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Quantum effects for particles channeling in a bent crystal

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ABSTRACT

Quantum mechanical theory for channeling of the relativistic charged particles in the bent crystals is considered in the paper. Quantum effects of under-barrier tunneling are essential when the radius of the curvature is closed to its critical value. In this case the wave functions of the quasi-stationary states corresponding to the particles captured in a channel are presented in the analytical form. The efficiency of channeling of the particles and their angular distribution at the exit crystal surface are calculated. Characteristic experimental parameters for observation the quantum effects are estimated.
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1. Introduction

The first experimental observation of the charged particle channeling in a bent single crystal was reported in Ref. [1]. This phenomenon was theoretically predicted by Tsyganov in Ref. [2]. At present, the effect is considered as an perspective method in high energy physics to control the charged particle beams. A lot of experimental works were done in order to investigate accurately various aspects of the phenomenon both for positively [3–7,11] and negatively charged particles [8–10] with different energies. The length of dechanneling for high-energy protons in the bent crystal was measured with high precision [11]. In the papers [12,13] the undulator on the basis of the bent crystal was considered theoretically and was realized recently in [14].

The angle of the particle beam rotation is defined by the crystal length and its curvature radius R_{cr}. This value was estimated in dependence on the particle energy in Ref. [2]. All above mentioned experiments were operated with the crystals having the bent radius $R \gg R_{cr}$. In this case the theoretical simulation of the particle channeling can be fulfilled in the framework of the classical mechanics as it takes place for the channeling in the straight crystal.

The maximal angle of the particle beam rotation corresponds to the minimal possible crystal curvature radius $R \approx R_{cr}$. However, as it was shown in Ref. [15], the classical theory is not applicable in this case. Therefore, it is of interest to investigate in detail the particle motion in the bent crystals taking into account the factors that are not described within the framework of the classical theory of the phenomenon.

In this paper (see also in [15]) the quantum theory of the planar channeling of the relativistic particles in a bent single-crystal is built and the quantum effects are described at the crystal curvature radius in the range $R \approx R_{cr}$. It is shown that in this case the particle states in a bent crystal are changed substantially because of tunneling under the barrier created by the crystallographic planes. It leads to the change of the efficiency of capture in the channeling modes and the angular distribution of the particles at the exit surface of the bent crystal. All numerical calculations are fulfilled for the proton channeling in the Si crystals but the analysis is valid also for the negatively charged particles.

2. Stationary states of the particle channeled by the bent crystal.

Let us consider the equation, which follows from the Dirac equation and determines the stationary states of the relativistic particle with energy E and mass $m \ll E$ in a crystal if the small spin effects are not taken into account [15,16] (the natural system of units with $\hbar = c = 1$ is used):

$$\left\{\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2} + \frac{\partial^2}{\partial z^2} + E^2 - m^2 - 2EV(\vec{r})\right\}\Psi(\vec{r}) = 0. \quad (1)$$

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The average potential of the crystallographic planes in the bent crystal has cylindrical symmetry [3] and is described by the following function

$$V(r) = \sum_{n=-n_1}^{n_1} V_1(r - R - nd).$$

Here $V_1(r-R-nd)$ is the potential of a single plane; R is the curvature radius of the central channel, $2n_1$ is the number of crystallographic planes in the direction perpendicular to the bend; $d \ll R$ is the interplane distance.

The variables in Eq. (1) can be separated in the cylindrical coordinate system due to the potential symmetry:

$$\Psi(\vec{r}) = \frac{u(r)}{\sqrt{r}} \exp[i(l\varphi + p_z z)]; \quad l = 0, \pm 1, \pm 2, \ldots.$$

To solve this equation it is convenient to introduce relative radial variable $x = r - R; |x| < n_1 d \ll R$ and use the condition $|V(r)| \ll E$. Then the equation for the function $u(r)$ becomes similar to Schrodinger equation for the particle transverse motion in the case of planar channeling [17]

$$\left\{ -\frac{d^2}{dx^2} + 2E_0 V_{eff}(x) \right\} u(x) = \varepsilon u(x).$$

