Theory of spontaneous emission of x rays from relativistic channeled particles

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(Submitted 28 April 1981)
Zh. Eksp. Teor. Fiz. **81**, 1639–1648 (November 1981)

Spontaneous emission of radiation from relativistic channeled particles (know as the Kumakhov radiation) is investigated for the first time allowing for the energy band structure. A study is made of the band populations as a function of the angle of incidence of electrons on a single crystal and of the divergence of the electron beam. It is shown that for optimal angles of incidence it should be possible to achieve a population inversion of the levels and stimulated emission, giving rise to lasing in the x-ray range. Three possible types of radiative transition during channeling are considered: within a potential well, from suprabarrier bands to a potential well, and between suprabarrier bands. Radiation of the first type is much stronger than those of the other two types, and it can find extensive applications in, for example, x-ray lithography. A detailed comparison is made between the Kumakhov radiation and coherent bremsstrahlung. It is shown that the theory of coherent bremsstrahlung fails to describe any one of the transitions considered.

PACS numbers: 61.80.Mk, 78.70.En

1. INTRODUCTION

Much work has been done on the theory of radiation emitted by relativistic channeled charged particles in crystals. The paper of Kumakhov,[1] predicting high-power radiation under channeling conditions, was followed by others presenting the classical and quantum theories of this new physical effect representing the results of experimental investigations (Wedell's review[2] is devoted to the Kumakhov radiation). The theoretical and experimental results are in satsifactory agreement.[2,3] The cited investigations have been concerned with the radiation emitted by particles of energies from hundreds to megaelectron volts to tens of gigaelectron volts. The number of experiments carried out at low energies (of the order of a few megaelectron volts) is small.[4-6] However, it would be desirable to investigate this range of energies more thoroughly because one could then use high-current electron accelerators, whose main advantages are the enormous current in a beam ($10^3 - 10^4$ A) and also compactness and relatively low cost. Such an accelarator could be used in a high-power source of x rays based on the emission of radiation by channeled particles, and also in a new type of laser operating without mirrors and stimulating radiation of channeled particles. Construction of such spontaneous and coherent sources of x ray radiation would be highly desirable because of possible numerous applications, particularly in x-ray lithography.

We shall report the first investigation of the radiation emitted by electrons moving in a planar channel with account taken of the produced energy band structure. We shall consider all three possible types of transition: inside a potential well, from suprabarrier states to a potential well, and between suprabarrier states. We shall consider the populations of the states as a function of the angle of entry of an electron relative to the atomic planes and also as a function of the electron beam divergence. We shall compare the results obtained with those for coherent bremsstrahlung.

2. RADIATION EMITTED IN THE COURSE OF PLANAR CHANNELING OF ELECTRONS. THEORY

We shall consider the passage of electrons through a crystal neglecting secondary dechanneling processes and also the energy losses due to the emission of radiation. The motion of an electron in a continuous potential of planes $U(x)$ is described by the Dirac wave equation.[7] Since the kinetic energy of the longitudinal motion of electrons is considerably greater than their potential energy in an interplanar field, the Dirac equation reduces to the Schrödinger equation for the transverse motion of a particle whose mass is relativistic $M = E/c^2$:

$$-\frac{\hbar^2}{2M}\frac{d^2\psi(x)}{dx^2} + U(x)\psi(x) = E_\perp\psi(x), \qquad (1)$$

where $\psi(x)$ is the wave function of the transverse motion of the particle and $E_\perp$ is the transverse energy.

The potential $U(x)$ of the transverse motion is a periodic function with a period d_p (d_p is the distance between the planes):

$$U(x) = U(x+d_p), \qquad (2)$$

so that in order to solve the wave equation we have to use the Bloch condition

$$\psi(x+d_p) = \exp(ik_\perp d_p)\psi(x), \qquad (3)$$

where $k_\perp$ is the quasimomentum of an electron in a crystal.

