we shall henceforth omit the prime of $\mathbf{x}'$), then we obtain finally a nonlinear differential equation for z (or $\tilde{\xi}$):

$$\Delta z + [\varepsilon - |\xi|]z = 0,$$
$$\sigma'(c_0+\tilde{\xi}) - \sigma'(c_0) = z^2\operatorname{sgn} v_0, \quad \varepsilon = \frac{E - v_0c_0}{|v_0|} \tag{2.17}$$

with the natural boundary condition

$$z|_{x\to\infty} = \tilde{\xi}|_{x\to\infty} = 0.$$

As follows from (2.17), the concrete connection between $\tilde{\xi}$ and z is determined by the entropy $\sigma(c)$. We present this dependence for the already discussed cases (2.7) and (2.8):

$$1)\ \sigma = -c\ln\frac{c}{e}, \quad \pm z^2 = \ln\frac{c_0+\tilde{\xi}}{c_0},$$
$$\tilde{\xi} = \begin{cases} c_0(e^{z^2}-1), & v_0 < 0 \\ c_0(e^{-z^2}-1), & v_0 > 0 \end{cases}. \tag{2.18}$$

$$2)\ \sigma = -c\ln c - (1-c)\ln(1-c),$$
$$\pm z^2 = \ln\left[\frac{1-c}{c}\frac{c_0}{1-c_0}\right], \quad c_0 + \tilde{\xi} = \frac{1}{e^{\gamma\pm z^2}+1}, \tag{2.19}$$
$$e^{-\gamma} = c_0/(1-c_0).$$

The functions z(x) and $\tilde{\xi}(x)$ obtained from (2.17) yield, respectively, the wavefunction corresponding to the fluctuation level ε and the distribution of the concentration in the region of the fluctuation responsible for this level.

After obtaining these functions, we get for the sought spectral density, in accord with (2.10), the expression

$$\ln\nu(E) = S\{\tilde{\xi}\} = \frac{1}{(ak_0)^3}g\left(\frac{E-c_0v_0}{|v_0|}\right),$$
$$g(\varepsilon) = \int[\sigma(c_0+\tilde{\xi}) - \sigma(c_0) - \tilde{\xi}\sigma'(c_0)]\,d^3x, \quad \tilde{\xi} = \tilde{\xi}(\mathbf{x}, \varepsilon). \tag{2.20}$$

If the potentials v_j cannot overlap greatly, that is, the maximum admissible concentration of the centers $c_{\max} \sim 1$, then the maximum possible value $|\varepsilon| \sim 1$. In particular, for the "lattice gas" (2.8) we have

$$c_0 < \xi < 1 - c_0, \quad |\varepsilon| < \begin{cases} 1-c_0, & v_0 < 0 \\ c_0 & v_0 > 0 \end{cases}.$$

Inasmuch as (2.17) contains only the parameters c_0 and ε, we have $g(\varepsilon) \sim 1$ when $\varepsilon \sim c_0 \sim 1$, and consequently

$$\ln\nu(E) \sim \frac{1}{(ak_0)^3} \sim \frac{1}{J}.$$

As will be shown in Sec. 4, at sufficiently small ε it turns out, for the extremal fluctuation, that $\tilde{\xi} \ll c_0$. In this case, the functional $S\{\xi\}$ in (2.6) takes on near the extremal the form

$$S\{\xi\} = \frac{\sigma''(c_0)}{2(ak_0)^3}\int\xi^2d^3x. \tag{2.21}$$

Equations (2.17) are suitably simplified

$$\tilde{\xi}\sigma''(c_0) = \pm z^2,$$
$$\Delta z + \varepsilon z - z^3/\sigma''(c_0) = 0. \tag{2.22}$$

Finally, (2.20) yields

$$g(\varepsilon) = \frac{1}{2\sigma''(c_0)}\int z^4d^3x. \tag{2.24}$$

Taking into account the natural spherical symmetry of the extremal fluctuation and choosing its center at the origin, we can put $z = z(r)$. Then assuming

$$z^2 = \varepsilon\sigma''(c_0)\varphi^2(\alpha r), \quad \varepsilon = -\alpha^2 \quad (\varepsilon\sigma''(c_0) > 0), \tag{2.25}$$

we obtain for φ an equation without parameters

$$\frac{1}{\rho^2}\frac{d}{d\rho}\left(\rho^2\frac{d\varphi}{d\rho}\right) - \varphi + \varphi^3 = 0, \quad \varphi|_{r\to\infty} = 0, \tag{2.26}$$

which can be solved numerically. From (2.24) and (2.25) we have

$$g(\varepsilon) = g(-\alpha^2) = \frac{\alpha\sigma''(c_0)}{2}\int_0^\infty\varphi^4(\rho)4\pi\rho^2d\rho. \tag{2.27}$$

