Spontaneous Symmetry Breaking of Optimum Fluctuations in Semiconductors

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The optimum fluctuation method (OFM) has been applied to the tails of the density of states, arising near the edges of the spherically symmetric degenerate bands. In this case the optimum fluctuations (OF) have been shown to undergo a qualitative change, as compared to the case of nondegenerate bands, they lose the spherical symmetry and become elongated or flattened. This means that spontaneous breaking of symmetry takes place. In addition to the usual mechanism of tailing due to the potential of impurities, another mechanism connected with the field of random deformations, arising due to difference in the size of the guest and host atoms, has been also considered. The method used for treating this problem is intimately related to the techniques of the theory of self-trapping. The density of states in the tails, and in some cases the shape of OFs, have been found for all the cases under consideration.

It seems natural to anticipate that the solution corresponding to the minimal "eigen value" is spherically symmetric. However, the absence of such a "symmetry breaking" has not been proved in the general form so far.
I. Lifshitz et al,[1] Section 15.1

1. INTRODUCTION

The above epigraph is a footnote from the monograph of Lifshitz *et al.*[1] It puts forward the problem and sounds as a challenge. This paper is aimed at introducing and considering a quite new aspect of this problem.

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Below we show that the symmetry breaking, mentioned in this footnote, is indeed absent in a simplest model only, when the band is nondegenerate. On the contrary, for degenerate bands the symmetry breaking is a general regularity.

First of all we present a brief introduction to the problem. Once a semiconductor or a dielectric crystal contains either impurities, or defects, the tails of the density of states arise in the forbidden gap. The part of these tails arising due to large impurity clusters can be described by the OFM, developed by Halperin and Lax,[2] Zittarz and Langer,[3] and by Lifshitz.[4] This method is used extensively and has been generalized in monographs.[1,5,6] For the model, in which the random potential is described as a white noise, the density of states $\rho(E)$ is

$$\ln \rho(E) \propto -|E/m^3|^{1/2} \tag{1}$$

where E is the energy (the bottom of the band is chosen as an origin), and m is the mass of a particle.

The tails of the density of states have been observed experimentally in heavily doped semiconductors, and also in solid semiconducting alloys, in which the random potential arises due to fluctuations of the content. The existence of tails in the edge absorption in some materials of the second group has been recently observed in optical spectra by a number of workers.[7-10] For the energy dependence of the absorption the theory[11] provides a formula which is similar to (1). It can be seen from (1) that the density of states in the tails decreases the slower, the larger the mass of the particles m is. Usually, the mass of heavy holes is the heaviest one in semiconductors. Therefore, the most extensive tails should arise near the valence band edge. However, the valence band in cubic semiconductors is usually degenerate. At the same time the theory of tails of the density of states has been developed previously for nondegenerate bands. As far as we know the only exceptions are our preliminary communications,[12,13] where the main peculiarity of OFs near the degenerate bands, the spontaneous breaking of symmetry, has been established. The results of the paper[12] were applied in Ref. 14 to zero-gap semiconductors, and in Ref. 15 to the spectra of mixed crystals $CdS_{1-x}Se_x$.

The general outline of the paper is the following. In Section 2 is presented the Hamiltonian of the system and a description of the variational principle which is applied for solving this problem. Section 3 presents the basic results of the calculations. Section 4 deals with the generalized problem in which the random strains caused by difference in the radii of particles forming a mixed crystal are taken into account.

2. HAMILTONIAN AND THE VARIATIONAL PRINCIPLE

The theory of bound states near the edges of degenerate bands, as is well known, requires cumbersome calculations. Having in mind the fact that we are going to consider a new phenomenon—spontaneous symmetry breaking of OFs—we simplify as much as possible the Hamiltonian under consideration.

First of all we limit ourselves to the cubic crystals possessing the inversion symmetry. Additional terms in the Hamiltonian arising when the inversion symmetry is absent are usually small; therefore, we do not take them into account. We also assume that the Hamiltonian can be written in the spherical approximation [group $O(3)$], i.e., the cubic invariants[16,17] can be omitted; this approximation may turn out to be more restrictive. Below we consider two most important cases in parallel.

1. *The threefold degenerate band.* It corresponds to holes under the conditions when the spin-orbit coupling is absent, or to Frenkel excitons when the optical transition is dipole-allowed but weak.

2. *A fourfold degenerate hole band under the conditions of a strong spin-orbit coupling.*

It is convenient to describe the band degeneracy by ascribing the spin to the corresponding quasiparticle: in the first case $S = 1$, and in the second case $S = 3/2$. We also use the second quantum number–helicity of the particle σ, i.e., the projection of spin onto the quantization axis. The effective mass in the state with the helicity σ is denoted by m_σ. Everywhere below the sign in the Hamiltonian of a hole will be changed by the opposite one, to eliminate the negative kinetic energy.

