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## Dynamics of high-energy charged particles in straight and bent crystals

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Abstract. The problems of the dynamics of high-energy charged particles in straight and bent crystals are discussed. Various methods for describing particle scattering in crystals are considered, including the Born approximation, classical electrodynamics, and the eikonal approximation. These problems belong to the theory of nonlinear systems in which both regular and chaotic motion is possible. Various types of channelling motion and abovebarrier motion of particles in a crystal along one of the crystallographic axes are discussed. Special attention is given to the studies of motion of particles in a bent crystal, which may be used to bend high-energy particle beams.

## 1. Introduction

The problem of the interaction of fast charged particles with crystals is of considerable interest from a number of viewpoints. Above all, the passage of high-energy particles

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Received 20 January 1995 Uspekhi Fizicheskikh Nauk **165** (10) 1165–1192 (1995) Translated by A Tybulewicz through a crystal is accompanied by coherence and interference effects, which are due to the interaction of a particle with different atoms in the lattice. These effects include the diffraction of x rays in crystals [1], the Bragg scattering [2], the coherent scattering, the radiation emitted by relativistic electrons, the formation of electron – positron pairs [3–6], and the rainbow scattering [7, 8]. These effects are the reasons why the probability of the interaction of a particle with lattice atoms may be considerably higher than the probabilities of analogous processes involving single atoms. Much has been published on this subject (details can be found in reviews and monographs [9–16]).

A crystal is a unique system with very strong internal electric fields. The average values of the internal crystal fields may be several orders of magnitude higher than macroscopic external fields. When particles move in such internal fields, they may experience channelling, which is a remarkable phenomenon in which a particle moves along open channels formed by atoms located in crystallographic planes or arranged along crystallographic axes.<sup>†</sup> The motion in a strong inhomogeneous crystal-lattice field is strongly nonlinear and it can be regular or chaotic. It would seem that any motion of a particle in a crystal should always be regular because of the periodic crystal structure.

†Attention to this effect was first drawn by Stark in 1912 [17]. The existence of open channels was established much later by Robinson and Oen [18] who simulated numerically the motion of a charged particle in a crystal. The foundation of the theory of channelling was provided by Lindhard [19]. Channelling is discussed in a number of reviews and monographs [20-27].

However, in view of the high intensity and nonlinearity of the fields in crystals, motion of a particle may be regular or chaotic [28-30], both in the presence and absence of channelling [14, 31].

Quantum-electrodynamic effects which appear during the motion of a charged particle in a strong crystal field have a number of interesting properties. The probabilities of such processes as bremsstrahlung and pair formation increase strongly at high particle energies (see, for example, Refs [14, 25, 32-36]). In describing these effects it is necessary to take account of the recoil which accompanies the emission of radiation and also of multiple processes. A very specific phenomenon is the growth of an electromagnetic shower in a crystal [37, 38].

There is also the problem of the interaction of highenergy particles with a bent crystal. In the presence of a strong internal crystal field the bending of a crystal bends the particle path, so that it is possible to bend a beam of moving particles in a crystal. The attention to this effect was first drawn by Tsyganov [39] and it can be used to bend beams of high-energy charged particles, extract particles from cyclic accelerators, and split a beam into several components (for reviews see Refs [40-43]). It is important to note that crystals can perform these tasks within much smaller spatial regions than can macroscopic external fields. This is due to the high intensity of internal crystal fields.

The interactions of high-energy charged particles with crystal fields have been investigated by a variety of theoretical methods, such as the Born perturbation theory, the semiclassical approximation, and classical electrodynamics. The problem then arises of the approximations which can be used for the internal crystal field. The approximation of a continuous row or string is used in the theory of channelling: in this approximation the lattice potential is averaged along the coordinate (crystallographic axis) parallel to such motion.

The purpose of this review is to consider in detail the dynamics of charged particles in the continuum potential of rows of atoms in a crystal and to determine the conditions under which such motion can be regular and those which make the motion chaotic. We shall discuss the characteristic features of the dynamics of such particles not only in straight, but also in bent crystals.

# 2. Scattering of fast charged particles by rows of atoms in a crystal

## 2.1 Scattering in the Born approximation

If a high-energy charged particle is moving in a crystal at a small angle relative to one of the crystallographic axes (z axis), a correlation appears between the subsequent collisions of the particle with the lattice atoms. In the presence of such correlations the scattering cross section of a particle in a crystal may be very different from the scattering cross section in an amorphous medium. Correlations appear even when a particle collides with atoms forming a single row oriented along the z axis. We shall therefore consider first the scattering by a single row of atoms in a crystal when a particle beam crosses the row at a small angle relative to its axis (Fig. 1).

The scattering by a row of atoms may be coherent because of the periodic structure of the row and the related possibility of the interference between the scattering amplitudes when a particle collides with different atoms.



Figure 1. Interaction of a fast charged particle with a row of atoms in a crystal.

We shall show that the effectiveness of such scattering is described by the parameter [14]

$$\zeta^{(N)} = N_c \, \frac{Ze^2}{\hbar c} \,, \tag{2.1}$$

where  $N_c \propto R/\psi a$  is the number of atoms in a row with which a particle interacts effectively when it crosses the row; Z|e| is the nuclear charge of a single atom; R is the screening radius of the atomic potential; a is the lattice constant (we shall use a system of units in which the quantum constant  $\hbar$  and the velocity of light c are taken to be unity).

The parameter  $\zeta^{(N)}$  can be small or large compared with unity. Depending on the value of this parameter, one has to use different methods in the description of scattering. If  $\zeta^{(N)} \ll 1$ , the Born approximation is applicable; if  $\zeta^{(N)} \ge 1$ , we can use the approximation of classical mechanics. Finally, the eikonal approximation is valid in the intermediate cases. We shall consider all these three approximations and we shall begin with the Born approach.

In the first Born approximation the scattering cross section is governed by the square of the modulus of a matrix element of the energy of the interaction between a particle and an external field, which is proportional to the Fourier component of the interaction energy  $U_q$ . Since we are interested in high energies and small scattering angles, we can ignore the spinor structure of the matrix element. The differential scattering cross section is then given by [14, 44]

$$\mathrm{d}\sigma = \frac{\varepsilon^2}{4\pi^2} \left| U_q \right|^2 \,\mathrm{d}o \;, \tag{2.2}$$

where do is an element of the solid angle in the direction of the scattering;  $\varepsilon$  is the energy of the particle; q = p - p' is the momentum transferred to the external field; p and p'are the momenta of the particle before and after the scattering.