From this we get, for sufficiently small ε,

$$\ln\nu(E)=\frac{\sigma''(c_0)}{2(ak_0)^3}\sqrt{|\varepsilon|}\,\varphi_4,\qquad \varphi_4=4\pi\int_0^\infty\varphi^4(\rho)\rho^2d\rho. \tag{2.28}$$

The case $\varepsilon \gtrsim 1$ will be considered in the following sections.

In the opposite limiting case, if the potentials can strongly overlap, and if the extremal fluctuations $\tilde{\xi}$ are realized in a volume $\sim a^3$ ($\tilde{\xi} \gg 1$), the form of the general equations (2.17) becomes somewhat complicated. Indeed, it is necessary to take (2.3) in lieu of the initial equation (2.4) or (2.13). Upon varying $\delta\lambda_0\{\xi\}$ we obtain

$$\delta\lambda_0=v_0\frac{(\psi_0,\psi_0\hat{\Theta}\delta\xi)}{\|\psi_0\|^2}=\frac{v_0(\delta\xi,\hat{\Theta}\psi_0^2)}{\|\psi_0\|^2}, \tag{2.29}$$

and the equation for the extremal of $\tilde{\xi}$ assumes in lieu of (2.15) the form

$$\sigma'(c_0+\tilde{\xi})-\sigma'(c_0)=-\hat{\Theta}\psi_0^2\frac{\beta v_0a^3}{\|\psi_0\|^2}. \tag{2.30}$$

After going over to the function z in accord with (2.16), and changing over to the variable $x' = k_0x$ in analogy with (2.17), we obtain jointly with (2.3) (if $v_0 < 0$)

$$\Delta z+(\varepsilon-\hat{\Theta}\tilde{\xi})z=0,\qquad \sigma'(c_0+\tilde{\xi})-\sigma'(c_0)=-\hat{\Theta}z^2. \tag{2.31}$$

3. FLUCTUATION LEVELS IN THE ONE-DIMENSIONAL CASE

In the one-dimensional case it is easy to obtain close formulas for all the quantities of interest to us: the wave functions corresponding to the fluctuation levels, the forms of the corresponding concentration fluctuations, and the spectral density.

The initial equation (2.17) for z takes the form

$$d^2z/dx^2-(\alpha^2-\tilde{\xi})z=0,\qquad \varepsilon=-\alpha^2\quad(v_0<0). \tag{3.1}$$

Recognizing that the fluctuation is symmetrical and choosing its center at the origin, we obtain the boundary conditions

$$z|_{x\to\infty}=0,\qquad z'|_{x=0}=0. \tag{3.2}$$

The first of these conditions can be written in the form

$$z'|_{z=0}=0. \tag{3.3}$$

The first integral of (3.1) under condition (3.3) takes the form

$$z'^2=2\int_0^z(\alpha^2-\tilde{\xi})zdz,\qquad z^2=\sigma'(c_0+\tilde{\xi})-\sigma'(c_0), \tag{3.4}$$

whence

$$dx=\left[2\int_0^z(\alpha^2-\tilde{\xi})zdz\right]^{-1/2}dz,\qquad 2zdz=\sigma''(c_0+\tilde{\xi})d\tilde{\xi}. \tag{3.5}$$

The wave function $z(x)$ is determined by the equation

$$x=\int_0^z\left[2\int_0^z(\alpha^2-\tilde{\xi})zdz\right]^{-1/2}dz. \tag{3.6}$$