The total energy eigenvalue in Eq. (1) is determined by the quantum numbers l, p_z and the energy of radial motion ε in the effective potential $V_{eff}(x)$:

$$E \approx E_0 + \varepsilon; \quad E_0^2 = m^2 + p_z^2 + \frac{l^2 - 1/4}{R^2};$$
$$V_{eff}(x) = V(x) + \frac{p_0^2}{E_0 R} x = V(x) + \frac{p_0 v}{R} x; \quad p_0 = \sqrt{E_0^2 - m^2 - p_z^2}, \quad (2)$$

with $v = p_0/E_0$ as the particle velocity.

From the classical point of view the bound state of the particle in a channel is appeared when the potential energy $V_{eff}(x)$ has a minimum in the range $-d/2 \leqslant x \leqslant d/2$. When considering Eq. (2) this condition takes the following form:

$$-\mid V'(x)|_{max} + \frac{p_0 v}{R} \leqslant 0. \quad (3)$$

The crystallographic plane potential is the monotonically increasing function for $x \to \pm d/2$, therefore the condition (3) is equivalent to the following inequality for the average radius of the crystal curvature:

$$R \geqslant \frac{p_0 v}{\mid V'(x)|_{max}} \equiv R_{cr}, \quad (4)$$

which coincides with expression obtained by Tsyganov [2].

In order to illustrate the further results quantitatively let us choose Si crystal bent along the planes (1 1 0) ($d = 1.92$ Å) as an example. In this case the potential of a single plane is well approximated by the Peschl-Teller potential [17]:

$$V_1(x) = a_{PT} \tanh^2(x/b_{PT}), \quad (5)$$

with the parameters $a_{PT} = 23$ eV, $b_{PT} = 0.145d$ and $V'_{1max} = 6.37$ GeV/cm.

Remind, that the channeling potential have already took into account averaging of the microscopic particle-crystal potential over the atomic thermal vibrations [17]. Deviations from this potential conditioned by the particle-phonon interaction lead to an incoherent scattering and define one of the contributions to the dechanneling processes.

If one considers the channeling of protons with the energy $E = 70$ GeV, for which one of the first experiments with a bent crystal was carried out [1], $R_{cr} \approx 11.01$ cm. Fig. 1 shows the potential $V_{eff}(x)$, obtained by (5) and (2) with $E_0 = 70$ GeV, and the curvature radius $R = 12.01$ cm.

However, in a quantum theory the condition (4) is not sufficient to ensure that the particle could be captured in channel and change the velocity direction at a large angle. It happens because of the possibility of the particle tunneling under potential barrier (between the points x_1 and x_0 in Fig. 1). In the result it passes to the continuous spectrum state corresponding to a direct motion of the particle. Lifetime of the particle in a bent channel, and consequently, the angle of the particle rotation depends on the concrete form of the potential.

Note that one can consider the quantum effect of under-barrier tunneling as an additional mechanism of the particle dechanneling along with the known classical processes [3,11]. At the considered particle energy such quantum effects are negligible in the case of planar channeling in the straight crystal. But the barrier penetrability grows significantly when the curvature radius of the crystal is close to its critical value. Fortunately in this case all calculations can be conducted analytically for arbitrary $V(x)$, because $V_{eff}(x)$ can be taken into account in the harmonic approximation. With the above parameters $R_{cr} \approx 11.01$ cm and we will choose the crystal bend radius close to this value, for example, $R = 12.01$ cm (Fig. 1). In this case, the potential of a bent channel near barrier can be approximately written in the following form:

$$V_{eff}(x) \approx \begin{cases} V_1 = \frac{1}{2} V''(x_0)(x - x_0)^2; & x' < x < x_0; \\ V_2 = \Delta V - \frac{1}{2} \mid V''(x_1) \mid (x - x_1)^2; & x < x'. \end{cases} \quad (6)$$

Here the point x' is determined from the matching condition $V_1(x') = V_2(x')$ and $\Delta V = V_{max}(x_1) - V_{min}(x_0)$.