In the scattering by a row of atoms the energy of the interaction of a particle with the row  $U(\mathbf{r})$  is the sum of all the energies of the interactions with the individual atoms  $u(\mathbf{r} - \mathbf{r}_n)$ :

$$U(\mathbf{r}) = \sum_{n=1}^{N} u(\mathbf{r} - \mathbf{r}_n) , \qquad (2.3)$$

where  $\mathbf{r}_n$  is the coordinate of the position of an atom in a row. Here,  $\mathbf{r}_n = \mathbf{r}_n^0 + \mathbf{u}_n$ ,  $\mathbf{r}_n^0$  is the coordinate of an equilibrium position of an atom in the row [it is assumed that the atoms are distributed along the z axis and are separated by equal distances d from one another (see Fig. 1)], and  $\mathbf{u}_n$  is the thermal displacement of each atom. The square of the modulus of the Fourier component of the potential described by expression (2.3) is

$$|U_q|^2 = \sum_{n,m=1}^N \exp\left[i\boldsymbol{q}\cdot(\boldsymbol{r}_n - \boldsymbol{r}_m)\right] |u_q|^2 . \qquad (2.4)$$

If we average the above expression over the thermal vibrations of atoms (by a procedure described, for example, in Refs [9, 12]) and if we bear in mind that at high values of N, we have

$$\left|\sum_{n=1}^{N} \exp(\mathrm{i}q_z dn)\right|^2 = N \frac{2\pi}{d} \sum_{g_z} \delta(q_z - g_z) ,$$

we find that

$$\langle |U_q|^2 \rangle = N \left\{ \frac{2\pi}{d} \sum_{g_z} \delta\left(q_z - g_z\right) \exp\left(-\boldsymbol{q}^2 \overline{\boldsymbol{u}^2}\right) + \left[1 - \exp\left(-\boldsymbol{q}^2 \overline{\boldsymbol{u}^2}\right)\right] \right\} |u_q|^2 , \qquad (2.5)$$

where  $\overline{u^2}$  is the mean square of the thermal displacement of an atom in a row;  $\delta(q_z)$  is the delta function;  $g_z = 2\pi n_z/d$  is a component of the reciprocal lattice vector  $(n_z = 0, \pm 1, \pm 2, \ldots)$ . The scattering cross section described by expression (2.2) can then be represented in the form

$$d\sigma = d\sigma_{\rm coh} + d\sigma_{\rm n} , \qquad (2.6)$$

where  $d\sigma_{coh}$  and  $d\sigma_n$  are the coherent and noncoherent scattering cross sections:

$$d\sigma_{\rm coh} = N \, \frac{2\pi}{d} \sum_{g_z} \delta\left(q_z - g_z\right) \exp\left(-\boldsymbol{q}^2 \overline{\boldsymbol{u}^2}\right) d\sigma_1(q) \,, \quad (2.7)$$

$$\mathrm{d}\sigma_{\mathrm{n}} = N \left[ 1 - \exp(-\boldsymbol{q}^2 \overline{\boldsymbol{u}^2}) \right] \mathrm{d}\sigma_1(\boldsymbol{q}) \;. \tag{2.8}$$

Here,  $d\sigma_1(q)$  is the scattering cross section of a particle in the field of a single atom in the row. When the potential of a single atom is the screened Coulomb potential

$$u(r) = (Ze |e|r^{-1}) \exp\left(-\frac{r}{R}\right), \qquad (2.9)$$

the cross section  $d\sigma_1$  is

$$d\sigma_1 = \frac{4Z^2 e^4 \varepsilon^2}{(q^2 + R^{-2})^2} \, do \,. \tag{2.10}$$

The quantity  $d\sigma_n$  is independent of the orientation of the row relative to the momentum of the incident particle and it represents noncoherent scattering, which differs only by the factor  $[1 - \exp(-q^2 u^2)]$  from the corresponding cross section for an amorphous medium. The coherent scattering cross section  $d\sigma_{\rm coh}$  depends strongly on the orientation of the atomic row relative to the momentum of the incident particle. We shall now consider in greater detail this term.

It follows from the laws of conservation of energy and momentum during scattering,  $\varepsilon = \varepsilon'$  and  $\mathbf{p} = \mathbf{p}' + \mathbf{q}$ , that  $2pq_{\parallel} = \mathbf{q}^2$ , where  $q_{\parallel}$  is the component of  $\mathbf{q}$  parallel to p. For small angles of incidence of a particle on the row ( $\psi \ll 1$ ), this relationship becomes

$$2p(q_z + \psi q_x) \approx q_z^2 + q_x^2 + q_y^2 , \qquad (2.11)$$

where the x axis is directed along the projection of the momentum p of the incident particle onto the (x, y) plane orthogonal to the row axis z. Formula (2.11) gives in fact the relationship between the components of the vector q. For small scattering angles, we have

$$q_z \approx -\psi q_x + \frac{q_y^2}{2p} \,. \tag{2.11a}$$

If we bear in mind that in the case of small scattering angles the cross section is  $do \approx dq_x dq_y p^{-2}$ , we find that

$$d\sigma_{\rm coh} = N \sum_{n} \delta \left( \psi q_x - \frac{q_y^2}{2p} - \frac{2\pi}{d} n \right)$$
$$\times \frac{dq_x \, dq_y}{2\pi dp^2} \, \varepsilon^2 |u_q|^2 \exp\left(-q^2 \overline{u^2}\right) \,. \tag{2.12}$$

The main contribution to this cross section comes from the term with n = 0. In fact, when n = 0, then  $q_x \approx q_y^2/2p\psi$ , whereas for n = 1, we have  $q_x \approx 2\pi/d\psi \gg q_y^2/2p\psi$ . Since  $u_q$  and  $\exp(-q^2u^2)$  decrease rapidly with increase in q, the contribution of the terms with  $n \neq 0$  to the scattering cross section is small. Consequently, after integration with respect to  $q_x$ , we find that

$$\mathrm{d}\sigma_{\mathrm{coh}} = N \, \frac{\mathrm{d}q_y}{2\pi \,\mathrm{d}\psi} \frac{\varepsilon^2}{p^2} \, |u_q|^2 \exp\left(-q^2 \overline{u^2}\right), \ q_x \approx \frac{q_y^2}{2p\psi} \,. \ (2.13)$$

The above cross section increases rapidly on reduction in  $\psi$ . This is due to the coherent mechanism of the scattering of a particle on  $N_c \propto R/\psi d$  atoms in a row. We can demonstrate this by noting that the cross section described by formula (2.13) can be represented as follows:

$$d\sigma_{\rm coh} \propto NN_{\rm c} \, d\sigma_1 \propto M_{\rm c} N_{\rm c}^2 \, d\sigma_1 \,, \qquad (2.14)$$

where  $d\sigma_1$  is the scattering cross section for one atom, integrated over  $q_x$ , at  $M_c \propto N/N_c$ .