Allowance for the periodicity of the interplanar potential (2) of a crystal and for the Bloch condition (3) gives rise to the energy band structure of the crystal. The band structure is determined in Ref. 8. The system (1)–(3) can be solved by representing the wave function of an electron and the interplanar potential as an expansion in terms of the reciprocal lattice vectors $g = 2\pi/d_p$:

$$U(x) = -\sum_m U_m \exp(imgx), \qquad (4)$$

$$\psi(x) = \sum_n C_n \exp[i(k_\perp - ng)x], \quad m, n = 0, \pm 1, \pm 2, \ldots \qquad (5)$$

when the conditions (2) and (3) are satisfied automatically.

Since the coefficients of the expansion of the potential U_m decrease rapidly on increase in m, the expansion given by Eq. (4) may be truncated at the term which satisfies $U_m/U_0 \ll 1$. Substituting Eqs. (4) and (5) into Eq. (1), we find that instead of a second-order differential equation we now have a system of algebraic equations:

$$\left[\frac{\hbar^2}{2M}(k_\perp + ng)^2 - E_\perp\right]C_n{}^j - \sum_m C_m{}^j U_{n-m} = 0. \tag{6}$$

The number of the equations considered, i.e., the number of Bloch waves in Eq. (1), should be sufficiently large so that the energy band structure goes over into a continuous spectrum. Therefore, n is governed by the condition[8]

$$\hbar^2 (ng)^2/2M \gg U_0. \tag{6'}$$

In Eq. (6) the symbol j labels the energy bands. We shall use the Molière potential,[9] although—in principle—one could utilize also other types of potential. Solution of the system (6) gives the values of C_m^j and the energy band structure $E_\perp$.

The band populations can be found by matching the electron wave functions inside and outside a crystal. Then, the probability of occupancy of a level $k_\perp$ located within an energy band j is governed by the square of the matrix element

$$\langle \psi^j(x) | \exp(ik_x x) \rangle = 2\pi \sum_m C_m{}^j \delta_{k_x, k_\perp - mg} \tag{7}$$

and the wave function of the transverse motion of electrons is

$$\psi(x) = \sum_j A_j \psi^j(x) = \sum_j A_j \sum_m C_m{}^j \exp[i(k_\perp - mg)x]. \tag{8}$$

We can calculate the number of photons emitted by a channeled particle employing the formulas obtained by Kumakhov,[7] because—as shown in Ref. 10—right up to electron energies of a few gigaelectron volts we can use the dipole approximation discussed in Ref. 7. Then, in the case of the radiation directed along the electron motion (this is the most interesting case) we find that the number of photons emitted by an electron per unit distance in a solid angle $d\Omega$ is

$$\frac{dN}{d\Omega} = \frac{e^2 \omega_{j',j} |p_{j',j}|^2}{\pi \hbar (m_0 c^2)^2}, \tag{9}$$

where

$$\omega_{j',j} = \Omega_{j',j}/(1-\beta_\parallel), \quad \Omega_{j',j} = (E_{\perp j} - E_{\perp j'})/\hbar,$$

and the matrix element of the transition $p_{j',j}$ can be found by direct calculation:

$$p_{j',j} = \frac{\hbar}{i} \int \psi^{j'}(x) \frac{d\psi^j(x)}{dx} dx = -\hbar g \sum_m m C_m{}^j C_m{}^{j'}. \tag{10}$$

The calculation factor $\delta_{k_\perp - mg, k_\perp' - ng}$ ($k_\perp$ and k' correspond to the states ψ^j and $\psi^{j'}$) demonstrates that in the dipole approximation the electron quasimomentum is conserved during emission of radiation.
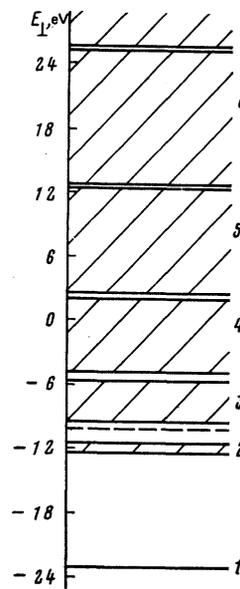
FIG. 1. Energy band structure of electrons with $E_{kin} = 4$ MeV in a (110) plane of Si.