In order to avoid misunderstanding it should be stressed that the harmonic approximation (6) for $V_{eff}(x)$ differs essentially from that one for channeling potential in the straight crystal. The latter one is used usually for x near the minimum of $V(x)$. On the contrary the points x_0, x_1 corresponding to the minimal value of $V_{eff}(x)$ are disposed near the point of inflection x_d for $V(x) : V'(x_d)_{max}$, $V''(x_d) = 0$; $|x_0 - x_d| \sim (R - R_{cr})$ (Fig. 1). All these points are close to the atomic planes and correspond to the potential maximum for the positively charged particles and to the potential minimum for the negatively charged particles. Interpolation (6) does not depend on the detailed form of the channeling potential on the whole interval but only on the values $V''(x_0), V''(x_1)$. It can be verified that these values change unessentially for all commonly used model channeling potential and for both particle charges [17].

For the potential (6) the quasi-stationary energy levels for the particle in the bent channel can be approximately calculated by means of the formula:

$$\varepsilon_k \approx \omega\left(k + \frac{1}{2}\right) - i\Gamma_k/2 \equiv \varepsilon_k^{(0)} - i\Gamma_k/2; \omega = \left[\frac{V''(x_0)}{E_0}\right]^{1/2}. \quad (7)$$

The width Γ_k of the level can be found by using the quasi-classical expression for the penetration coefficient of the potential barrier [18]

$$\Gamma_k = A\omega \exp\left[-2\int_b^a \sqrt{2E_0(V_{eff}(x) - \varepsilon_k^{(0)})} dx\right], \quad (8)$$

where $A \approx 1$ is pre-exponentials and the two turning points a and b are defined by the expression:

$$a, b = x_1 \pm \sqrt{\frac{2\Delta V - (2k+1)\sqrt{\frac{V''(x_0)}{E_0}}}{\mid V''(x_1) \mid}}.$$

Maximal number of the levels corresponding to the particle bound states is defined by the condition:

$$k_{max} < \frac{\Delta V}{\omega} - \frac{1}{2}$$

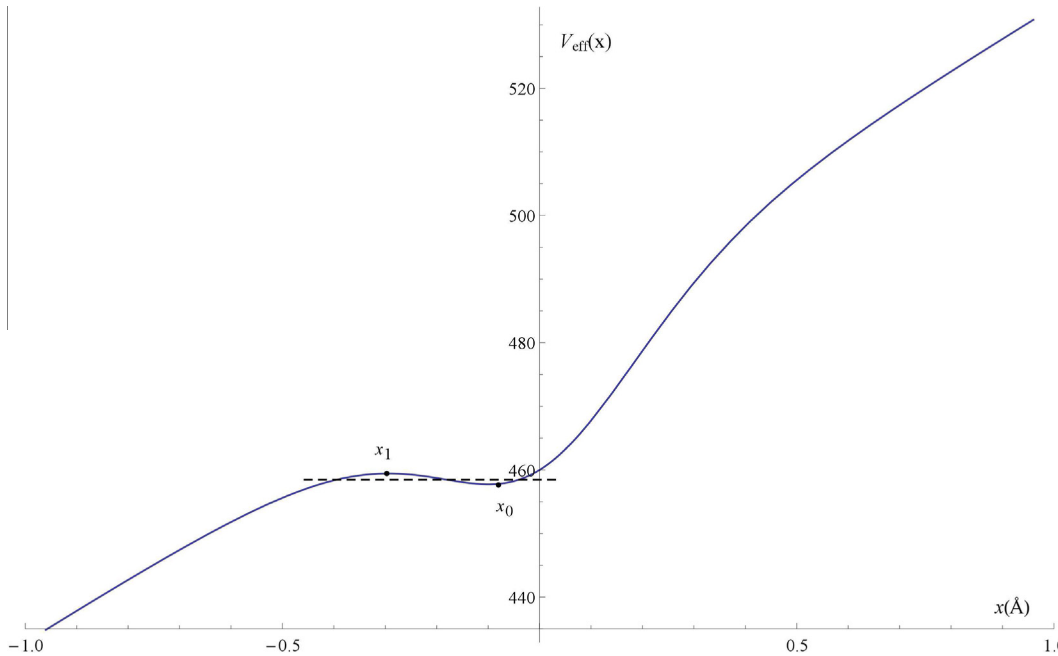

Fig. 1. Effective potential for the particle in the bent crystal.

For example, when the particle energy $E_0 = 70$ GeV it leads to:

$$V_{min} = 456.788;\ V_{max} = 457.193;\ \omega = 0.112,$$

so that

$$k_{max} < \frac{V_{max} - V_{min}}{\omega} - \frac{1}{2} = 3.12$$

This means that there are 4 bound levels with quantum numbers k = 0, 1, 2, 3. Widths of these levels were calculated using the formula (8). Analogous calculations can be executed for other particle energy. Table 1 shows some results.

By the definition of width, the particle that is trapped at the kth bound level in the bent channel remains at it moving through entire crystal length L if the following condition is fulfilled

$$\Gamma_k L < 1. \tag{9}$$

It allows one to introduce the characteristic value $L_k = 1/\Gamma_k$ as the distance which the particle at the k-th bound level moves being captured in the bent channel. This length should be taken into account only for the levels close to the top of the barrier. Its values strongly depend on the particle energy and also presented in Table 1. As one can see at the considered energies only two lowest levels are effective for the capture of particles.

3. Efficiency of the particle capture in the bent channels.

Let us consider the following geometry for observation of a beam rotation by a bent crystal (Fig. 2). Here $\vec{p}_0$ is the incident particle momentum. Crystal is supposed to be homogeneous in the z-axis direction, so without violation of generality it is possible

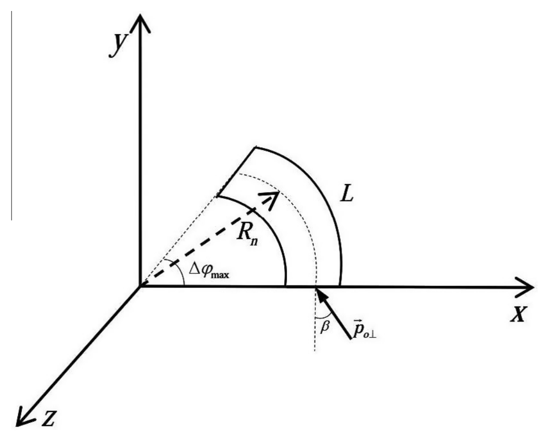

Fig. 2. Rotation of a beam in a bent crystal.

to choose $p_{0z} = 0$; $p_{0x} \approx E_0 \sin\beta$; $p_{0y} \approx E_0 \cos\beta$; angle β determines divergence of the momentum in the incident beam; $L_x = 2n_1 d$ is the crystal width, $L_z = h$ is its height and L is its length.

In order to calculate the population of the bound levels in a bent channel one should use the continuity condition at $\varphi = 0$ for the wave function, describing the incident wave packet and superposition of the stationary wave functions being solutions of the Schrödinger equation in the crystal.

For the levels satisfying the condition (9) the wave function of bound state of the particle in the bent channel with number p is written as follows:

$$\Psi_{p_z,l,p,k} = \frac{e^{ip_z z}}{\sqrt{2\pi h}} \frac{e^{il\varphi}}{\sqrt{2\pi}} \left(\frac{1}{k! 2^k} \sqrt{\frac{\alpha}{\pi}} \right)^{1/2} e^{-\frac{1}{2}\alpha x^2} \frac{H_k[\sqrt{\alpha} x]}{\sqrt{r}}, \tag{10}$$

where $x = r - R_n - x_0 - pd = r - r_p; \alpha = \sqrt{E_0 V''(x_0)}; H_k$ is the Hermite polynomials.