We can see that the cross section  $d\sigma_{coh}$  is proportional to  $N_{\rm c}^2$ , i.e. it is proportional to the square of the number of atoms in the row with which the particle interacts effectively as it crosses the row [14]. This is due to the coherent nature of the scattering of particles by a row. It is worth noting that formula (2.14) does not contain the total number N of atoms in the row but only the square of  $N_c$ , i.e. the coherent scattering does not involve all the N atoms in the row, but only some of the atoms  $N_{\rm c}$ , which is defined by the angle of incidence of a particle on the row:  $N_c \propto R/\psi d$ . In other words, the coherent scattering process does not apply to all the row atoms, but only to some of them,  $N_c$  ( $N_c \ll N$ ). The number  $N_c$  increases on reduction in the angle  $\psi$ . However, the angle  $\psi$  cannot be regarded as zero, because then the Born approximation becomes meaningless (this is discussed below).

Formula (2.14) includes also the number  $M_c$ , which is proportional to the ratio of the total number N of atoms in the row to  $N_c$ . The occurrence of this factor can be interpreted as follows. If the whole atomic row is divided into  $M_c$  blocks and each of these blocks contains  $N_c$  atoms, then separate blocks do not interfere with one another during scattering, i.e. they do not result in coherent scattering, and, consequently, the scattering cross section should be proportional to the number  $M_c$  of such blocks (and not to the square of this number!).

We shall now consider the conditions of validity of the adopted Born approximation. The Born approximation can be used to describe the scattering by a single atom if  $Ze^2/\hbar c \ll 1$  [44]. Here, Z is the charge of the scattering centre (in units of |e|). If the scattering is coherent and it involves a complex system of, for example,  $N_c$  atoms in a row, the charge of the scattering centre is  $N_cZ$ . Therefore, the coherent scattering can be described by the Born approximation if  $N_cZe^2/\hbar c \ll 1$ . The quantity  $\zeta^{(N)} = N_cZe^2/\hbar c$  is the parameter mentioned above.

Finally we shall discuss the circumstances in which the main contribution to the cross section of the small-angle scattering by a row of atoms comes from the Fourier components of the potential energy characterised by  $g_z = 0$ . This means that the inhomogeneity of the potential along the row axis is unimportant and that the scattering is governed primarily by the continuum potential of the row, i.e. the row potential averaged over the coordinate z:

$$U_R(x, y) = \frac{1}{Nd} \int_{-\infty}^{\infty} dz \sum_{n=1}^{N} u(\mathbf{r} - \mathbf{r}_n) . \qquad (2.15)$$

If we substitute this potential in expression (2.2), we obtain the coherent scattering cross section described by formula (2.13).

The concept of the continuum potential was first introduced by Lindhard in the description of the channelling of fast particles in a crystal [19]. A channelling particle moves in one of the channels formed by rows of atoms in a crystal or by crystallographic planes of atoms, and is deflected periodically by small angles relative to the channel axis. Such particle motion in a crystal is possible if the angle  $\psi$  between the momentum of a particle and the channel axis does not exceed a certain specific angle  $\psi_c = \sqrt{4Z} \frac{e^2}{ed}$ , known as the critical angle for axial channelling.

The concept of the continuum potential can be used also in studies of the scattering of particles by a row of atoms when the angle  $\psi$  is small so that the condition of validity of the Born approximation  $RZe^2/\psi d\hbar c \ll 1$  is satisfied. This condition differs from the channelling condition  $\psi \lesssim \psi_c$ .

It is worth noting that the channelling angle appears in a natural manner in higher orders of perturbation theory when studies are made of the scattering of fast charged particles by a row of atoms in a crystal. In particular, this angle occurs in the expression for the scattering cross section obtained in the second Born approximation, which should make only a small contribution compared with the scattering cross section derived in the first Born approximation.

In fact, if the second Born approximation is used, the scattering cross section of a fast particle incident on a row of atoms in a crystal is [45]:

$$d\sigma = N \frac{8\pi Z^2 e^4 dq_y}{\psi d(q_y^2 + R^{-2})^2} \left[ 1 + \frac{e}{|e|} \frac{\psi_c^2}{\psi^2} \eta(Rq_y) \right], \qquad (2.16)$$

where the dimensionless coefficient  $\eta$  depends on the transferred momentum  $q_y$ :  $\eta \sim 1$ , if  $Rq_y \sim 1$ , and  $\eta \approx 2 \ln(Rq_y)$  if  $Rq_y \gg 1$ . Expression (2.16) is derived on the assumption that the potential of a single atom in a row is the screened Coulomb potential.

We can see that the relative contribution of the second Born approximation depends on the ratio  $(\psi_c/\psi)^2$ . This contribution is small if  $\psi^2 \ge \psi_c^2$ . The latter condition should be added to the condition  $\zeta^{(N)} \ll 1$  considered above. The inequality  $\psi^2 \ge \psi_c^2$  is satisfied automatically at high values of the particle energy, so that at high energies the validity of the Born approximation is governed by the condition  $\zeta^{(N)} \ll 1$ , which is independent of the particle energy. The last inequality means physically that the amplitude of the incident wave. Although the second Born approximation leads to small effects at high energies, it can nevertheless play an important role if we are interested in the dependence of the scattering cross section on the sign of the particle charge. This dependence is not predicted by the first Born approximation, and in the second approximation the particles with opposite signs of the charge are scattered differently.