In these notations the kinetic energy operator of a particle with the spin $S = 1$ has the form $(\hbar = 1)$

$$\hat{T}_1 = \frac{1}{2m_1} \text{ rot rot} - \frac{1}{2m_0} \text{ grad div} \tag{2}$$

or, another form, which is the same:

$$\hat{T}_1 = \frac{1}{2m_1} [-\nabla^2 + (\mathbf{S}\nabla)^2] - \frac{1}{2m_0} (\mathbf{S}\nabla)^2 \tag{3}$$

Vector $\mathbf{S} = (S_x, S_y, S_z)$ is constructed of matrices of the angular momentum operator. The corresponding spectrum of free particles is shown in Fig. 1a.; the eigenfunctions are spherical vectors.

For a particle with the spin $S = 3/2$ the Hamiltonian is

$$\hat{T}_{3/2} = \frac{1}{4m_{1/2}} \left[(\mathbf{S}\nabla)^2 - \frac{9}{4} \nabla^2 \right] + \frac{1}{4m_{3/2}} \left[\frac{1}{4} \nabla^2 - (\mathbf{S}\nabla)^2 \right] \qquad (4)$$

Its spectrum is shown in Fig. 1b; the eigenfunctions are spinors.

The operators $\hat{T}_1$ and $\hat{T}_{3/2}$ are invariants of group $O(3)$.

In semiconductors usually $\mathcal{M}_1 = m_1/m_0 > 1$ and $\mathcal{M}_{3/2} = m_{3/2}/m_{1/2} > 1$, that is, the masses m_1 and $m_{3/2}$ are heavy masses, whereas m_0 and $m_{1/2}$ are light masses.

As for the random potential $U(\mathbf{r})$, we assume that its mean value $\langle U(\mathbf{r}) \rangle = 0$, and $U(\mathbf{r}) \propto \delta n(\mathbf{r})$, where $\delta n(\mathbf{r})$ is the deviation of the concentration of a solid solution from its mean value. Such modeling seems to be reasonable enough for the systems with isoelectronic substitution and corresponds to the Faulkner description[18] of the isoelectronic guests. For instance it can be applied to the systems of the $Al_x Ga_{1-x} As$ type. Let us introduce the functional $\mathcal{S}[U]$, which differs from entropy only by the sign. Then assuming the composition distribution to be random, we may obtain the expression for entropy from the relation $U(\mathbf{r}) \propto \delta n(\mathbf{r})$ and simple statistical considerations:

$$\mathcal{S}[U] = \frac{1}{2B} \int U^2(\mathbf{r}) \, d\mathbf{r} \qquad (5)$$

B is the constant. This scheme is equivalent to the white noise model with the correlation function

$$\langle U(\mathbf{r}) U(\mathbf{r}') \rangle = B\delta(\mathbf{r} - \mathbf{r}') \qquad (6)$$

The OFM consists in finding the most probable fluctuation providing the quantum level position equal to E. Since the probability of the fluc-
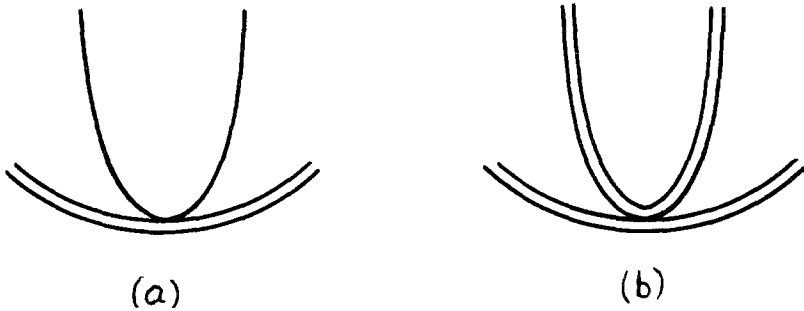

(a) **(b)**

Fig. 1. Spectrum of free particles with spins $S = 1$ (a) and $S = 3/2$ (b). The twofold degenerate branches of the spectrum are shown by double lines. It is assumed that $m_0 < m_1$, $m_{1/2} < m_{3/2}$.

tuation is proportional to $\exp\{-\mathscr{S}[U]\}$, this means that the minimum of $\mathscr{S}[U]$ should be found under the additional condition that the equation

$$(\Psi|\,\hat{T} + U(\mathbf{r})\,|\,\Psi) = E \tag{7}$$

is satisfied. Here E is the lowest quantum level in the potential $U(\mathbf{r})$, and $\Psi(\mathbf{r})$ is the normalized wave function. The corresponding equation can be written as follows:

$$\delta_U\{\mathscr{S}[U] + \beta E[U]\} = 0 \tag{8}$$

where β is the Lagrange factor, which is determined by the condition $E[U] = E$. Performing the variation in (8) we get

$$U(\mathbf{r}) = -\beta B(\Psi(\mathbf{r})\,\Psi(\mathbf{r})) \tag{9}$$

and

$$\hat{H}_\beta\,\Psi = \{\hat{T} - \beta B(\Psi(\mathbf{r})\,\Psi(\mathbf{r}))\}\,\Psi(\mathbf{r}) = E(\beta)\,\Psi(\mathbf{r})$$
$$E(\beta) = E \tag{10}$$