3. RESULTS OF CALCULATIONS

Our numerical calculations were carried out for electrons with a kinetic energy of 4 MeV moving in a (110) channel in silicon. Figure 1 shows the transverse-energy band structure obtained in this case. The dashed line represents the top of a potential well. It is clear from this figure that two bands are formed inside the potential well and are separated by a wide gap. The first band is narrow and it can be regarded as practically a level, i.e., the transverse energy is independent of the quasimomentum. Above the potential well there are suprabarrier bands whose width increases rapidly on increase in the transverse energy, but the gaps between them decrease. The dependence of $E_\perp$ on the quasimomentum is nearly parabolic for these bands, and the deviations from the parabola decrease on increase in the band number. The lower suprabarrier bands correspond to quasi-channeling.

The energy band pattern indicates that there are three types of radiative transition in the Kumakhov effect: 1) transitions within a potential well between strongly coupled states; 2) transitions from suprabarrier states to a potential well; 3) transitions between suprabarrier states. The last type of transition corresponds to the emission of radiation in the course of quasichanneling analyzed classically in Ref. 11. The radiation which appears as a result of all three types of transition may be investigated within the framework of a quantum theory developed in Refs. 7 and 12.

Figure 2 shows the dependences of the band populations on the angle of incidence of electrons on a single crystal. The beam divergence is ignored and the populations are normalized to unity. The angle is expressed in units of the Bragg angle, which in
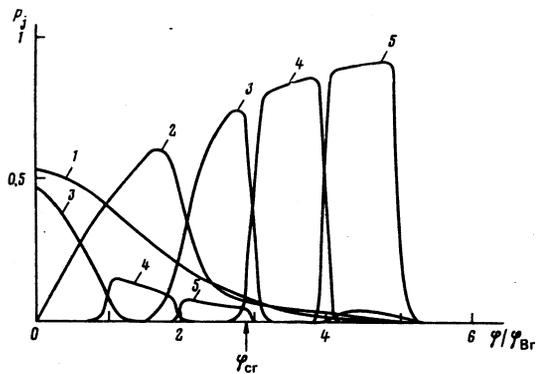
FIG. 2. Band populations vs the angle of incidence of electrons. The numbers of the curves are the same as the numbers of the bands in Fig. 1.

FIG. 3. Band populations plotted vs. the angle of incidence of an electron beam: a) beam divergence $0.3\varphi_{cr}$; b) $0.5\varphi_{cr}$, c) $0.7\varphi_{cr}$. The numbers of the curves are the same as the numbers of the bands in Fig. 1.

our case is $\varphi_{Br} = 0.35\varphi_{cr}$ (φ_{cr} is the critical channeling angle). It is clear from Fig. 2 that in the range $\varphi < \varphi_{cr}$ the channeling is dominated by the first three bands and a suitable selection of the angle of incidence can ensure preferential population of any one of them. It is thus possible to achieve a population inversion immediately on entry of electrons into a crystal.

This result is important from the point of view of stimulated emission. The appearance of an inversion as a result of a change in the angle means that there is no need for pumping. Moreover, one should point out that the bands 2 and 3 are longer-lived from the point of view of inelastic scattering and, therefore, allowance for inelastic processes will clearly increase the population inversion.

If the angle of incidence is $\varphi = 0$, almost half the particles (~47%) are captured by the third (suprabarrier) band, indicating that the first suprabarrier states play an important role in the channeling process.

If $\varphi > \varphi_{cr}$, then the weakly coupled suprabarrier bands begin to fill in turn and they now capture practically all the electrons.

Figure 3 shows the results of a calculation of the populations of bands 1–4 as a function of the angle of incidence of an electron beam whose divergence is $\Delta\varphi = 0.3\varphi_{cr}$, $0.5\varphi_{cr}$, $0.7\varphi_{cr}$. The populations of the fifth and higher bands do not exceed 2% if $\varphi < \varphi_{cr}$.