### 2.2 Scattering in classical mechanics

It is demonstrated above that the scattering of fast charged particles by a row of atoms in a crystal can be described on the basis of the Born approximation if the parameter  $\zeta^{(N)} = N_c Z e^2 / \hbar c$  is small compared with unity. If this parameter is of the order of or greater than unity, we cannot use quantum mechanical perturbation theory. The scattering problem should then be solved rigorously in terms of quantum mechanics. If the parameter  $\zeta^{(N)}$  is large compared with unity, the situation corresponds formally to the limit  $\hbar \to 0$  (the large value of the parameter  $\zeta^{(N)}$  is due to the smallness of the angle  $\psi$  between the momentum of a particle and the axis of a row). This limit means going over from quantum to classical mechanics, so it is natural to consider the scattering for  $\zeta^{(N)} \ge 1$  on the basis of the classical theory of scattering. If the parameter  $\zeta^{(N)}$  is compared with unity, i.e. if we are dealing with the intermediate case, the eikonal theory of scattering of fast particles can be used (see Section 2.3).

In classical electrodynamics the motion of a relativistic charged particle in an external field  $U(\mathbf{r})$  is described by equation [46]

$$\frac{\mathrm{d}\boldsymbol{p}}{\mathrm{d}t} = -\vec{\nabla}U(\boldsymbol{r}) \;, \tag{2.17}$$

where p(t) is the particle momentum defined by  $p = mv(1 - v^2/c^2)^{-1/2}$ , and  $v = p/\varepsilon$ .

In the scattering of a particle by a row of atoms the potential  $U(\mathbf{r})$  is understood to be the sum of the potential energies of the interaction of a particle with individual atoms in the row, described by expression (2.3). We are interested in the scattering when the energy  $\varepsilon$  of a particle is sufficiently high and the angle  $\psi$  between the momentum p and the row axis is sufficiently small. Under these conditions the change in the impact parameter between consecutive collisions of the particle with the row atoms is small compared with the impact parameter b itself. For this reason the particle motion in the field of a row of atoms occurs as if in an effective continuum potential described by expression (2.15) and representing a row of atoms averaged over the coordinate z parallel to the row axis. Therefore, the effective potential  $U_R(x, y)$  is a function of just two coordinates, x and y, which are both perpendicular to the row axis. In the simplest case we can regard  $U_R(x, y)$  as having cylindrical symmetry along the z axis. We are then dealing with the problem of the motion of a particle in a field with cylindrical symmetry (Fig. 2). Obviously, in a field of this kind the component  $p_z$  of the particle momentum is conserved along the row axis:  $p_z = \text{const.}$  The motion in a transverse plane is then described, in accordance with Eqn (2.17), by the following equation:

$$\ddot{\boldsymbol{\rho}} = -\frac{1}{\varepsilon_{\parallel}} \frac{\partial}{\partial \boldsymbol{\rho}} U_R(x, y) , \qquad (2.18)$$

where  $\boldsymbol{\rho} = (x, y)$ ,  $\boldsymbol{\rho}$  is the distance between the particle and the row axis;  $\boldsymbol{\varepsilon}_{\parallel} = (p_z^2 + m^2)^{1/2}$ ;  $\boldsymbol{\varepsilon}_{\parallel} \approx \boldsymbol{\varepsilon}$ .



Figure 2. Scattering of a fast particle in the field of the continuum potential of a single row of atoms.

Since the function  $U_R(\rho)$  has cylindrical symmetry, Eqn (2.18) has two integrals of motion which are the energy of transverse motion

$$\boldsymbol{\varepsilon}_{\perp} = \frac{1}{2} \, \boldsymbol{\varepsilon} \boldsymbol{\dot{\rho}}^2 + U_R(\boldsymbol{\rho}) \tag{2.19}$$

and the angular momentum

$$M = \varepsilon \rho^2 \dot{\varphi}(t) , \qquad (2.20)$$

where  $\varphi(t)$  is the azimuthal scattering angle in a transverse plane (Fig. 2). At large distances from a row of atoms, where  $U_R = 0$ , the integral of the energy of transverse motion is  $\varepsilon_{\perp} = \frac{1}{2} \varepsilon \psi^2$ .

These integrals of motion can be used to find the azimuthal angle  $\varphi(b)$  of the scattering of a particle by a row as a function of the impact parameter of the row [14]:

$$\varphi(b) = \pi - 2b \int_{\rho_0}^{\infty} \frac{\mathrm{d}\rho}{\rho^2} \left[ 1 - \frac{U_R(\rho)}{\varepsilon_\perp} - \frac{b^2}{\rho^2} \right]^{-1/2}, \qquad (2.21)$$

where  $\rho_0$  is the distance of closest approach of the particle to the axis of the atomic row. Expression (2.21) is derived using the relationship  $M = p\psi b$  between the angular momentum M and the impact parameter of the row. The quantity  $p\psi$  occurring in this relationship is the projection of the momentum of the incident particle onto the (x, y) plane.

The total angle of the scattering of a particle by a row is

$$\theta(b) = 2\psi \sin\left[\frac{1}{2}\,\varphi(b)\right] \,. \tag{2.22}$$

In the classical theory of scattering the function  $\varphi(b)$  is called the function of particle deflection in an external field.

The differential cross section of the scattering of a particle by a row of atoms is

$$\mathrm{d}\sigma = L\psi\,\mathrm{d}b\;,\tag{2.23}$$

where  $L\psi$  is the projection of the row length onto a plane orthogonal to the momentum of the incident particle and b is the impact parameter of the row representing the shortest distance between the particle and the row axis in the absence of scattering (Fig. 2). According to expression (2.21), the quantity db can be expressed in terms of the azimuthal scattering angle and, therefore, we have

$$\mathrm{d}\sigma = L\psi \sum_{n} \frac{\mathrm{d}\varphi}{|\mathrm{d}\varphi(b)/\mathrm{d}b|_{n}} \,. \tag{2.24}$$

This expression is obtained bearing in mind that the function  $b(\varphi)$ , which is the inverse of the deflection function  $\varphi = \varphi(b)$ , is generally a multivalued dependence on the scattering angle [14, 47, 48]. The summation over *n* in expression (2.24) corresponds to the summation over single-valued branches of the deflection function  $\varphi(b)$ .