Here

$$(\Psi(\mathbf{r})\,\Psi(\mathbf{r})) = \Psi_\alpha^*(\mathbf{r})\,\Psi_\alpha(\mathbf{r}) \tag{11}$$

is the scalar square of Ψ, taken over the vector (spinor) index α. Vector Ψ is assumed normalized, $(\Psi\,|\,\Psi) = 1$, this notation includes integration in $\mathbf{r}$ [quite similarly to (7)].

In the simplest case $\hat{T} = -\Delta/2m$. Then Ψ is substituted by the scalar function ψ; the nonlinear equation (10) can be rewritten in nondimensional form and solved numerically. Then the minimal $\mathscr{S}(E)$ and the density of states $\rho(E) \propto \exp\{-\mathscr{S}(E)\}$ are calculated by Eqs. (9) and (5) (see, for instance, Ref. 1). In this case

$$\mathscr{S}_{\text{sc}}(E) = \frac{13.3}{Bm^{3/2}}\,|E|^{1/2} \tag{12}$$

In order to solve Eq. (10) for the multicomponent Ψ, we shall use the procedure, closely connected to the theory of self-trapping barrier.[19,20] Equation (10) can be regarded as an equation for the stationary points of the functional

$$H_\beta[\Psi] = (\Psi|\,\hat{T} - \tfrac{1}{2}\beta B(\Psi\Psi)\,|\,\Psi) \tag{13}$$

This representation makes it possible to obtain the virial theorem.[21,19] Performing the substitution $\Psi(\mathbf{r}) \to \nu^{3/2}\Psi(\nu\mathbf{r})$, we get

$$H_\beta(\nu) = \nu^2(\Psi|\,\hat{T}\,|\,\Psi) - \frac{1}{2}\nu^3\beta E \int (\Psi\Psi)^2\,d\mathbf{r} \tag{14}$$

$\Psi(\mathbf{r})$ is an extremal of $H_\beta[\Psi]$, hence $dH_\beta(v)/dv|_{v=1} = 0$. This leads immediately to the virial theorem:

$$(\Psi| \hat{T} | \Psi) = \tfrac{3}{4}\beta B \int (\Psi\Psi)^2 \, d\mathbf{r} \tag{15}$$

It follows from Eqs. (10), (13), (15) that for extremal paths of Eq. (13) the following relation holds:

$$E(\beta) = -H_\beta < 0 \tag{16}$$

And from Eqs. (5), (9), (10), and (15) we have

$$\mathscr{S}(E) = 2\beta(E) |E| \tag{17}$$

The functional $H_\beta[\Psi]$ is not bounded from below. This can be seen from (14), its right-hand side tends to $-\infty$ when $v \to \infty$. As a result, Eq. (10) has an infinite number of negative levels E_n; their moduli increase with the quantum number n. According to (16), each of E_n corresponds to a positive stationary point of the functional $H_\beta[\Psi]$. Below we show [see Eq. (20)] that $\beta(E) \propto |E|^{1/2}$. Therefore, according to (17), the $E = E_0$, i.e., the negative eigen value with the minimal modulus corresponds to the minimum of $\mathscr{S}$. The lowest saddle point of the functional $H_\beta[\Psi]$ may be set into correspondence to this eigenvalue. Indeed, according to (14) $H_\beta = 0$ at $v = 0$ and $H_\beta \to -\infty$ when $v \to \infty$. Therefore, the lowest stationary point with $H_\beta > 0$ should be a saddle point of the functional $H_\beta[\Psi]$.

In order to estimate the order of magnitude of the basic physical quantities without performing numeracal calculations, it is convenient to pass to nondimensional variables. When introducing them, one has to take account of the fact proved in the next section, that these quantities are scaled by the mass of heavy holes m_h. This means that while varying $\mathscr{M}$ on the semiaxis $(0, \infty)$, these basic quantities vary in finite limits (cf. Figs. 2–4).