If allowance is made for the beam divergence, it is found that the population of the second band differs from zero already at $\varphi = 0$ (Fig. 2) and it increases on increase in the divergence, becoming practically comparable with the population of the first band when $\Delta\varphi = 0.7\varphi_{cr}$ (Fig. 3c), whereas the population of the first band decreases. In contrast to a parallel beam (Fig. 2), the divergence has the effect that not only the third but also the fourth band captures a considerable number of particles if $\varphi < \varphi_{cr}$.

When the beam divergence is low (Fig. 3a), the curves obtained have humps, i.e., a population inversion is
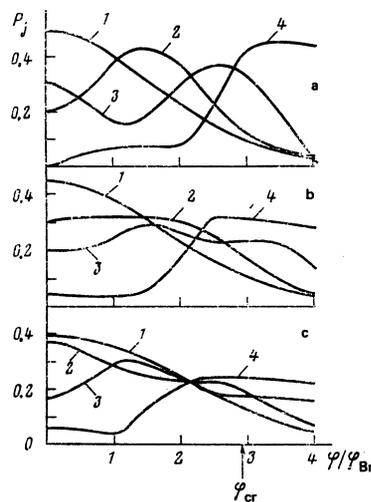
observed in a certain range of angles of incidence. An increase in the divergence flattens the humps and reduces the inversion. Therefore, stimulated emission is obtained for beams of angular divergence $\sim 0.3\varphi \sim 0.3\varphi$ or less, which should be possible to ensure in practice.

Figure 4 gives the number of photons emitted by an electron per unit path length as a function of the angle of incidence. For each transition there is an optimal range of angles within which the number of the emitted photons is maximal. For angles of incidence smaller than the critical channeling angle the strongest radiation corresponds to the transition 2–1 (curve 1 in Fig. 4a), exceeding the number of bremsstrahlung photons by more than one order of magnitude. A comparison of the number of photons emitted as a result of this transition with the maximum numbers generated by other transitions gives a ratio of 4–10 or greater. We shall show later that allowance for the electron beam divergence increases this ratio.

A characteristic feature of the spectra is that a change in the angle of incidence affects less the number of photons generated as a result of the 2–1 transition than the number of photons resulting from all the other transitions. These changes are due to a steep rise and fall of the populations of the suprabarrier bands at specific angles of incidence (Fig. 2). A comparison of the transitions between suprabarrier bands (third type) and from suprabarrier states to a potential well (second type) shows that transitions of the second type are the more intense (curves 2 and 3 in Fig. 4a, curves 1, 2 and 3, 4, 5 in Fig. 4b). The 5–4 and 5–2 transitions are not shown in Fig. 4b because the intensities of the corresponding radiations are far too low, i.e., the transitions of the third type with an odd value of Δj are not very likely.

Figure 5 is the emission spectrum representing transitions between the various bands, calculated for

$(2\pi)^2\, N$, photons/μ
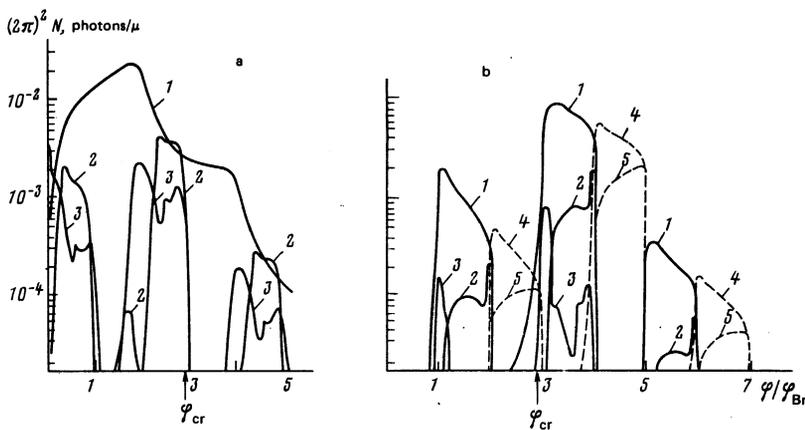
FIG. 4. Numbers of photons emitted per unit path length vs. the angle of incidence of electrons for the following transitions: a1) 2–1; a2) 3–2; a3) 3–2; b1) 4–1; b2) 4–2; b3) 4–3; b4) 5–1; b5) 5–3.