These expressions demonstrate that the scattering of a fast charged particle in the field of the continuum potential of a row of atoms in a crystal is possible only along an azimuthal angle  $\varphi$  in a plane orthogonal to the row axis.

The quantity  $U_R/\varepsilon_{\perp}$  occurring in expression (2.21) is of the order of magnitude of the ratio of the square of the critical axial channelling angle to the square of the angle of incidence of the particle on the row:  $U_R/\varepsilon_{\perp} \approx (\psi_c/\psi)^2$ . According to expression (2.21), small values of this parameter correspond to small values of the azimuthal scattering angle:

$$\varphi(b) \approx -\frac{1}{2\varepsilon_{\perp}} \frac{\mathrm{d}}{\mathrm{d}b} \int_{-\infty}^{\infty} \mathrm{d}x \ U_R\left[ \left( x^2 + b^2 \right)^{1/2} \right] \,. \tag{2.25}$$

The path of a particle in the field of a row of atoms is nearly rectilinear. This corresponds to the motion under conditions far from those which apply in the case of axial channelling.

If  $\psi \ge \psi_c$ , it follows from expression (2.25) that the quantity  $|\varphi(b)|$  is independent of the sign of the particle charge and that it increases rapidly on reduction in  $\psi$ . If in the deflection function described by expression (2.21) we include the next term of the expansion in terms of the parameter  $U_R/\varepsilon_{\perp}$ , we obtain the dependence of  $|\varphi(b)|$  on the sign of the particle charge. Therefore, a reduction in  $\psi$  rapidly enhances the dependence of the deflection function on the sign of the particle charge.

Expression (2.21) is valid not only when  $\psi \gg \psi_c$ , but also when  $\psi \leq \psi_c$ . In the latter case we cannot expand in terms of the parameter  $U_R/\varepsilon_{\perp}$  and numerical integration of relationship (2.21) is needed in order to determine the deflection function and the scattering cross section. The deflection functions and the scattering cross sections are given in Ref. [14] for some continuum potentials of a row of atoms. Therefore, we shall not consider these results in detail. We shall simply mention that if  $\psi \leq \psi_c$ , the deflection functions and the scattering cross sections of particles scattered by a row of atoms differ very greatly for opposite charges of the particles and that typical forms of the functions  $U_R(\rho)$  are such that in a field of this kind the particle deflection function is a double-valued function of the impact parameter. In other words, the rainbow scattering of particles is then possible [49, 50].

### 2.3 Scattering in the eikonal approximation

Let us consider the scattering of high-energy charged particles on a row of atoms in a crystal in the intermediate case when the relevant parameter is  $\zeta^{(N)} \sim 1$ . Let us discuss the transition from the Born to the classical mechanics approximation. In the case of high energies of interest to us such a transition can be investigated on the basis of the quantum-mechanical semiclassical approximation, analo-

gous to the geometric optics approximation which is valid if the wavelength is short and the changes of the wavelength in a distance equal to the wavelength are small. We shall be interested in small-angle scattering  $(\theta \ll \psi)$  and if  $\psi \gg \psi_c$ , we can then expand the scattering amplitude in terms of reciprocal powers of the particle energy. Such motion corresponds to a path close to rectilinear. We thus find that the eikonal approximation is appropriate and in this approximation the scattering amplitude is [14, 48]

$$a(\boldsymbol{q}) = -\frac{\mathrm{i}\rho}{2\pi\hbar} \int \mathrm{d}^2\rho \exp\left(\frac{\mathrm{i}}{\hbar} \,\boldsymbol{q} \cdot \boldsymbol{\rho}\right) \left\{ \exp\left[\frac{\mathrm{i}}{\hbar} \,\chi(\boldsymbol{\rho})\right] - 1 \right\} \quad (2.26)$$

and the scattering cross section is

$$\mathrm{d}\boldsymbol{\sigma} = |\boldsymbol{a}(\boldsymbol{q})|^2 \,\mathrm{d}\boldsymbol{o} \;, \tag{2.27}$$

where do is an element of the solid angle in the scattering direction,  $\rho$  is the radius vector in a plane orthogonal to the momentum p of the incident particle, and

$$\chi(\boldsymbol{\rho}) = -\frac{1}{\nu} \int_{-\infty}^{\infty} \mathrm{d}l \, U(\boldsymbol{r}) \; . \tag{2.28}$$

Integration of Eqn (2.28) with respect to l is carried out along a path traversed by the particle in a field  $U(\mathbf{r})$ ;  $v = p/\varepsilon$ .

Formula (2.26) is valid if the motion of a particle in an external field is nearly rectilinear. We then find that formulas (2.26) and (2.27) allow us to go over, in the limit, to the range of validity of both the Born approximation  $(|\chi| \leq \hbar)$ , and of the classical scattering theory  $(|\chi| \geq \hbar)$ . These formulas can therefore be regarded as intermediate between those for the scattering cross sections in the Born approximation and the classical scattering theory.

We can see that in the Born approximation and in the treatment based on classical mechanics the scattering of a fast charged particle in the field of a row of atoms in a crystal is governed mainly, for low angles of incidence  $\psi$  on a row, by the continuum potential of the row described by expression (2.15). We can use the same expression for the potential in the intermediate case under discussion here and calculate the quantity  $\chi$  which occurs in formula (2.26):

$$\chi = \chi(y) = -\frac{1}{\psi v} \int_{-\infty}^{\infty} \mathrm{d}x \ U_R(x, y) \ . \tag{2.29}$$

Integration with respect to l in Eqn (2.28) is now replaced with integration with respect to x:  $dl = dx/\psi$ . Bearing in mind that  $\chi(y)$  is a function of the coordinate y alone, we find that

$$a(\boldsymbol{q}) = -\mathrm{i}p\delta(q_x) \int_{-\infty}^{\infty} \mathrm{d}y \exp\left(\frac{\mathrm{i}}{\hbar} q_y y\right) \left\{ \exp\left[\frac{\mathrm{i}}{\hbar} \chi(y)\right] - 1 \right\}. (2.30)$$

Substitution of the scattering amplitude given by formula (2.3) into expression (2.27) describing the scattering cross section and elimination of the delta function  $\delta(q_x)$  gives

$$d\sigma = \frac{L\psi}{2\pi\hbar} dq_y \left| \int_{-\infty}^{\infty} dy \exp\left(\frac{iq_y y}{\hbar}\right) \left\{ \exp\left[\frac{i}{\hbar} \chi(y)\right] - 1 \right\} \right|^2.$$
(2.31)

The above expression is obtained bearing in mind that  $\delta^2(q_x) = (L\psi/2\pi\hbar)\,\delta(q_x).$ 

The function  $\chi/\hbar$  occurring in expression (2.31) is of the order of  $RZ e^2/\psi d\hbar c \approx \zeta^{(N)}$ . We have encountered this quantity in discussing the range of validity of the Born approximation and of the classical scattering theory. In the former case this quantity is small compared with unity, but in the latter case it is larger than unity. We can now see that it occurs in fact in the scattering amplitude obtained in the eikonal approximation and it can then be small or large compared with unity. It therefore follows that formula (2.31) is suitable for the description of the scattering both in the Born approximation and in the classical theory.

