Anisotropy of optimum fluctuations in crystals with a degenerate spectrum

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It is shown that in crystals with degenerate spherical bands optimum fluctuations, which form tails in the density of states in the forbidden band, are nonspherical: They are elongated or flattened.

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Impurities and defects in semiconductors give rise to tails in the density of states $\rho(E)$, which penetrate deeply into the forbidden band. In order to describe them, Halperin and Lax,[1] Zittarz and Langer,[2] and Lifshitz[3] developed the method of optimum fluctuations (OF). This method was further developed in subsequent papers; the present status of the problem is summarized in Refs. 4–6. In all work performed using the OF method, it is assumed that in the presence of spherically symmetrical OF bands the distribution of impurities is also spherically symmetrical. Below we shall show that

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this assumption is valid only for nondegenerate bands. In contrast, for degenerate spherical bands in the entire quantum region the optimum fluctuations are anisotropic fluctuations which are considerably elongated or flattened. For A_{III} B_V semiconductors an energy specturm with spherical bands is typical: nondegenerate conduction band and degenerate valence band.[1)] Relative to them, our result shows that the tail of the conduction band is formed by symmetrical fluctuations, while the much more elongated (due to the large mass of heavy holes) tail of the valence band is formed primarily by nonsymmetrical fluctuations.

In the quantum region $r_\psi \gg r_c$ (r_ψ is the radius of the ψ function, r_c is the correlation radius of the random potential $U(\mathbf{r})$). The problem is especially simple for white noise $\langle U(\mathbf{r})U(\mathbf{r}')\rangle = B_0\delta(\mathbf{r}-\mathbf{r}')$. In this case according to the standard procedure of the OF method,[5,6] finding the tails of Ψ reduces to solving the Schrödinger equation

$$H_\beta \Psi = \{ T - \beta B_0(\Psi^*(\mathbf{r}), \Psi(\mathbf{r})) \} \Psi(\mathbf{r}) = E\Psi(\mathbf{r}). \tag{1}$$

Here T is the kinetic energy operator, which for bands with angular momentum (spin) S is an operator $(2S+1)\times(2S+1)$ matrix, Ψ is the normalized vector (spin) wave function; the braces in (1) indicate a scalar product. The product $(\Psi^*(\mathbf{r}),\Psi(\mathbf{r})$ is a form factor of the fluctuations. The operator appearing on the left side of (1) has an infinite number of negative characteristic values ϵ_n which increase in modulus with increasing n. The factor β in (1) is a Lagrangian multiplier, which is chosen in such a way that ϵ_1 is the characteristic value of H_β with smallest modulus. This value appearing on the left side of ($\epsilon_1 = E$). is equal to E. In this case,

$$\rho(E) \propto \exp(-S(E)), \quad S(E) = \frac{1}{2}B_0\beta^2(E)\int(\Psi^*(\mathbf{r}), \Psi(\mathbf{r}))^2 d^3r. \tag{2}$$

Equation (1) determines the stationary points of the functional

$$\mathcal{J}[\Psi] = \int\left\{(\Psi^*, T\Psi) - \frac{1}{2}\beta B_0(\Psi^*, \Psi)^2\right\}d^3r. \tag{3}$$

Writing the virial theorem for it,[7,8] we obtain

$$\int(\Psi^*(\mathbf{r}), \Psi(\mathbf{r}))^2 d^3r = -\frac{4E}{\beta B_0}, \quad \mathcal{J} = |E| \tag{4}$$

and

$$S(E) = 2|E|\beta(E). \tag{5}$$

Everything said above concerns an arbitrary T operator. In particular, for a degenerate band $T = -\hbar^2/2m\nabla^2$, $\Psi(\mathbf{r})$ is a scalar, and substituting $\Psi(\mathbf{r}) = \Psi(|\mathbf{r}|)$ is self-consistent. For $S = 1$ or $3/2$ the operator T is a linear function of two spherical invariants: ∇^2 and $(S\nabla)^2$, where $S = \{S_x, S_y S_z\}$ are the spin matrices for spin S; the coefficients in front of them are related in a known manner to the masses of heavy and light holes (m_h and m, respectively). In this case the assumption of sphericity of OF is not self-consistent: It would lead to the fact that $\Psi(\mathbf{r})$ are spherical vectors, but a direct calculation shows that for spherical vectors with angular momentum $J \neq 0$ the expression (Ψ^*, Ψ) is not spherically symmetrical. Here there is a spontaneous breakdown of symmetry, typical for vector nonlinear equations.[2)]

It follows from a comparison of separate terms in (1) that $\beta(E) \sim \hbar^3/B_0 m_h^{3/2} E^{1/2}$ depends on the mass ratio $\mu = m_h/m_l$. For this reason, it is convenient to represent $S(E)$ in the form

$$S(E) = S_0(E) f(\mu), \quad S_0(E) \approx 13.3 \frac{\hbar^3 E^{1/2}}{B_0 m_h^{3/2}}, \quad f(\mu) = \left(\frac{m_h}{m_{\text{эк}}(\mu)} \right)^{3/2}. \tag{6}$$

Here $S_0(E)$ is the value of $S(E)$ for the nondegenerate band with mass m_h, while $m_{\text{equiv.}}(\mu)$ is the equivalent mass which permits finding S from S_0.