The form of the concentration fluctuation is given by the equation

$$x=\int_0^{\tilde{\xi}}\frac{\sigma''(c_0+\tilde{\xi})d\tilde{\xi}}{2z(\tilde{\xi})}\left\{\int_0^{\tilde{\xi}}\sigma''(c_0+\tilde{\xi})[\alpha^2-\tilde{\xi}]d\tilde{\xi}\right\}^{-1/2}, \tag{3.7}$$

and finally, for the logarithm of the spectral density we have

$$\ln\nu(E)=g(\varepsilon)/ak_0,\qquad \varepsilon=(E-c_0v_0)/|v_0|,$$

$$g(\varepsilon)=2\int_0^\infty\left[\sigma(c_0+\tilde{\xi})-\sigma(c_0)-\tilde{\xi}\sigma'(c_0)\right]dx$$
$$=2\int_0^{z_0}[\sigma(c_0+\tilde{\xi})-\sigma(c_0)-\tilde{\xi}\sigma'(c_0)]\left[2\int_0(\alpha^2-\tilde{\xi})zdz\right]^{-1/2}dz. \tag{3.8}$$

Here z_0 is the first positive root of the equation

$$\int_0^{z_0}[\alpha^2-\tilde{\xi}(z)]zdz=0.$$

We write out the obtained formulas in explicit form for the simplest case of an "ideal gas" of scattering centers. Here

$$\tilde{\xi}=c_0(e^{z^2}-1),$$
$$\sigma(c_0+\tilde{\xi})-\sigma(c_0)-\tilde{\xi}\sigma'(c_0)=c\ln\frac{c}{e}-(c-c_0)$$
$$=c_0[e^{z^2}(z^2-1)+1].$$

Therefore, according to (3.6) and (3.8), we obtain for the wave function $z(x)$

$$x=\int_0^z\frac{dz}{z[\alpha^2-c_0(e^{z^2}-1-z^2)/z^2]^{1/2}} \tag{3.9}$$

and for the spectral density

$$\ln\nu(E)=\frac{c_0}{a}\int_0^{z_0}\frac{[e^{z^2}(z^2-1)+1]dz}{\{Ez^2-c_0v_0[e^{z^2}-1]\}^{1/2}}. \tag{3.10}$$

In the one-dimensional case, in the absence of correlation and when $v(x) = A\delta(x)$, there exists an exact solution of the problem[3] of the spectral density $\nu(E)$. This solution, however, does not yield any information on the character of the wave functions and, most importantly, it cannot be generalized to the case of a large number of dimensions. The obtained expression (3.10) for the argument of the exponent $\ln\nu(E)$ coincides with this exact solution and we shall therefore not stop to investigate it.

4. FLUCTUATION LEVELS IN THE THREE-DIMENSIONAL CASE

It is natural to assume that the extremal fluctuation is spherically symmetrical. Then the initial equation (2.17) takes the form

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial z}{\partial r}\right)-(\alpha^2-|\tilde{\xi}|)z=0,\quad \tilde{\xi}=\tilde{\xi}(z),\quad z|_{r\to\infty}=0,\quad \alpha^2=|\varepsilon|, \tag{4.1}$$

or, putting $z = \chi/r$,

$$\chi''(r)-(\alpha^2-|\tilde{\xi}|)\chi=0,\qquad \tilde{\xi}=\tilde{\xi}(\chi/r),\qquad \chi(0)=\chi(\infty)=0. \tag{4.2}$$

Equation (4.2) cannot be integrated in quadratures and can be solved only approximately. Since the function $\tilde{\xi}(z)$ is as a rule monotonic, a convenient method for its solution is, say, the subdivision of the region of variation of $\tilde{\xi}(z)$ into several intervals and replacing $\tilde{\xi}(z)$ in each of these intervals by a constant value ξ_k. Here, naturally, the first value ξ_0 determines the maximum depth of the potential well, and the last value $\xi_n = 0$. The values of ξ_k and the points r_k corresponding to the jumps $\Delta\xi_k = \xi_{k+1} - \xi_k$ should be determined by solving the corresponding variational problem.

Qualitatively good results are obtained already for n = 1 and n = 2; an approximation of the exact solution can be obtained not only by increasing n, but also by an iteration method, in which each succeeding approximation $\chi_{k+1}(r)$ is obtained from the preceding one $\chi_k(r)$ $(r = r_k(\chi))$

$$\chi''(r) - \left[\alpha^2 - \tilde{\xi}\left(\frac{\chi}{r_k(\chi)}\right)\right]\chi = 0, \quad \chi = \chi_{k+1}. \tag{4.3}$$

Since it is not our aim in the present article to develop such approximate methods, we present only the simplest calculation with n = 1. This case corresponds in (4.2) to a potential well of constant depth $|\xi_0|$ and of radius R

$$|\tilde{\xi}| = \begin{cases} |\tilde{\xi}_0| = \mu^2, & r < R \\ 0, & r > R \end{cases}, \tag{4.4}$$

where the self-consistent quantities ξ_0 and R are to be determined from the extremal conditions.