The energy corresponding to the wave function (10) is defined by four quantum numbers

Table 1
Parameters of the bound states for particle in the bent channel.

E_0(GeV)	ω(eV)	k	Γ_2/ω	Γ_3/ω	L_2(cm)	L_3(cm)
70	0.112	0,1,2,3	0.24×10^{-3}	0.42	0.24	0.0002
80	0.099	0,1,2	1.32×10^{-3}	–	0.06	–

$$E_{p_z,l,p,k} = \sqrt{m^2 + p_z^2 + \frac{l^2 - 1/4}{R_n^2}} + p\Delta V + \omega\left(k + \frac{1}{2}\right).$$

It should be noted that the expression (10) is similar to the formula for the wave function of the channeled particle in a plane crystal [17]. However, because of absence periodicity of the potential in the radial direction the energy levels for isolated pits do not form energy zone with $2n_1$ sublevels but they stay different for each channel. Then the quantum number p determines the channel number.

Before proceeding to study the boundary problem, let us remind the classical estimation for the capture efficiency ("acceptance") of the particle in the bent channels. This value A_{cl} in framework of the classical theory can be estimated as ratio of the phase volume corresponding to the finite movement of the particles in the channel to the total phase volume of the incident beam [3,12]:

$$A_{cl} \approx \left(1 - \frac{R_{cr}}{R}\right)^2 F\left(\frac{\pi\theta_c}{4\Delta\beta}\right);$$
$$\begin{cases} F(u) = 1;\ u > 1; \\ F(u) = u;\ u < 1, \end{cases} \qquad (11)$$

with $\theta_c = \sqrt{2a_{PT}/E_0}$ and $\Delta\beta$ determine the Lindhard angle and the angular divergence of the incident beam, correspondingly.

Strictly speaking, Eq. (11) is valid for $R \gg R_{cr}$. However, we will use it also for $R \sim R_{cr}$ for approximate comparison with our results.

Let us now deduce the formula for the acceptance A_q in the quantum case. The wave function of the incident particle in the range $\varphi < 0$ is defined by the following wave packet:

$$\Psi_0 = \int \frac{d\vec{q}}{(2\pi)^{3/2}} a(\vec{p}_0 - \vec{q}) \exp[i(q_z - \vec{q}\vec{r}_i)] \sum_l (-1)^l J_l(q_\perp r) e^{il(\varphi-\beta)}.$$

Here the function $a(\vec{p}_0 - \vec{q})$ determines distribution of the particle momentum relatively its central value $\vec{p}_0$. It is normalized by the condition $\int d\vec{q} \mid a(\vec{p}_0 - \vec{q})|^2 = 1$. The vector $\vec{r}_i$ determines the point, where the single-particle wave packet is localized when it gets to the crystal; $J_l(q_\perp r)$ is the Bessel functions.

Wave function of the electron in the bent crystal is defined by the following superposition:

$$\Psi_1 = \sum_\lambda C_\lambda \Psi_\lambda(r), \qquad (12)$$

where λ includes all quantum numbers p_z, l, k, p; $\Psi_\lambda(r)$ is the stationary wave function (10) and the coefficients C_λ are defined by the integral:

$$C_\lambda = \int_{-\infty}^{\infty} dz \int_0^\infty r dr [\Psi_0 \Psi_\lambda^*]_{\varphi=0} = \int \frac{d\vec{q}}{(2\pi)^{3/2}} a(\vec{p}_0 - \vec{q}) \exp[-i(\vec{q}\vec{r}_i + l\beta)]$$
$$\times \int_{-\infty}^{\infty} dz \frac{e^{i(q_z - p_z)z}}{\sqrt{2\pi h}} \int_0^\infty dr \sqrt{r} J_l(q_\perp r) C_k e^{-\frac{\alpha x^2}{2}} H_k(\sqrt{\alpha}x), \qquad (13)$$

$C_k = \left(\frac{1}{k!2^k}\sqrt{\frac{\alpha}{\pi}}\right)^{1/2}$ is the normalization constant.