The nondimensional variables are introduced according to the definition:

$$\mathbf{r} = r_0\boldsymbol{\xi}, \qquad \Psi(\mathbf{r}) = r_0^{-3/2}\tilde{\Psi}(\boldsymbol{\xi}), \qquad r_0 = m_h\beta B$$

$$E = \mathscr{E}/m_h r_0^2, \qquad H_\beta = \mathscr{H}/m_h r_0^2, \qquad \hat{t} = \hat{T}/m_h r_0^2 \tag{18}$$

Then functional (13) is substituted by

$$\mathscr{H}[\tilde{\Psi}] = (\tilde{\Psi}| \hat{t} - \tfrac{1}{2}(\tilde{\Psi}\tilde{\Psi}) | \tilde{\Psi}) \tag{19}$$
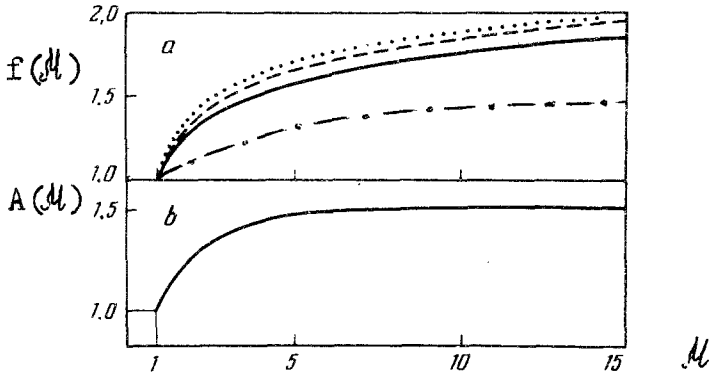
Fig. 2. The functions $f(\mathcal{M})$ and $A(\mathcal{M})$ for the band with $S = 1$: (a) Solid line, $M = 0$; dashed line, $M = \pm 1$ (nonsymmetric fluctuations); dotted line, optimum spherical fluctuation; dash-and-dot line, the state with $M = \pm 1$ in the field of optimum fluctuation corresponding to $M = 0$; (b) The function $A(\mathcal{M})$ for $M = 0$.

Using (17) and (18) we get

$$\beta(E) = \frac{1}{Bm_h^{3/2}} \left(\frac{\mathcal{H}}{|E|} \right)^{1/2} \tag{20}$$

$$\mathcal{S}(E) = \frac{2}{Bm_h^{3/2}} \left(\mathcal{H} |E| \right)^{1/2} \tag{21}$$
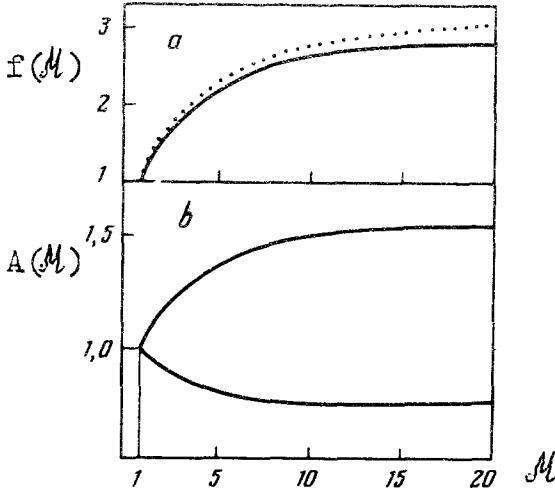

Fig. 3. The functions $f(\mathcal{M})$ and $A(\mathcal{M})$ for the band with $S = 3/2$: (a) Solid line, nonsymmetric fluctuations ($M = \pm 1/2$ and $M = \pm 3/2$); dotted line, optimum spherically symmetric fluctuations; (b) the upper curve, $M = \pm 1/2$, the lower one, $M = \pm 3/2$. All the curves almost do not change, if the holes with $\sigma = \pm 1/2$ are heavy, and A and f are plotted versus $\mathcal{M}^{-1}$.
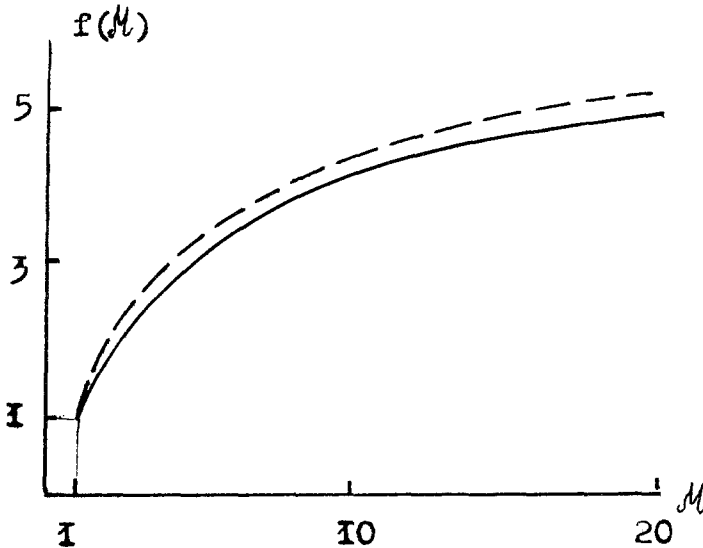
Fig. 4.   The function $f(\mathcal{M})$ for the band with $S = 1$ at $m_0 > m_{\pm 1}$: Solid line, $M = 0$; dashed line, $M = \pm 1$.