Joining together the solution $\chi = A \sin \kappa r$, $r < R$ and $\chi = Be^{-\alpha r}$, $r > R$, $\kappa^2 + \alpha^2 = \mu^2 = |\xi_0|$, we obtain the first condition relating R, ξ_0, and ε (or R, μ, and α):

$$\operatorname{tg}(\pi - \kappa R) = \kappa/\alpha, \quad \pi/2 < \kappa R < \pi.$$

Putting

$$\frac{\alpha}{\mu} = \left|\frac{\varepsilon}{\xi_0}\right|^{1/2} = \cos\vartheta, \quad \frac{\kappa}{\mu} = \sin\vartheta,$$

we get

$$\operatorname{tg}(\pi - \mu R \sin\vartheta) = \operatorname{tg}\vartheta, \quad 0 < \pi - \mu R \sin\vartheta < \pi/2,$$

whence

$$R = \frac{\pi - \vartheta}{\mu \sin\vartheta} = \frac{\pi - \vartheta}{\kappa} = \frac{\pi - \vartheta}{\alpha \operatorname{tg}\vartheta}, \quad 0 < \vartheta < \frac{\pi}{2}. \tag{4.5}$$

for $\alpha/\mu \ll 1$ we get $\vartheta \to \pi/2$ and $R \to \pi/2\mu$; for $\kappa/\mu \ll 1$ we get $\vartheta \to 0$ and $R \to \pi/\kappa$.

The fluctuation of the entropy S as a function of ξ_0 and R is of the form

$$S = \frac{1}{(ak_0)^3}\frac{4\pi}{3}R^3 s(c, c_0),$$
$$s(c, c_0) = \sigma(c) - \sigma(c_0) - (c - c_0)\sigma'(c_0), \quad c - c_0 = \xi_0 = \pm\mu^2. \tag{4.6}$$

For the limiting concentrations c = 0 and $c = c_g$ we get

$$\sigma(0) = \sigma(c_g) = 0,$$

and for sufficiently small c we get $\sigma(c) = -c \ln c$. Finally, for small $c - c_0 = \xi_0 \ll c_0$ we have

$$s = \frac{\xi_0^2}{2}\sigma''(c_0) = \frac{\mu^4}{2}\sigma''(c_0), \tag{4.7}$$

whence, according to (4.5) and (4.7)

$$S = \frac{4}{3}\frac{\pi}{(ak_0)^3}\mu\left(\frac{\pi - \vartheta}{\sin\vartheta}\right)^3 \sigma''(c_0) = \frac{4}{3}\frac{\pi}{(ak_0)^3}\alpha\sigma''(c_0)\frac{(\pi - \vartheta)^3}{\cos\vartheta \sin^3\vartheta}. \tag{4.8}$$

To obtain in $\nu(E) = \max S$ it is necessary to obtain the extremum of S as a function of R and ξ_0, subject to condition (4.5) and for fixed $\varepsilon = -\alpha^2$. We present the results of these calculations in some of the simplest cases.

1. $v_0 > 0$. In this case the true boundary of the spectrum coincides with the initial boundary E = 0. Then for the levels close to this boundary, $E \ll c_0 v_0$ $(\varepsilon + c_0 \ll c_0)$, we get from (4.6) and (4.4)

$$R \approx \pi(\varepsilon + c_0)^{-1/2} = \pi\sqrt{v_0/E},$$
$$(ak_0)^3 \ln \nu(E) = {}^4/_3\, \pi^{5/2}(v_0/E)^{3/2}[c_0\sigma'(c_0) - \sigma(c_0)]$$
$$= {}^4/_3\, \pi^{5/2}|\varepsilon + c_0|^{-3/2}[c_0\sigma'(c_0) - \sigma(c_0)]. \tag{4.9}$$

This formula coincides with that obtained earlier in [1] and is asymptotically correct, since the exact form of the potential well $\tilde{\xi}(z(r))$ is rectangular when $E \to E_g$.