If  $|\chi| \ll \hbar$ , formula (2.31) reduces to formula (2.13) for the scattering cross section in the Born approximation.

If  $|\chi| \ge \hbar$ , then the integral with respect to y, which occurs in formula (2.31), can be calculated by the stationary phase method. The stationary phase points (there may be several of them) are given by the relationship [36]

$$q_y = -\frac{\mathrm{d}}{\mathrm{d}y} \,\chi(y) \;. \tag{2.32}$$

We then have

$$\int_{-\infty}^{\infty} dy \exp\left(\frac{i}{\hbar} q_{y}y\right) \left\{ \exp\left[\frac{i}{\hbar} \chi(y)\right] - 1 \right\}$$
$$\approx \sum_{n} \sqrt{\frac{2i\pi\hbar}{d^{2}\chi/dy_{n}^{2}}} \exp\left(\frac{i}{\hbar} F_{n}\right),$$

where  $F_n = q_y y_n + \chi(y_n)$  and the summation is carried out over different stationary phase points  $y_n$ . The scattering cross section is then described by the following formula:

$$d\sigma = L\psi \, dq_y \left| \sum_n \left( \frac{d^2 \chi}{dy_n^2} \right)^{-1/2} \, \exp\left( \frac{i}{\hbar} \, F_n \right) \right|^2 \,. \tag{2.33}$$

If the interference between the terms corresponding to different stationary phase points is ignored in the above formula, the result is given by expression (2.24), which is obtained in the classical scattering theory. [In this case we should take account of formula (2.32) and of the fact that for small scattering angles we have  $\theta \approx \psi \varphi$  and  $q_y \approx p \psi \varphi$ .] It should be stressed that the parameter  $\zeta^{(N)}$ , which

It should be stressed that the parameter  $\zeta^{(N)}$ , which occurs in formula (2.31), increases rapidly on reduction in  $\psi$  and for  $\zeta^{(N)} \ge 1$  the scattering of a particle on a row of atoms becomes classical. This parameter is  $\zeta^{(N)} \sim 1$  when  $\psi \sim RZ \ e^2/d\hbar c$ . At high energies the latter angle is considerably higher than the critical angle for axial channelling  $\psi_c = (4Z \ e^2/\epsilon d)^{1/2}$ , i.e. the scattering becomes classical well before the onset of channelling.

## **2.4** Motion of a charged particle in a field created by an ensemble of atomic rows in a crystal

We have considered the motion of a charged particle in the field of a row of atoms and we have shown that this motion is governed primarily by the continuum potential of the chain, described by expression (2.15), which represents the potential averaged over the coordinate z along the row axis. We shall now consider the motion of a particle in the field of an ensemble of rows of atoms in a crystal, described by the potential

$$U(x,y) = \sum_{n} U_{R}(\boldsymbol{\rho} - \boldsymbol{\rho}_{n}) , \qquad (2.34)$$

where  $U_R(\rho)$  is the potential energy of the interaction of a particle with the continuum potential of a single row of atoms and  $\rho_n$  is the radius vector of the row in a plane orthogonal to the z axis.

As in the case of motion in the field of the continuum potential of a single row of atoms, the component of the particle momentum, parallel to the crystallographic z axis near which motion takes place, is conserved in the field given by expression (2.34). The motion in a plane transverse to the z axis is then described by

$$\ddot{\boldsymbol{\rho}} = -\frac{1}{\varepsilon} \frac{\partial}{\partial \boldsymbol{\rho}} U(x, y) . \qquad (2.35)$$

In general, the continuum potentials of the rows of atoms in a crystal overlap so that the motion occurs in a very complex periodic field of a row of atoms. Nevertheless,



**Figure 3.** Equipotential surfaces of the continuum potential energy U(x, y) representing the interaction of a positive particle with rows of atoms in a silicon crystal in a plane orthogonal to the  $\langle 111 \rangle$  axis, calculated at room temperature of the crystal. The numbers alongside the curves represent the potential energy in electron volts. The dashed curves correspond to zero curvature of the potential-energy surface described by expression (3.11).



Figure 4. Same as in Fig. 3, but for the  $\langle 110 \rangle$  crystallographic axis.

the main features of the motion in such a field can be analysed with the help of the integral of the energy of transverse motion

$$\boldsymbol{\varepsilon}_{\perp} = \frac{1}{2} \, \boldsymbol{\varepsilon} \boldsymbol{\dot{\rho}}^2 + U(x, \, y) \; . \tag{2.36}$$

Figs 3 and 4 show typical equipotential surfaces of the continuous potential energy U(x, y) for the positively charged particles moving in a silicon crystal near the  $\langle 111 \rangle$  and  $\langle 110 \rangle$  crystallographic axes. The equipotentials for negatively charged particles have the negative sign.

These equipotentials show that the function U(x, y) for positively charged particles has maxima at the points corresponding to the positions of atomic rows in a transverse plane and that the potential wells in the regions between the rows are shallow. The motion in such a field, considered as a function of the transverse motion energy  $\varepsilon_{\perp}$ , may be both finite and infinite relative to the atomic rows. The motion is finite if  $\varepsilon_{\perp} < U_{\rm H}$ , where  $U_{\rm H}$  is the potential energy at a saddle point. The particles then move in channels (they become 'channelled') along helical paths with their axes parallel to the channel axis.

If  $\varepsilon_{\perp} > U_{\rm H}$ , the motion becomes infinite relative to the atomic rows. The particle then has a sufficient energy  $\varepsilon_{\perp}$  to pass above the existing potential barriers and, therefore, such particles can be called 'above-barrier'.