Using the integral representation for the Bessel function and the saddle-point method with the condition $q_\perp R \gg 1$ [19] one can find the value C_λ in the following form:

$$C_\lambda = \int \frac{d\vec{q}}{(2\pi)^{3/2}} a(\vec{p}_0 - \vec{q}) \exp[-i(\vec{q}\vec{r}_i + l_\beta)] C_k (i)^{k+1/2} \frac{\sqrt{R}}{q_\perp}$$
$$\times \frac{\delta(p_z - k_z)}{\sqrt{h}} \times e^{-\frac{\alpha}{2q_\perp^2}(l - q_\perp r_p)^2} H_k\left(\frac{q_\perp}{\sqrt{\alpha}} \mid q_\perp r_p - l \mid\right). \qquad (14)$$

Let us suppose that the incident beam is monochromatic by energy and has the Gaussian distribution over the angles with the angular width $\Delta\beta = \theta \approx \theta_c$. Then the probability of the particle will be captured at one of the bound levels in the bent channel is defined by the following expression:

$$P(r_i, r_p) = \sum_{k=0}^{k_1} \sum_l \frac{\theta}{\sqrt{\pi}} e^{-\theta^2(l - p_0 r_i)^2} \frac{h}{k! 2^k} \sqrt{\frac{\alpha}{\pi}} \frac{V''(x_0)}{p_0} \left(r_p - \frac{l}{p_0}\right)^2$$
$$\times \frac{R\alpha}{p_0 \Delta V} e^{-\frac{\alpha}{p_0^2}(l - p_0 r_p)^2} H_k^2\left(\frac{\sqrt{\alpha}}{p_0} \mid l - p_0 r_p \mid\right), \qquad (15)$$

where k_1 is maximal value of k for which the inequality (9) is fulfilled.

The acceptance A_q can be calculated in the result of averaging the value $P(r_i, r_p)$ over the coordinates of the incident particles within the cross-sectional area $S_b = hL_b$ of the beam and summation over numbers of the channels $-n_1 < p < n_1$. Besides, the sum over l in Eq. (15) can be replaced by the integral because in the considered case of the relativistic particles the number of various values of l contributed to this sum is very large ($\Delta l \approx p_0 n_1 d \gg 1$).

In a result of calculation of all integrals one can find the acceptance A_q in the following form:

$$A_q = \sum_{-n_1}^{n_1} \int \frac{dx_i dz_i}{S_b} P(r_i, r_p) = \sum_{k=0}^{k_1} \left(k + \frac{1}{2}\right) \frac{L_x}{L_b} \frac{V''(x_0) R}{dp_0^2 \Delta V}$$
$$\approx \frac{L_x}{L_b} \sum_{k=0}^{k_1} \left(k + \frac{1}{2}\right) \frac{\omega^2}{dV'(x_0)\Delta V} = \frac{L_x}{L_b} \frac{\omega}{dV'(x_0)} \frac{k_1(k_1 + 2)}{2k_1 + 1}. \qquad (16)$$

It is assumed that the beam width L_b is wider than the crystal width L_x.

Table 2 shows a comparison of the acceptance A_q value with its classical values of A_{cl}, which was calculated according to the formula (11), for the particle energies $E_0 = 70$ GeV and 80 GeV.

In our knowledge, the existing experiments with bent crystals corresponded to the case $R \gg R_{cr}$ and we could not compare the theoretical values (16) with experimental data. Therefore we used an extrapolation of Eq. (11) beyond the framework of its validity for rough estimation of the classical acceptance (last column in Table 2) in the case $R \sim R_{cr}$. One can see that the simple geometrical calculation (11) underestimates essentially the acceptance value because the larger phase volume is taken into account in the quantum calculation of the occupation coefficients (13).