four angles of incidence of the beam. The ordinate gives the number of photons emitted per unit path length in a unit spectral interval per second. The beam divergence is assumed to be $0.3\varphi_{cr}$. All the levels within the bands become filled for this beam divergence. Since the suprabarrier bands are very wide, the lines representing transitions from these bands are also wide. The dependence of the number of photons on their energy for some transitions (for example, 4–3 and 5–3) is close to a constant value extending from zero to a certain energy limit. In contrast, the 2–1 line is much narrower and stronger (in some parts of Fig. 5 it is reduced by a factor indicated alongside the line profile), because photons are emitted in a narrow spectral interval. Such broadening of the emission lines of suprabarrier particles demonstrates ineffectiveness of the transitions in question compared with the 2–1 case. Line narrowing could be observed if beams with angular divergence $\Delta\varphi < \varphi_{Br}$ are used. One should point out that we have ignored the intraband relaxation, whose influence is clearly low.

It is interesting to compare the total number of photons emitted in the course of various transitions. The results are presented in Table I. The last column

$N\cdot 10^5$
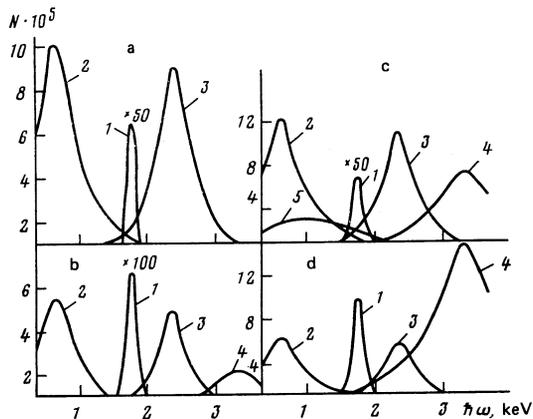
FIG. 5. Number of photons emitted, per unit length in a unit spectral interval, in the forward direction, as a result of excitation with an electron beam of $0.3\varphi_{cr}$ divergence incident at the following angles: a) 0; b) $0.5\varphi_{cr}$; c) $0.9\varphi_{cr}$; d) $1.2\varphi_{cr}$. Transitions: 1) 2–1; 2) 3–2; 3) 3–1; 4) 4–1; 5) 4–3.

of this table gives the ratio of N_{2-1} to the total number of photons emitted as a result of all the other transitions.

It follows from these results that at energies of the order of a few megaelectron volts and angles of incidence of an electron beam not exceeding the critical channeling angle, the main emission mechanism in the process of channeling is in the form of transitions between strongly coupled states lying within the potential well (radiation of the first type). Calculations show that at low angles of incidence there is an increase in the ratio of the total number of photons emitted as a result of transitions within a well to the number of photons emitted as a result of transitions from the suprabarrier states.

4. COMPARISON OF THE KUMAKHOV RADIATION WITH COHERENT BREMSSTRAHLUNG

The Kumakhov radiation has been compared with coherent bremsstrahlung in a number of studies. For example, the radiation emitted by a particle moving in a transient channeling regime and incident at a small angle to the axis and plane of a crystal is considered in Ref. 13. It is found that coherent bremsstrahlung cannot generally be described adequately without allowance for the channeling. Akhiezer et al.[14,15] compared the channeling radiation and coherent bremsstrahlung also under conditions of transient channeling, but the two types of emission have been considered as independent processes. A comparison of transitions of the first type with coherent bremsstrahlung was also made by Wedell.[2]

TABLE I. Ratio of the number of photons emitted along all directions due to 2–1 transition to numbers of photons emitted as a result of other transitions.