For levels close to the renormalized boundary ($|\varepsilon| \ll c_0$) we have in accordance with (4.5) and (4.8), minimizing S with respect to ϑ with $\alpha = \sqrt{|\varepsilon|}$ fixed,

$$R \sim |\varepsilon|^{-1/2}, \quad |\xi_0| \sim |\varepsilon|,$$
$$(ak_0)^3 \ln \nu(E) = \gamma\sigma''(c_0)|\varepsilon|^{1/2}, \quad \gamma \sim 1. \tag{4.10}$$

Since we get $|\varepsilon| \ll c_0$ when $|\xi_0| \sim |\varepsilon| \ll c_0$, the exact solution of (4.1) simplifies greatly and, as was shown above, leads to (2.23), (2.26), and (2.28).

Thus, the exact value of the numerical constant γ in (4.10) is

$$\gamma = \frac{\varphi_4}{2} = 2\pi\int_0^\infty \varphi^4(\rho)\rho^2 d\rho. \tag{4.11}$$

2. $v_0 < 0$. In this case the position of the true boundary of the spectrum is determined by the permissible overlap of the potentials v_j.

If there is no correlation (ideal gas of scattering centers) and arbitrary overlap is permissible, then the true boundary is located at $-\infty$.

Then, as can be readily verified, there is no solution of the extremal problem formulated above, within the framework of equation (4.1). Indeed, putting $\xi_0 \gg 1$, and consequently c_0, $|\varepsilon| \ll c$ $(c = c_0 + \xi_0 \approx \xi_0)$ we obtain, in accord with (4.5) and (4.6),

$$R = \frac{\pi}{\alpha}c^{-1/2},$$

$$-S = \frac{4\pi R^3}{3(ak_0)^3}c \ln\frac{c}{c_0} = \frac{\pi^4}{6(ak_0)^3}\frac{\ln(c/c_0)}{\sqrt{c}}\left(1 + O\left(\sqrt{\frac{|\varepsilon|}{c}}\right)\right). \tag{4.12}$$

The minimum of this expression is equal to zero and is attained at $c \to \infty$ and $R \to 0$. This means that the level ε is realized not on the fluctuations of the macroscopic volume ($R \gg ak_0$), but at the maximum overlap of the centers, which corresponds to $R \sim ak_0$ and $c = \xi_0 \sim (ak_0)^{-2}$; consequently, in accord with (4.6),

$$(ak_0)^3 \ln \nu(E) = \gamma_1 ak_0 \ln[c_0(ak_0)^2](1 + O(ak_0\sqrt{|\varepsilon|}),$$
$$\gamma_1 \sim 1, \quad |\varepsilon| \ll c \sim (ak_0)^{-2}. \tag{4.13}$$

The exact solution of the problem is described in this case by (2.23).

On the other hand, for levels that are sufficiently close to the renormalized boundary ($|\varepsilon| \ll c_0$) there exists, as in the case $v_0 > 0$, a solution of the extremal problem corresponding to fluctuations in a large volume and described by formula (2.28) or (4.10)

$$g(\varepsilon, c_0) = (ak_0)^3 \ln \nu(E) = -\frac{\gamma|\varepsilon|^{1/2}}{c_0}, \quad \sigma''(c_0) = -\frac{1}{c_0}. \tag{4.14}$$

The true solution is (asymptotically with respect to $(ak_0)^3$) the smaller of the two values of $|\ln \nu(E)|$ given by (4.13) and (4.14). Thus,

$$(ak_0)^3 \ln \nu(E) = \begin{cases} -\gamma|\varepsilon|^{1/2}/c_0, & |\varepsilon| < \varepsilon_k(c_0), \\ -\gamma_1 ak_0 \ln c_0(ak_0)^2, & |\varepsilon| > \varepsilon_k(c_0), \end{cases} \tag{4.15}$$
$$\varepsilon_k(c_0) \sim c_0^2(ak_0)^2 \ln^2[c_0(ak_0)^2].$$

If large overlaps of the potentials v_j are not admissible and there exists a maximum concentration c_g ($\sigma(c_g) = 0$) corresponding to the true boundary of the spectrum $E_g = c_g v_0$, then solution (4.13) cannot be realized for sufficiently small $(ak_0)^3$. Then, in accordance with the general formula (2.20), $g(\varepsilon, c_0) = (ak_0)^3 \ln \nu(E)$ does not contain ak_0 at any energy ε up to the true boundary E_g. Near this boundary, in analogy with (4.9), we get

$$g(\varepsilon, c_0) = -\frac{4}{3}\pi^{5/2} y^{-3/2} s(c_g, c_0), \quad y \ll s(c_g, c_0), \tag{4.16}$$

$$y = (E - E_g)/|v_0| = \varepsilon + c_g - c_0, \quad s(c_g, c_0) = -\sigma(c_0) - (c_g - c_0)\sigma'(c_0).$$