4. Angular distribution of the particles exited from the crystal

In the present paper let us consider the pure quantum effects neglecting the dechanneling and volume capture processes [3]. In this case the particles that occupied the levels with quantum number $k < k_1$ will move on the circular trajectory with radius R. It leads to rotation of the occupied part of the beam at the angle

$$\beta(L_r) = \frac{L_r}{R},$$

where $L_r \leqslant L$ is the length of the particle path in the bent crystal.

In the framework of the quantum–mechanical description the state of the beam after passing of the way L_r is determined by evolution of the population coefficients in the expansion of the wave function (12) over the quasi-stationary states:

$$\Psi_1(L_r) = \sum_\lambda C_\lambda \Psi_\lambda(r) e^{i\epsilon_\lambda L_r}. \qquad (17)$$

Taking into account the level widths of the bound levels (7) one can calculate the probability to find the particle at kth level after passing the distance L_r as follows:

Table 2
Acceptance of the particle capture in the bent channel.

E_0	k_1	A_q	A_{cl}
70	3	3.94%	0.69%
80	2	2.44%	0.54%

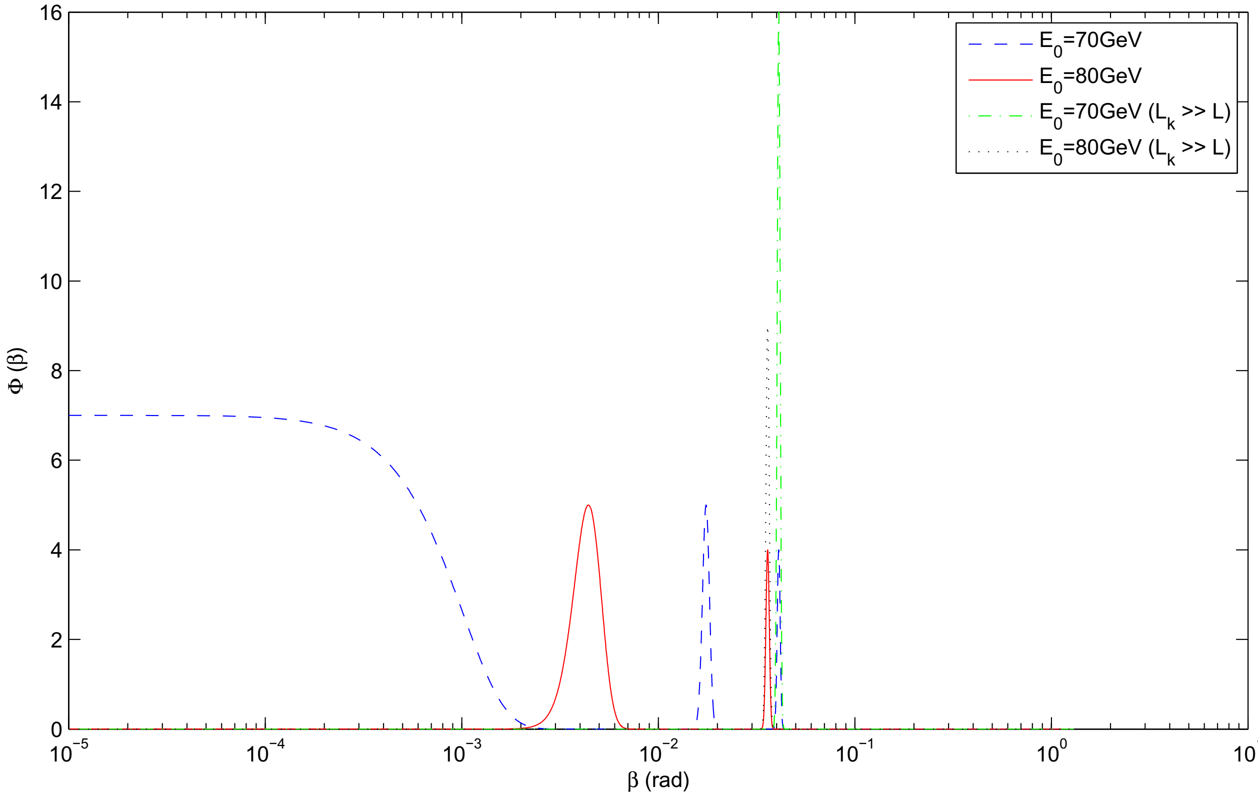

Fig. 3. Angular distribution of the particles exited from the crystal.