Equation (21) agrees with (12): the quantity $\mathcal{H} = \mathcal{H}(\mathcal{M})$ involved in it is determined by finding the extremal of the functional (19) corresponding to its lower saddle point. Formula (21) is a rather general one, but for more realistic models $\mathcal{H}$ should be determined by variation of the functional (19) with a more complicated operator $\hat{t}$.

3. ANISOTROPY OF OPTIMUM FLUCTUATIONS

Now we consider functional (19) or its equivalent, the Schrödinger equation

$$\{\hat{t} - (\tilde{\Psi}\tilde{\Psi})\} \tilde{\Psi} = \mathscr{E} \tilde{\Psi} \tag{22}$$

If we assume that the form factor $(\tilde{\Psi}\tilde{\Psi})$ of the OF is spherically symmetric, the eigenfunctions of Eq. (22) can be classified to the total angular momentum J. And it would be natural to assume that just the states with $J = S$ provide the minimal value of $|\mathscr{E}|$; arguments are the same as in the Kohn–Shechter theory of acceptor centers.[17] For instance, for $S = J = 1$ the wave function of the state having the projection of the angular momentum $M = 0$ in the basis X, Y, Z has the form

$$\Psi_0(\mathbf{r}) = \varphi_1(r) \begin{vmatrix} 0 \\ 0 \\ 1 \end{vmatrix} + \varphi_2(r) \begin{vmatrix} xz \\ yz \\ z^2 - r^2/3 \end{vmatrix} \tag{23}$$

Here $\varphi_1(r)$ and $\varphi_2(r)$ are spherically symmetric functions. Using Eq. (23) one may easily see that the assumption on the spherical symmetry of $(\Psi\Psi)$ is contradictory. Indeed, we have

$$(\Psi_0\,\Psi_0) = \left(\varphi_1^2 - \frac{2}{3}\,r^2\varphi_1\varphi_2 + \frac{r^4}{9}\,\varphi_2^2\right)$$
$$+ z^2\left(2\varphi_1\varphi_2 + \frac{1}{3}\,r^2\varphi_2^2\right) \tag{24}$$

The last term is nonsymmetrical, and the condition that both its summands cancel each other $6\varphi_1\varphi_2 + r^2\varphi_2^2 = 0$ imposes the restrictions upon φ_1 and φ_2, which are inconsistent with (22). The only exception is the case $\mathcal{M} = 1$, when Eq. (22) falls into independent scalar Schrödinger equations, as follows from Eq. (3). The situation is analogous for $S = 3/2$.

Therefore, the vector (spinor) nature of Ψ leads to the spontaneous symmetry breaking of OFs. This phenomenon is similar to the spontaneous symmetry breaking of a self-trapping barrier, where the Jahn–Teller mechanism is acting.[19,20]

The numerical calculation for the lowest saddle point of the functional (19) has been performed for the bands with $S = 1$ and $S = 3/2$. It has been supposed that the minimal breaking of symmetry which violates the degeneracy sets in, therefore, the group $D_{\infty h}$ is retained. In this case the states are classified according to the projection M of the angular momentum on the symmetry axis. Since before the breaking of the spherical symmetry the eigenstates were assumed to belong to the angular momentum $J = S$, only the states with $M = 0, \pm 1$ and $M = \pm\frac{1}{2}, \pm\frac{3}{2}$ were calculated. The most detailed calculations were carried out for $\mathcal{M}_1$, $\mathcal{M}_{3/2} > 1$. The method of calculation is similar to that described in Ref. 20, as applied to a self-trapping barrier. At large $\mathcal{M}$ the change in the asymptotic behavior of $\tilde{\Psi}(\xi)$ at $\xi \gg 1$ is taken into account: at any finite $\mathcal{M}$ the Ψ decreases exponentially, and at $\mathcal{M} = \infty$, following the power law ($\tilde{\Psi} \propto \xi^{-3}$).

The final results of calculation are shown in Figs. 2 and 3 in the form of two functions: $f(\mathcal{M})$ and $A(\mathcal{M})$. The first of them,

$$f(\mathcal{M}) = \left(\frac{\mathcal{H}(\mathcal{M})}{\mathcal{H}(1)}\right)^{1/2} \equiv \left(\frac{m_h}{m_{eq}}\right)^{3/2} \tag{25}$$

allows one to calculate $\mathscr{S}(E)$ by Eq. (21). The second part of Eq. (25) can be considered as a definition of the equivalent mass $m_{eq} = m_{eq}(\mathcal{M})$. Using (25) one way write [cf. (12)]

$$\mathscr{S}(E) = \frac{13.3}{Bm_h^{3/2}}f(\mathcal{M})\,|E|^{1/2} = \frac{13.3}{Bm_{eq}^{3/2}(\mathcal{M})}\,|E|^{1/2} \tag{26}$$

The second function $A(\mathscr{M})$ describes anisotropy of fluctuations. It is defined as $A(\mathscr{M}) = z_0(\mathscr{M})/\rho_0(\mathscr{M})$, where z_0 and ρ_0 are positions of the points on the axis of quantization and in the plane normal to it, in which $(\tilde{\Psi}\tilde{\Psi})$ shows a twofold decrease, as compared to the point $\mathbf{r} = 0$. It is seen from Fig. 3b that at a given S the states with different values of $|M|$ have the opposite asymmetry.