At small concentrations $c_0 \ll 1$ ($\sigma''(c_0) = -1/c_0$) we can obtain for $g(\varepsilon, c_0)$ an asymptotically exact expression in the entire region of energies ε.[7] Recognizing that near the limiting concentration c_g the entropy is $\sigma(c) \sim -(c - c_g) \ln (c - c_g)$, and $|s(c_g, c_0)| = |c_g \ln c_0| \gg 1$, we obtain, finding the extremum of the expression $S = R^3(c, \varepsilon) s(c, c_0)$ with $c_g - c \ll c_g$,

$$R = y^{-1/2}\left(\pi - \arcsin\sqrt{\frac{y}{c_g}}\right), \quad c = c_g - \exp\left\{3c_g \ln c_0\left(-\frac{\partial \ln R}{\partial c_g}\right)\right\} \cong c_g,$$

$$g(\varepsilon, c_0) = \frac{4}{3}\pi y^{-3/2}\left(\pi - \arcsin\sqrt{\frac{y}{c_g}}\right)^3 c_g \ln c_0, \quad y \ll |c_g \ln c_0|.$$

Together with the solution (4.14) obtained earlier in the region of low energies $|\varepsilon| \ll c_0$, we get

$$\begin{gathered} g(\varepsilon, c) = -\gamma|\varepsilon|^{1/2}/c = g_{\mathrm{I}}, \quad |\varepsilon| \ll c, \\ g(\varepsilon, c) = \frac{4}{3}\pi y^{-3/2}\left(\pi - \arcsin\sqrt{\frac{y}{c_g}}\right)^3 c_g \ln c = g_{\mathrm{II}}, \\ y = \varepsilon + c_g - c \ll c_g \ln c. \end{gathered} \tag{4.17}$$

As seen from (4.17), the regions of existence of solutions (I) and (II) overlap when c is sufficiently small. Therefore the functions $g_{\mathrm{I}}(\varepsilon, c)$ and $g_{\mathrm{II}}(\varepsilon, c)$ represent two different branches of a solution of the extremal problem. As before, the true extremum for each ε and c is given by the smaller of the quantities $|g_{\mathrm{I}}|$ or $|g_{\mathrm{II}}|$ and thus $g = g_{\mathrm{I}}$ when $|\varepsilon| < \varepsilon_k(c)$ and $g = g_{\mathrm{II}}$ when $|\varepsilon| > \varepsilon_k(c)$, where

$$\varepsilon_k(c) = Ac^2 \ln^2 c, \quad A = \pi^8/36\gamma^2 c_g. \tag{4.18}$$

The result shows that a line of singularities $\varepsilon = \varepsilon_k(c)$ appears in the function $g(\varepsilon, c)$ at sufficiently small concentrations c (in analogy with the case of (4.15)). This line is located (for small c) in the vicinity of the renormalized boundary E_c and separates the states generated by the weak "long-wave" fluctuations of concentration from the states corresponding to the local fluctuations of the large concentration. A similar situation should apparently exist also when $ak_0 \sim 1$; in this case the local fluctuations of the concentration for the levels $|\varepsilon| < \varepsilon_k$ reduce to "collisions" of a rather small number of scatterers—possibly two or three, which in themselves generate local levels near the renormalized boundary (see [1]).

In conclusion we return to the question of the limits of applicability of the obtained results.

Replacement of the initial macroscopic equation (1.1) by the macroscopic equation (2.4) confirms the correctness of the results, as seen from the derivation of (2.5) and (2.10), and finally verifies the final formula (2.30), provided the following requirements are met:

$$(ak_0)^3 \ll 1, \quad |\ln \nu(E)| \gg 1.$$

Therefore it might seem from the exact formula (4.14) that the formulated macroscopic theory of fluctuation levels is valid for all energies $\varepsilon = (E - E_c)/|v_0|$ to the left of the renormalized boundary, satisfying the inequality