Divergence	Angle of incidence	N_{2-1}/N_{3-2}	N_{2-1}/N_{3-1}	N_{2-1}/N_{4-3}	N_{2-1}/N_{4-1}	N_{2-1}/N
$0.3\varphi_{cr}$	0	7	8.8	–	–	3.9
	$0.5\varphi_{cr}$	25	37	74	37	9.3
	$0.9\varphi_{cr}$	6.3	9.5	9.5	7.6	2
	$1.2\varphi_{cr}$	3.3	5	1.3	0.9	0.4
$0.5\varphi_{cr}$	0	13	26	52	52	6.5
	$0.5\varphi_{cr}$	11	14	54	54	4.9
	$0.9\varphi_{cr}$	11	15	9	5.6	2.3
	$1.2\varphi_{cr}$	3.3	4.3	2.6	1.9	0.7
$0.7\varphi_{cr}$	0	22	33	65	65	9.3
	$0.35\varphi_{cr}$	9.8	12	49	49	4.5
	$0.9\varphi_{cr}$	13	20	10	6.7	2.7
	$1.2\varphi_{cr}$	8.3	13	6.3	5	1.8

In the present section we shall discuss transitions of the third type, i.e., the case when the angle of incidence of a beam relative to a plane is outside the range of the critical channeling angle, whereas the angle between the beam and the atomic chains forming the plane is large. As pointed out earlier, the dependence of the transverse energy on the electron quasimomentum in subbarrier states is nearly parabolic. Consequently, we face the question of whether transitions of the third type can be described using the existing theory of coherent bremsstrahlung. Such bremsstrahlung is usually investigated in the Born approximation and the wave functions of electrons are represented in the form of plane waves.[16] We shall show that the Born approximation is inappropriate for suprabarrier transitions.

According to Ref. 16, the interference effects appear in bremsstrahlung when the momentum transferred to a medium $q = \mathbf{k}_0 - \mathbf{k}_f - \mathbf{k}_p$ ($\mathbf{k}_0$ is the initial electron momentum, $\mathbf{k}_f$ is the final electron momentum; $\mathbf{k}_p$ is the momentum of an emitted photon) is close to the reciprocal lattice vector. The contribution of the emitted radiation is made only by those reciprocal lattice vectors which lie in a pancake-shaped layer characterized by the following parameters: the plane of the layer is perpendicular to the direction of $\mathbf{k}_0$, the radius is of the order of the electron mass m, and the distance from the origin of the coordinate system to the nearest layer surface is $m^2 k_p / 2k_0 k_f$ and is equal to the layer thickness (for convenience we are employing units with $\hbar = c = 1$). We shall now follow Schiff's treatment.[17] The energy of a free electron is related to its momentum by

$$E = (k^2 + m^2)^{1/2}; \qquad (11)$$

if the allowance is made for the periodic potential of the crystal planes, the above relationship changes to

$$E = (k^2 + m^2)^{1/2} + E', \qquad (12)$$

where E' denotes the influence of the interplanar potential. This modification shifts the pancake and alters $m^2 k_p / 2k_0 k_f$ to

$$m^2 k_p / 2k_0 k_f - (E_0' - E_f'). \qquad (13)$$

The validity of the Born approximation is now governed by the ratio of the first to the second term in Eq. (13). The Born approximation can be used if the second term is smaller than the first; otherwise, the layer in question becomes smeared out and the predictions of the theory of coherent bremsstrahlung[16] become inaccurate.

In our case, we find that the various suprabarrier transitions are characterized by $m^2 k_p / 2k_0 k_f = 13-20$ eV, $E_0' - E_f'$ is of the order of the band gap and it amounts to $\Delta E_{3-4} = 92$ eV, $\Delta E_{4-5} = 66$ eV, and $\Delta E_{5-6} = 58$ eV; we thus find that the theory of coherent bremsstrahlung gives incorrect results.