Let us discuss the results presented in Figs. 2 and 3. It is clear from Figs. 2b and 3b that the anisotropy of optimum fluctuations is high. This fact follows from Fig. 2a too, where the dash-and-dot curve shows $f(\mathscr{M})$ for the states $M = \pm 1$ in the field of the OF corresponding to $M = 0$. It strongly differs from a solid curve, whereas in a spherically symmetric potential they should have coincided. At the same time the difference in $f(\mathscr{M})$ for different values of M is small (Fig. 2a and 2b); in the case $S = 3/2$ it is less than the accuracy of calculations (several percent). This result seems puzzling and we cannot interpret it now. The fact that the values of $f(\mathscr{M})$ for rather different (elongated and flattened) fluctuations are close one to another forced us to calculate also the function $f(\mathscr{M})$ corresponding to the fluctuation, which is optimal in the class of spherically symmetric functions. In this calculation in Eq. (19) the substitution

$$(\tilde{\Psi}(\xi)\tilde{\Psi}(\xi)) \Rightarrow \langle(\tilde{\Psi}(\xi)\tilde{\Psi}(\xi))\rangle_\Omega \tag{27}$$

was performed in Eq. (19). Here the brackets designate averaging over the angles. From Figs. 2a and 3a it follows that the values of $f(\mathscr{M})$ obtained only slightly exceed the values of $f(\mathscr{M})$ for self-consistent nonspherical functions. It should be noted that the states with $M = \pm 1$ are self-consistent, but are not extremals, since the functions $\Psi_{\pm 1}$ do not make a Kramers doublet. So, a second symmetry breaking is to set in: the fluctuations violating the axial symmetry will result in the splitting of level $\mathscr{E}_{\pm 1}$. It seems most probable that for $S = 1$ the only saddle point arising from the first multiplet $J = 1$ corresponds to the states with $M = 0$, but the directions of the quantization axis are distributed randomly.

One may conclude from the foregoing that in the functional space there is a vast region of fluctuations of quite different shape (from considerably elongated to the flattened ones), but providing close values of f, and consequently of $\mathscr{S}$ as well. So, the usual method of finding a preexponential factor $\rho_0(E)$ in $\rho(E) = \rho_0(E) \exp\{-\mathscr{S}(E)\}$ by expanding the functional $\mathscr{S}[U]$ near its minimal value and by subsequent functional integration in the vicinity of the minimum is not applicable, and the factor $\rho_0(E)$ should be anomalously large.

For comparison, Fig. 4 presents the results of calculating of $f(\mathscr{M})$ for the band $S = 1$ and for the state $M = 0$ in the case when $m_0 > m_1$. Here $f(\mathscr{M})$ varies over a much wider range than it did in the previous case.

It was assumed above that the initial Ψ (before the symmetry breaking!) belonged to irreducible representation with the angular momentum $J = S$. In principle, the other possibility exists that the minimal $\mathscr{S}$ is reached with the function Ψ transforming according to the completely symmetric representation. Such a Ψ has the form $\Psi_i(\mathbf{r}) = x_i\, g(r)$, i numerates the Cartesian coordinates x_i, and no spontaneous symmetry breaking exists. However, the calculation shows that such a function always leads to a larger $\mathscr{S}$ than the functions arising from the states with $J = S$. Apparently, the reason is that the given Ψ has a node at $\mathbf{r} = 0$, whereas in the (23)-type functions the first term which has no nodes is usually predominating.