If  $\frac{1}{2} \varepsilon \psi_c^2 > \varepsilon_\perp > U_H$ , where  $\psi_c$  is the critical angle for axial channelling, it follows from expression (2.36) that a positively charged particle cannot approach very closely the nuclei of the lattice atoms. Therefore, the processes related to small impact parameters (nuclear reactions, large-angle scattering, etc.) are suppressed in the case of such a particle. The term 'channelled particle' was first introduced in Ref. [19] in order to identify a group of particles which cannot approach the atomic nuclei very closely. We shall use the term 'channelled particle' for the particles in finite motion and the term 'above-barrier particle' for the particles in above-barrier motion.

If  $\varepsilon_{\perp} \gtrsim U_{\rm H}$  there are small spatial regions between the rows where a particle that enters one channel can switch to another channel. In this motion between the atomic rows a positive particle may spend a long time in one of the channels (until it reaches a region of this kind near a saddle point). Therefore, such motion can be called 'quasifinite'. The probability of such motion decreases rapidly with increase in  $\varepsilon_{\perp}$ , because this increase is accompanied by a rapid expansion of the spatial region near a saddle point where a particle can go over to a neighbouring channel.

The finite motion of a negative particle is possible if  $|\varepsilon_{\perp}| \lesssim 1/2\varepsilon \psi_c^2$ , i.e. if the particle is incident on a row of atoms at an angle  $\psi \lesssim \psi_c$ . We can then have situations in which a particle moves in a channel formed by one of the atomic rows or by several such rows.

The finite motion of particles in a crystal occurs not only for  $\psi \leq \psi_c$ , but also for  $\psi \geq \psi_c$ . In fact, there are open planar channels formed by atomic rows and a particle inside such a channel oscillates between the rows. This is known as planar channelling. Such motion occurs only for small values of the angle  $\theta$  between the component of the particle momentum orthogonal to the row axis z and the planar channel axis; moreover, the condition  $\psi \geq \psi_c$  has to be satisfied.

It therefore follows that the nature of motion in the field of atomic rows in a crystal depends strongly on the energy of transverse motion, the sign of the particle charge, the orientation of the particle momentum in a plane orthogonal to the row axis, and the nature of the distributions of the rows of atoms in this plane. The motion can be finite or infinite relative to a row of atoms.

We can solve Eqn (2.35) if we know not only the integral of the energy of transverse motion, but also one more integral of motion. For the scattering by a single row of atoms this integral of motion is the angular momentum. However, in the case under discussion, the second integral of motion exists only in a few cases, and these cases include both finite and infinite motion of a particle in a plane transverse to the z axis [28–31]. If the second integral exists, the variables in Eqn (2.35) can be separated and the motion is quasiperiodic. However, if the second integral does not exist, there are no periodically repeated sections of the path and the motion as chaotic.

It follows that the problem of motion of a charged particle in a two-dimensional periodic field of atomic rows is a typical problem in the theory of nonlinear systems which deals with the regular and chaotic nature of motion and with the stability of motion. We shall now discuss these topics in detail.

## 3. Chaos in dynamic systems

#### 3.1 Motion in the Henon-Heiles potential

The motion of a particle in a relatively complex field can be not only regular, but also stochastic [51, 52]. This is related to the instability of the motion of a particle in such a field. The instability means that a small change in the initial conditions leads to an exponential divergence of the initially closely spaced paths. If we follow the motion of a particle for a sufficiently long time, it will then appear to be chaotic (random). This situation occurs even in the case when the particle is in finite motion in a field that depends on two coordinates. Let us consider, for example, the motion in what is known as the Henon-Heiles potential [53]

$$U_{\rm H-H} = \frac{1}{2} \left( x^2 + y^2 \right) + x^2 y - \frac{1}{3} y^3 .$$
 (3.1)

For simplicity, all the variables are assumed to be dimensionless.

We obtain the potential energy described by expression (3.1) if three identical like charges are located at the vertices of an equilateral triangle and we consider the motion in a plane formed by these charges near the centre of the triangle. Then, expanding the potentials created by the separate charges along the coordinates x and y relative to the centre of the triangle and retaining the terms up to the third order, we obtain the potential described by expression (3.1).

Fig. 5 shows the equipotential surfaces of the potential energy described by the above expression near its minimum value.

The motion of a particle in a field described by expression (3.1) conserves the particle energy

$$E = \frac{1}{2} \left( p_x^2 + p_y^2 \right) + U_{\text{H-H}}(x, y)$$
(3.2)

(the energy *E* and the components of the momentum  $p_x$  and  $p_y$  are assumed to be dimensionless). The particle is then in the finite motion if  $E < \frac{1}{6}$  [51].



Figure 5. Equipotential surfaces of the Henon-Heiles potential described by expression (3.1).

The path of a particle in the field described by expression (3.1) can not only have the energy integral, but also the second integral of motion. This is not possible in general, but only under certain conditions.

The second integral of motion exists at low energies when the cubic terms in the expansion of the potential can be ignored. Then, not only the energy, but also the angular momentum of motion  $M = \rho^2 \dot{\varphi}$  are conserved; here,  $\rho$  and  $\varphi$  are the polar coordinates of the particle path. The variables in the equation of motion can be separated and the particle path is described by

$$t = \pm \int \frac{\mathrm{d}\rho}{\sqrt{2[E - U(\rho)] - M^2 \rho^{-2}}} + \mathrm{const} ,$$
  
$$\varphi = M \int \mathrm{d}t \, \rho^{-2}(t) + \mathrm{const} , \qquad (3.3)$$

where  $U(\rho) = \frac{1}{2}(x^2 + y^2)$ .

The second integral of motion can exist also if the cubic terms of the expansion are included in the potential energy. If this integral of motion exists, then the motion is regular. If the second integral does not exist, the motion is chaotic [51, 52]. The nature of motion can be determined by the Poincare section method (see, for example, Refs [14, 51]), which can be described as follows.