The wave function of an electron in a suprabarrier state cannot be represented by a plane wave. If it were close to a plane wave, one of the coefficients in the expansion (5) would have been of the order of unity and the others would have been very small. In fact,

we find that at least two coefficients of the expansion are comparable with the maximum value. For example, the highest values of the coefficients for the third band are 0.53, 0.82, and 0.2, for the fourth band they are 0.18, 0.92, and 0.35, and for the fifth band they amount to 0.26, 0.95, and 0.16. Deviations from a plane wave are sufficiently strong, i.e., the influence of the interplanar potential is considerable. An increase in the band number reduces these deviations and the states with a large transverse energy (in the region of the tenth to twelfth bands) can be described by plane waves. However, at these transverse energies the above method for calculating the band structure is clearly invalid because the approximation of a continuous potential of the planes is no longer obeyed.

Our conclusion of the invalidity of the theory of coherent bremsstrahlung in the case of transitions of the third type is supported also by the fact that the positron and electron emission spectra are identical in the Born approximation. This is obviously incorrect in our case. The potential well for positrons is wider than that for electrons, and, therefore, the influence of the neighboring wells in the former case is greater. This means that the energy bands of positrons are wider than those of electrons and their distribution is different. Hence, it is clear that the emission spectra must be different. In the case of the bands corresponding to large transverse energies the band gaps are practically zero and the difference between the spectra disappears.

[1]M. A. Kumakhov, Phys. Lett. A 57, 17 (1976).
[2]R. Wedell, Phys. Status Solidi B 99, 11 (1980).
[3]V. A. Bazylev, V. V. Beloshitskiǐ, V. I. Glebov, N. K. Zhevago, Kh. Trikalinos, and M. A. Kumakhov, Dokl. Akad. Nauk SSSR 253, 1100 (1980) [Sov. Phys. Dokl. 25, 624 (1980)].
[4]J. U. Andersen and E. Laegsgaard, Phys. Rev. Lett. 44, 1079 (1980).
[5]N. Cue, E. Bondepur, B. B. Marsh, H. Bakhru, R. E. Benenson, R. Haight, K. Inglis, and G. O. Williams, Phys. Lett. A 80, 26 (1980).
[6]Yu. N. Adishchev, V. V. Kaplin, D. E. Popov, A. P. Potylitsin, E. I. Rozum, and S. A. Vorobiev, Phys. Lett. A 81, 40 (1981).
[7]M. A. Kumakhov, Zh. Eksp. Teor. Fiz. 72, 1489 (1977) [Sov. Phys. JETP 45, 781 (1977)].
[8]A. V. Tulupov, Fiz. Tverd. Tela (Leningrad) 23, 46 (1981) [Sov. Phys. Solid State 23, 25 (1981)].
[9]M. T. Robinson, Phys. Rev. 179, 327 (1969).
[10]N. K. Zhevago, Zh. Eksp. Teor. Fiz. 75, 1389 (1978) [Sov. Phys. JETP 48, 701 (1978)].
[11]M. A. Kumakhov and C. G. Trikalinos, Phys. Status Solidi B 99, 449 (1980).
[12]V. A. Bazylev and N. K. Zhevago, Zh. Eksp. Teor. Fiz. 73, 1697 (1977) [Sov. Phys. JETP 46, 891 (1977)].
[13]V. V. Beloshitskiǐ and M. A. Kumakhov, Dokl. Akad. Nauk SSSR 251, 331 (1980) [Sov. Phys. Dokl. 25, 196 (1980)].
[14]A. I. Akhiezer, B. F. Boldyshev, and N. F. Shul'ga, Fiz. Elem. Chastits At. Yadra 10, 51 (1979) [Sov. J. Part. Nucl. 10, 19 (1979)].
[15]A. I. Akhiezer, I. A. Akhiezer, and N. F. Shul'ga, Zh. Eksp. Teor. Fiz. 76, 1244 (1979) [Sov. Phys. JETP 49, 631 (1979)].
[16]H. Überall, Phys. Rev. 103, 1055 (1956).
[17]L. I. Schiff, Phys. Rev. 117, 1394 (1960).

Translated by A. Tybulewicz

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