4. THE EFFECT OF RANDOM STRAINS

The isoelectronic impurities create both the random potential $U(\mathbf{r})$ and the field of random strains connected with difference in covalent or ionic radii of the guest and of the host atoms.[22] In an isotropic medium the equation for the vector of the displacements $\mathbf{u}(\mathbf{r})$, caused by the spatially inhomogeneous composition $n(\mathbf{r})$, has the form

$$-(\lambda + 2\mu)\,\text{grad div}\,\mathbf{u} + \mu\,\text{rot rot}\,\mathbf{u} = \Gamma_0\,\text{grad}\,n(\mathbf{r}) \qquad (28)$$

Here λ and μ are the Lamé constants, and the constant Γ_0 is proportional to the difference in the atomic radii. As in Section 2, we assume that $U(\mathbf{r}) \propto \delta n(\mathbf{r})$. Therefore, the right-hand side of (28) can be rewritten as $\Gamma\,\text{grad}\,U(\mathbf{r})$. We apply the macroscopic equation (28) as a most simple one, neglecting the inaccuracy which it introduces for low-scale inhomogeneities. The solution of Eq. (28) has the form

$$\mathbf{u}(\mathbf{r}) = \frac{\Gamma}{4\pi(\lambda + 2\mu)}\,\text{grad} \int \frac{U(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}\,d\mathbf{r}' \qquad (29)$$

Deformation $\mathbf{u}(\mathbf{r})$ arising due to the crystal inhomogeneity affects the electrons through the deformation potential. Under these conditions the equation generalizing (7) has the form

$$E = (\Psi|\,\hat{T} + U(\mathbf{r}) + [\mathscr{D}_1 + S(S + 1)\,\mathscr{D}_2]\,\varepsilon_{ii}(\mathbf{r})$$
$$- 3\mathscr{D}_2\,\varepsilon_{ij}(\mathbf{r})\,S_i S_j\,|\,\Psi) \qquad (30)$$

Here $\varepsilon_{ij} = \frac{1}{2}(\partial u_i/\partial x_j + \partial u_j/\partial x_i)$ are the components of the deformation tensor, and $\mathscr{D}_1$ and $\mathscr{D}_2$ are deformation potentials. From Eq. (8), using (5)

and the relation $\varepsilon_{ii}(\mathbf{r}) = -[\Gamma/(\lambda + 2\mu)]\, U(\mathbf{r})$, following from (29), we get a formula for $U(\mathbf{r})$:

$$U(\mathbf{r}) = -\beta B \gamma \hat{K} \Psi(\mathbf{r}), \qquad \gamma = 1 - \frac{\Gamma \mathscr{D}_1}{\lambda + 2\mu} \equiv -\frac{\Gamma \mathscr{D}'_1}{\lambda + 2\mu} \qquad (31)$$

where $\hat{K}$ is the nonlinear integral operator transforming $\Psi(\mathbf{r})$ into a scalar function:

$$\hat{K} \Psi(\mathbf{r}) = (\Psi(\mathbf{r})\, \Psi(\mathbf{r}))$$

$$+ \frac{3d}{4\pi} \int \frac{d\mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|} \frac{\partial^2}{\partial x'_i \partial x'_j} \Psi_\alpha(\mathbf{r}') \qquad (32)$$

$$\times\, (S_i S_j - S(S+1)\, \delta_{ij})\, \Psi_\beta(\mathbf{r}')$$

here $d = \mathscr{D}_2/\mathscr{D}'_1$. The generalized Eq. (13) acquires the form

$$H_\beta[\Psi] = (\Psi|\, \hat{T}\, |\Psi) - \tfrac{1}{2}\beta B \gamma^2 \int (\hat{K}\Psi)^2\, d\mathbf{r} \qquad (33)$$

The theorem of virial which follows from it,

$$(\Psi|\, \hat{T}\, |\Psi) = \tfrac{3}{4}\beta B \gamma^2 \int (\hat{K}\Psi)^2\, d\mathbf{r} \qquad (34)$$

leads to the relations

$$E = -H_\beta = -\frac{1}{4\beta B} \int U^2(\mathbf{r})\, d\mathbf{r} \qquad (35)$$

It follows from (5) and (35) that Eq. (17) for $\mathscr{S}$ remains valid.

Transformation to non-dimensional units is performed analogously to (18) with the only difference being that $r_0 = m_h \beta B \gamma^2$. As a result, $\beta^{-1} = B m_h^{3/2} \gamma^2 \, (|E|/\mathscr{H})^{1/2}$, and the final expression for $\mathscr{S}$ has the form

$$\mathscr{S}(E) = \frac{2}{B m_h^{3/2} \gamma^2} \, (\mathscr{H}\, |E|)^{1/2} \qquad (36)$$

The quantity $\mathscr{H}$ in (26) is a stationary value of the nondimensional functional

$$\mathscr{H}[\tilde{\Psi}] = (\tilde{\Psi}|\, \hat{t}\, |\tilde{\Psi}) - \tfrac{1}{2} \int (\hat{K}\tilde{\Psi})^2\, d\mathbf{r} \qquad (37)$$

which generalizes (19). $\mathscr{H}$ depends on two parameters, $\mathscr{M}$ and d.