$$P_k(L_r) \approx \frac{L_y}{L_b} \frac{(2k+1)}{(2k_1+1)} \frac{\omega}{dV'(x_0)} e^{-\frac{L_r}{L_k}}. \tag{18}$$

Under barrier tunneling is significant only for the upper levels, for which the values of L_k at the considered parameters are shown in Table 1 (for the lower levels $L_k \gg L$).

One can see from Eq. (18) that this process is described by the exponential law similarly to other dechanneling mechanisms conditioned by the particle multiple scattering on the crystal electrons and nuclei [11]. The latter processes are characterized by the dechanneling lengths L_e and L_n correspondingly and can be considered as over barrier processes. In the present paper we are restricted by the qualitative estimation of their influence on the quantum effect because the existing experimental data refer to the case $R \gg R_{cr}$. As it was mentioned above the point x_0 (Fig. 1) is arranged near the crystal plane where the electron density is small [11] and $L_e \gg L_k$. From the other side the estimation shows that this point is situated out of the "nuclear corridor" [11] for the considered experimental parameters. Therefore one can expect that $L_n \succeq L_k$ from Table 1 and the tunneling effect still can be observed.

In the crystal with length L the angle of the particle rotation is determined only by that part of trajectory when particle was staying at the bound level and it can be calculated using the following formula:

$$\beta_k = \frac{L_k}{R}\left[1 - e^{-\frac{L}{L_k}}\right]. \tag{19}$$

Let us, for example, consider a model of the incident beam with the uniform density along the axis x ($L_b = L_x$) and the Gaussian distribution on angle β with a width θ:

$$\frac{\theta}{\sqrt{\pi}}\Phi_0(\beta); \;\; \Phi_0(\beta) = e^{-\frac{\beta^2}{\theta^2}}.$$

Then the angular distribution of beam intensity at the exit of the crystal is described by the following expression:

$$I(\beta) = I_0\Phi(\beta); \;\; I_0 = \frac{\theta}{(2k_1+1)\sqrt{\pi}} \frac{\omega}{dV'(x_0)};$$

$$\Phi(\beta) = \sum_{k=0}^{k_1}(2k+1)\Phi_0(\beta - \beta_k), \tag{20}$$

where the values β_k are defined by the formula (19). Characteristic form of this function is shown in Fig. 3, for two energies of the particles and the crystal length $L = 0.5\ cm$, $\theta = 10^{-3}$ rad. The logarithmic scale for the exit angles was used.

One can see that the angular distributions have only one peak for each of the particle energies if the quantum tunneling is not taken into account ($L_k \gg L$ were chosen artificially for all levels). However, several fractions of the particles rotated at different angles were appeared if the real values of the tunneling lengths L_k from Table 1 were used. Such fine structure in the particle angular distribution could confirm qualitatively the considered quantum-size effect.

5. Conclusions

In the result, it shown in the paper that a fine structure of angular distribution in the rotated beam should appear in the framework of the quantum–mechanical effects for the particles channeled by the bent crystal. Its characteristic form depends on the number of the particle localized states in the average potential of the planes. Experimental investigation of this phenomenon may demonstrate the quantum-size effects for high energy physics and may be useful for optimization of the bent crystal parameters.

When the crystal curvature radius is closed to its critical value the quantum tunneling of the captured particles should be taken into account together with the classical dechanneling processes. The sample calculations were fulfilled for the positively charged particles (protons) but the qualitative results can be also corrected for electrons. It seems that the main problem for observation of the considered quantum effects is defined by manufacturing of the crystal with rather small bend radius.

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