We computed OF numerically under the assumption that they conserve the axis and center of symmetry; in this case, the quantum states are classified according to the projection of the angular momentum M on the axis of symmetry Oz. Since before loss of spherical symmetry ϵ_1 corresponds to the condition with $J = S$, we examined only the values $M = 0, \pm 1$ and $M = \pm 1/2, \pm 3/2$. The results are presented in Figs. 1 and 2; it assumed, as usual, that the helicity of heavy holes is $\lambda = \pm 1$ (for $S = 1$) and $\lambda = \pm 3/2$ (for $S = 3/2$). It is evident from Fig. 1a that $f(\mu)$ for $M = 0$ is only a little smaller than for $M = \pm 1$; for $M = \pm 1/2$ and $M = \pm 3/2$ (Fig. 2a) both curves nearly coincide. In addition, the anisotropy of the states that arise is large, as is evident from Figs. 1b and 2b. The anisotropy parameter $A(\mu) = z_0/\rho_0$ is indicated on them, where $z_0(\mu)$ and $\rho_0(\mu)$ are the coordinates of points on the Oz axis and in the $z = 0$ plane, where $(\Psi^*\Psi)$ decreases by a factor of two (compared with the point $\mathbf{r} = 0$). States with different projection M have the opposite anisotropy (see Fig. 2b).

We also calculated $f(\mu)$, limiting OF to the class of spherically symmetric functions. This was done by substituting in (1)

$$(\Psi^*(r), \Psi(r)) \Rightarrow = \Psi(|r|) \langle (\Psi^*(r)\Psi(r)) \rangle_\Omega;$$

the angular brackets indicate averaging over angles. The results are shown in Figs. 1a and 2a by the dashed line: $f(\mu)$ increases negligibly.

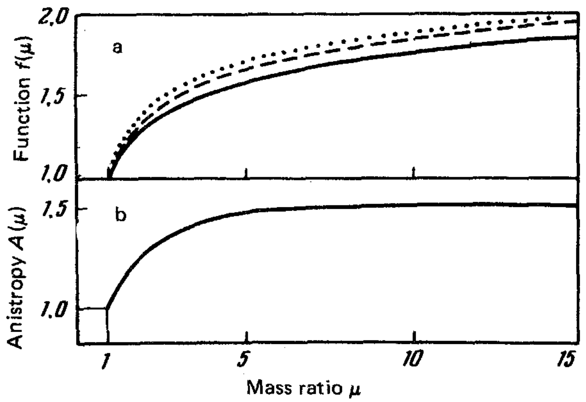

FIG. 1. The dependences $f(\mu)$ and $A(\mu)$ for bands with $S = 1$. (a) Solid curve is for $M = 0$ and the dashed curve is for $M = \pm 1$ (unsymmetrical fluctuations), the dotted curve is for spherically symmetrical fluctuations; (b) the curve $A(\mu)$ is for $M = 0$.

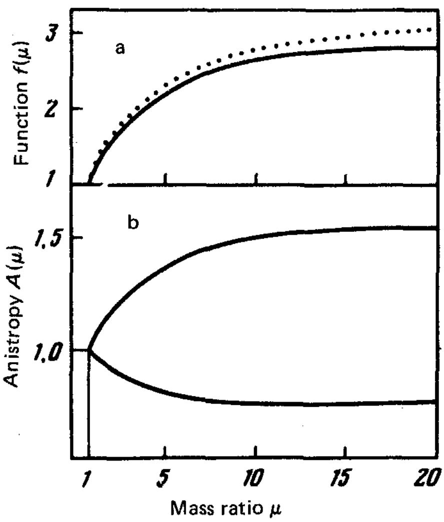

FIG. 2. The dependences $f(\mu)$ and $A(\mu)$ for bands with $S = 3/2$. (a) Solid curve is for unsymmetrical fluctuations ($M = \pm 1/2$ and $M = \pm 3/2$); dashed curve is for spherically symmetrical fluctuations; (b) upper curve is for $M = \pm 1/2$ and the lower curve is for $M = \pm 3/2$. If $L_1 \pm 1/2$ is for heavy holes, then the curves change places, remaining essentially the same.

Thus the spherical fluctuations are not OF; axial fluctuations correspond to the smallest $f(\mu)$. If we rule out the assumption that OF do not have axial symmetry, then it follows from Figs. 1 and 2 that there is a very wide class of fluctuations which give close values of $f(\mu)$. The reason for this is not clear, but from the result obtained it follows that the pre-exponential factor in $\rho(E)$ is large and its calculation is very difficult.

The most important and physically interesting result is the fact that the tails are formed primarily due to strongly anisotropic fluctuations. It raises the question of finding experimental methods for observing them directly. It is evident that the anisotropy can be directly manifested only in effects described by tensors with rank $n > 2$. For example, the indicatrix of resonant Rayleigh scattering in the region of long-wavelength absorption tail, corresponding to Frenkel excitons ($S = 1$), is described by $\cos^2\gamma + 1/2$ for large $|E|$, when $S_0(E)(f_\pm - f_0) \gg 1$, since under these conditions only dipoles with $M = 0$ will survive; γ is the angle between the electric vectors of the incident and scattered light. For smaller $|E|$ is the angle between the electric vectors of the incident and scattered light. For smaller the contribution of other scatterers increases (for example, spherical scatterers), leading to the law $\cos^2\gamma$. The methods of polarized luminescence,[10] polarized induced absorption, etc., can also be used. It may be expected that in specimens with a Fermi level in the region of the tail $\rho(E)$ uniaxial deformations will create, due to refilling of levels, an artificial anisotropy with an appreciable "memory."

In the classical region $r_\psi \ll r_c$, where $\ln\rho \propto -E^2$, OF remain spherically symmetrical.

[1)]We ignore the fluting of bands, caused by the cubic symmetry of the crystal.

[2)]It is closely related to the Jahn-Teller effect in the theory of self-localization (compare Ref. 9); in particular, the height of the self-localization barrier is $f(\mu)$ [see Eq. (6)].

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