Figure 5 shows the results of calculation of the function

$$f(\mathcal{M}, d) = \left(\frac{\mathcal{H}(\mathcal{M}, d)}{\mathcal{H}(1, 0)} \right)^{1/2} \tag{38}$$

The basic result which can be distinctly seen in the figure is that the difference in the values of f for $M = 0$ and $M = \pm 1$, which was small at
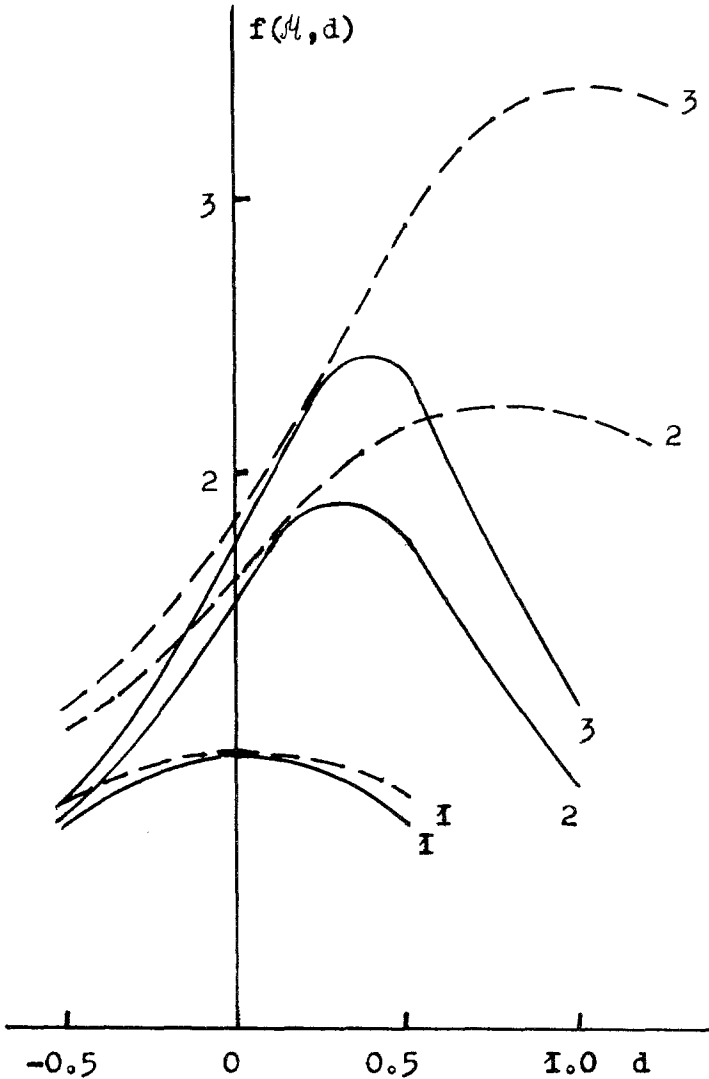

Fig. 5. Function $f(\mathcal{M}, d)$ for the band with the spin $S = 1$. The mass ratio is the parameter of the curves: (1) $\mathcal{M} = 1$, (2) $\mathcal{M} = 4$, (3) $\mathcal{M} = 10$. Solid lines, $M = 0$; dashed lines, $M = \pm 1$.

$d = 0$, strongly depends on d. When $\mathscr{M} \neq 1$, the curves corresponding to $M = 0$ and $M = \pm 1$ within the accuracy of calculation almost touch one another at $d \neq 0$. The difference in the values of ordinates at these points is within the accuracy of calculation, and at these values of d the parameter $A \approx 1$, i.e., the OFs are almost spherically symmetrical. Away from these points the curves, corresponding to $M = 0$ and $M = \pm 1$, are widely spaced. This fact has important consequences, since in the functional space there arises a distinctly marked region of anisotropic fluctuations with entropy, which is close to the maximal one. It should be stressed that this effect is completely due to the "second" deformation potential $\mathscr{D}_2$, introducing the spin-depending terms into the total potential.

The presence of large spin-depending terms in $U(\mathbf{r})$ should lead to a similar result.

5. CONCLUSION

The above results make it possible to draw some conclusions. On an example of bands with the spins $S = 1$ and $S = \frac{3}{2}$ it has been shown that degeneracy of bands results in a spontaneous symmetry breaking of the optimum fluctuations. This conclusion is of a general character. It remains unclear (Section 3) why in a rigid lattice fluctuations from a vast region of the functional space possess comparable entropy. It has been shown, however, that the lattice deformations arising due to disorder eliminate this degeneracy, at least partly. The symmetry of OFs should itself be manifested in a number of physical phenomena, such as luminescence and light scattering.[12] But at least in the white noise model this asymmetry does not change the analytical behavior of the density of states, which has a universal form: $-\ln \rho(E) \propto |E|^{1/2}$, and influences only the value of the numerical coefficient at $|E|$. A change in the analytical behavior of $\rho = \rho(E)$ arises when the hole-phonon coupling is taken into account. In this case even the abrupt termination of the tail of $\rho(E)$ is possible[23]; but this problem is beyond the framework of our paper.

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