$$|\varepsilon|^{1/2} \gg (ak_0)^3/\gamma\sigma''(c_0).$$

However, it is possible that the formula (4.14) is violated somewhat earlier, owing to the fact that no account is taken in it of the actually existing smearing of the level $\lambda_0\{\xi\}$, which is specified by the macroscopic density $n(\mathbf{x}) = (c_0 + \xi(\mathbf{x}))/a^3$ and vanishes on going to the macroscopic equation (2.13). Microscopic displacements of the centers are equivalent to addition of a field of random "dipoles"

$$\delta U = \sum_j [v(\mathbf{x} - \mathbf{x}_j) - v(\mathbf{x} - \mathbf{x}_j - \delta x_j)]$$

and leads to a shift and smearing of the macroscopic level $\lambda_0\{\xi\}$. The shifts of the levels $\lambda_0\{\xi\}$ reduce to an inessential refinement of the renormalized boundary E_c, but the smearing of these levels at sufficiently low $\varepsilon = E - E_c/|v_0|$ becomes appreciable and limits the possibility of approaching the point $\varepsilon = 0$ in the formulas for the probability $p_0(E)$.

For the same reason, within the framework of the macroscopic approximation, calculation of the factor in front of the exponential in $\nu(E)$ far from the renormalized boundary E_c (at $\varepsilon \sim 1$) is of no interest. Such a factor is the result of integration of (2.9) over the macroscopic fluctuations in the vicinity of the point of the extremum $\tilde{\xi}$, and the addition that it makes to $F(E) = \ln \nu(E)$ corresponds, when $\varepsilon \sim 1$, to a shift of the level ε by an amount $\delta\varepsilon \sim (ak_0)^3 \ln ak_0$; such a shift turns out to be, generally speaking, smaller than the shift of this level due to macroscopic fluctuations of the density.

However, the pre-exponential factor in the macroscopic approximation (2.5) gives apparently the correct value in the most interesting region near the renormalized boundary. On the other hand, in the direct vicinity of the boundary, and all the more in the region of smearing of this boundary, the probability $p_0(E)$, for which formulas (2.5), (2.9), etc. have been written out, no longer coincides with the spectral density $\nu(E)$. On approaching E_c, the overwhelming contribution to $\nu(E)$ is made already not by the states corresponding to the lower level at the given fluctuation, but by the higher levels. Such levels lose their fluctuation character in the smearing region, although they still do not correspond to states of the plane-wave type, since they are damped at distances smaller than the wavelength.

Nonetheless, the problem of the exact calculation of the probability $p_0(E)$ in the macroscopic approximation with the aid of formula (2.9) is of independent interest, and it is therefore meaningful to obtain the pre-exponential factor in this expression. The calculation of this factor is given in the Appendix.

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[7] When $|\ln c_0| \gg 1$, as can be verified from (2.19), the true form of the potential well coincides with (4.4).

APPENDIX

CALCULATION OF THE PRE-EXPONENTIAL FACTOR

According to (2.9), we can write

$$F(E)=\ln p_0(E)=\ln\left[\frac{\int\exp\{S+\beta[\lambda_0\{\xi\}-E_0]\}\delta(\lambda_0\{\xi\}-E)D\xi}{\int e^S D\xi}\right] \tag{A.1}$$

In the zeroth approximation, (2.10) takes the form

$$F_0(E)=S\{\tilde{\xi}\},\qquad \lambda_0\{\tilde{\xi}\}=E.$$

Hence

$$F(E)-F_0(E)$$
$$=\ln\left[\frac{\int\exp\{S\{\xi\}-S\{\tilde{\xi}\}+p[\lambda_0\{\xi\}-\lambda_0\{\tilde{\xi}\}]\}\delta(\lambda_0\{\xi\}-\lambda_0\{\tilde{\xi}\})D\xi}{\int e^S D\xi}\right] \tag{A.2}$$

where β, as before, is such that the extremum of the functional $S+\beta\lambda_0$ satisfies the condition $\lambda_0\{\tilde{\xi}\}=E$.

Near the renormalized boundary, when $\xi \ll c_0$, the functional S is given by the formula (2.21)

$$S=-A(\xi,\xi),\qquad A=-\sigma''(c_0)/2a^3. \tag{A.3}$$

Putting in the numerator of (A.2) $\xi=\tilde{\xi}+\eta$ and calculating $\lambda_0\{\tilde{\xi}+\eta\}-\lambda_0\{\tilde{\xi}\}$ by perturbation theory, accurate to terms of second order, we have

$$\lambda_0\{\tilde{\xi}+\eta\}-\lambda_0\{\hat{\xi}\}=(\eta,q)+(\eta,\hat{Q}\eta). \tag{A.4}$$

Here $q(\mathbf{x})=v_0\psi_0^2(\mathbf{x})\|\psi_0\|^{-2}$, and the kernel $Q(\mathbf{x},\mathbf{y})$ of the operator $\hat{Q}$ is

$$Q(\mathbf{x},\mathbf{y})=v_0^2\psi_0(\mathbf{x})\psi_0(\mathbf{y})G(\mathbf{x},\mathbf{y};E),\; G(\mathbf{x},\mathbf{y},E)=\sum_k\frac{\psi_k(\mathbf{x})\psi_k(\mathbf{y})}{E-c_0v_0-k^2}, \tag{A.5}$$

where $G(\mathbf{x},\mathbf{y};E)$ has the meaning of the Green's function of the equation

$$\Delta\psi+(E-c_0v_0-\tilde{\xi}v_0)\psi=0$$

from which the pole term $\psi_0(\mathbf{x})\psi_0(\mathbf{y})/(E-\lambda_0)$ is subtracted ($\lambda_0=E$).

Thus

$$F(E)-F_0(E)=\ln\left[\frac{\int\exp\{-A(\eta,\eta)+\beta(\eta,\hat{Q}\eta)\}\delta((q,\eta))D\eta}{\int e^{-A(\eta,\eta)}D\eta}\right]. \tag{A.6}$$

If η_0 is the projection of η on the vector q ($(\eta,q)=\eta_0\|q\|$), $\hat{Q}'$—projection of the operator $\hat{Q}$ on the subspace $\eta_0=0$ (hyperplane in functional space η), and $D\eta'$—volume element in the subspace $\eta_0=0$ ($D\eta=d\eta_0\cdot D\eta'$), then

$$F(E)-F_0(E)=$$
$$=\ln\left[\frac{\int e^{-A\eta_0^2}\delta(\eta_0)d\eta_0\int\exp\{-A(\eta',\eta')+\beta(\eta',\hat{Q}'\eta')\}D\eta'}{\|q\|\int e^{-A\eta_0^2}d\eta_0\int e^{-A(\eta',\eta')}D\eta'}\right]$$
$$=\ln\frac{\sqrt{A}}{\|q\|\sqrt{\pi}}-\frac{1}{2}\operatorname{Sp}\ln\left(1+\frac{\beta}{A}\hat{Q}'\right). \tag{A.7}$$

From (2.16) follows an expression for β:

$$\beta=\|z\|^2/v_0a^3. \tag{A.8}$$

Inasmuch, according to (2.25), $\psi_0\sim z\sim\varphi(r\sqrt{E_c-E})$ the role of the coordinate r in (2.25) is assumed by the dimensionless quantity k_0r), it follows that

$$\|z\|^2=\varepsilon\sigma''(c_0)\frac{\varphi_2}{|E-E_c|^{3/2}}=-\frac{\varphi_2\sigma''(c_0)}{|\varepsilon|^{1/2}k_0^3}. \tag{A.9}$$

Thus,

$$\beta=-\frac{\sigma''(c_0)}{v_0(ak_0)^3}\varphi_2|\varepsilon|^{-1/2},\qquad \varphi_n=\int_0^\infty\varphi^n(\rho)\cdot 4\pi\rho^2\,d\rho,$$
$$\beta/A=2\varphi_2|\varepsilon|^{-1/2}/v_0k_0^3. \tag{A.10}$$

Similarly, we get

$$\|q\|=|v_0|k_0^{3/2}|\varepsilon|^{3/4}\sqrt{\varphi_4/\varphi_2^2} \tag{A.11}$$

and for the first term in (A.7)

$$\left[\frac{A}{\pi\|q\|^2}\right]^{1/2}=\left[\frac{-\sigma''(c_0)\varphi_2^2}{2\pi(ak_0)^3\varphi_4}\right]^{1/2}\frac{|\varepsilon|^{-3/4}}{|v_0|}. \tag{A.12}$$

The form of the kernel of the operator $\hat{Q}$ ensures convergence of the term $\operatorname{Sp}\ln(1+\beta A^{-1}\hat{Q}')$ and the relative smallness of its contribution compared with $F_0(E)$ (not too close to E_c). However, a more detailed analysis of this kernel is beyond the scope of the present article.

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