Let us consider the path of a particle in the phase space  $(x, p_x, y, p_y)$ . It follows from the law of conservation of energy (3.2) that the path lies on a three-dimensional surface in this space. This surface is defined by  $E(x, p_x, y, p_y)$ . Let us consider the points of intersection of the path with a plane, for example, the  $(y, p_y)$  plane. In other words, let us assume that x = const in the relationship  $E(x, p_x, y, p_y) = \text{const}$ . Such points may lie on a curve or they may be distributed at random in a certain part of the plane  $(y, p_y)$ . If the points lie on a curve, there is a second integral of motion; otherwise there is no such integral. It follows that the existence of the second integral of motion is related to the positions of points along a certain curve. There is no criterion for finding the points on a certain curve and the existence of the curve can be determined only approximately by numerical integration of the equation of motion. Therefore, there is no general criterion of the existence of the second integral of motion.

The occurrence of chaotic motion allows us to use the methods of statistical physics in the description of the physical processes associated with such motion. Since we have seen that chaotic motion can appear even for two degrees of freedom, it follows that the methods of statistical physics can be used not only when there is a very large number of degrees of freedom, but also when there are relatively few of them. In the case under discussion, there are two degrees of freedom.

Fig. 6 gives the results of calculations of the Poincare sections and of the corresponding paths of the particles moving in the Henon-Heiles potential. The sections are plotted for various energies. At low energies E, when the motion occurs near the bottom of the potential well



Figure 6. Poincare sections and the corresponding paths of particles moving in the Henon-Heiles potential, described by expression (3.1), calculated for E = 1/20 (a) and E = 1/6 (b). Curves 1, 2, and 3 correspond to different initial conditions governing the path.

described by expression (3.1), the motion is regular for practically all the initial conditions. This is due to the fact that at low energies *E* a particle does not reach a region with a strong nonlinearity and, therefore, we are in fact dealing with the problem of motion in a centrally symmetric field.

It should be noted that there are several regions where the motion is stable in the sense that a small change in the initial conditions alters little the nature of the phase curves [51, 52]. Such regions are separated by certain lines and crossing of these lines modifies greatly the nature of motion: one stable regime changes to another.

An increase in the particle energy expands the regions in which the motion is unstable, so that these regions fill an ever-increasing part of the phase space in the Poincare sections, separating 'islands' in a section where the motion is stable. This means that, depending on the initial conditions, the nature of motion may differ greatly, i.e. it can be either regular and stable or irregular and chaotic.

When the energy reaches  $E \approx \frac{1}{6}$ , the motion will be chaotic for practically all the initial conditions.

It therefore follows that the motion of a particle in a two-dimensional field described by expression (3.1) can be both regular and chaotic.

#### 3.2 Stability of motion

In the simplest example of the motion of a particle in the Henon-Heiles potential we have seen that at low values of the energy the motion is stable. As the energy increases and a particle reaches a region where the forces are strongly nonlinear, the nature of the motion then depends on the initial conditions and can be regular or chaotic. At energies close to the top of the potential well the motion is unstable for practically all the initial conditions.

The growth of chaotic motion is due to local instability of motion in the sense that a small change in the intial conditions results in an exponentially rapid divergence of paths. Therefore, we shall consider in greater detail the stability of motion of a particle in an external field [31, 54]. With this in mind we shall discuss the rate of divergence of two initially close phase paths. Their motion is unstable if the paths diverge exponentially with time:

$$d(t) = d(0) \exp(\lambda t), \quad \operatorname{Re} \lambda > 0, \qquad (3.4)$$

where d(0) is the distance between two paths in the phase space at t = 0.

It is natural to relate the value of the parameter Re  $\lambda$  at the onset of an instability to the boundary of transition to chaotic motion. However, this condition of motion instability is only the necessary condition of transition to chaotic regime, but it is not sufficient because if Re  $\lambda > 0$ , a change from one stable motion to another can also take place. The necessary condition is very important and it is used widely in an analysis of the nature of motion in various systems.

We shall now discuss in greater detail this necessary criterion of stability [54]. We shall consider two initially close paths in the phase space  $-r_1(t)$ ,  $p_1(t)$  and  $r_2(t)$ ,  $p_2(t)$  — for two-dimensional motion; here,  $r_{1,2}$  and  $p_{1,2}$  are two-dimensional vectors representing the coordinates and the momenta of the particles. Let us introduce the variables

$$\boldsymbol{\xi} = \boldsymbol{r}_1 - \boldsymbol{r}_2, \quad \boldsymbol{\eta} = \boldsymbol{p}_1 - \boldsymbol{p}_2.$$

We then have  $\dot{\xi} = \eta$  (for simplicity, we shall assume—as in the preceding section—that the variables r and p are dimensionless). Then, linearisation of the equation of motion

$$\dot{\boldsymbol{j}} = -\nabla U(\boldsymbol{r}_1) + \nabla U(\boldsymbol{r}_2) , \qquad (3.5)$$

where  $\mathbf{r}_2 = \mathbf{r}_1 - \boldsymbol{\xi}$  on the assumption that  $\boldsymbol{\xi}$  is small, gives the following equations for  $\boldsymbol{\xi}$  and  $\boldsymbol{\eta}$ :

$$\dot{\boldsymbol{\xi}} = \boldsymbol{\eta}, \quad \dot{\boldsymbol{\eta}} = -\hat{\boldsymbol{S}} \boldsymbol{\xi} , \qquad (3.6)$$

where  $\hat{S}$  is a matrix deduced from the second derivatives of the potential along the path

$$S_{ij} = \frac{\partial^2 U}{\partial r_i \partial r_j} \Big|_{\boldsymbol{r} = \boldsymbol{r}_1(t)}$$

Eqns (3.6) can be written in the matrix form:

$$\begin{pmatrix} \dot{\boldsymbol{\xi}} \\ \dot{\boldsymbol{\eta}} \end{pmatrix} = \hat{\Gamma} \begin{pmatrix} \boldsymbol{\xi} \\ \boldsymbol{\eta} \end{pmatrix}, \quad \hat{\Gamma} = \begin{pmatrix} \hat{O} \ \hat{I} \\ -\hat{s} \ \hat{O} \end{pmatrix}, \quad (3.7)$$

where  $\hat{O}$  and  $\hat{I}$  are the zero and identity (unit) matrices of the second rank. Application of unitary transformation  $\hat{T}$  can reduce the matrix  $\hat{\Gamma}$  to the diagonal form:

$$\left(\hat{T}\hat{\Gamma}\hat{T}^{-1}\right)_{ij} = \lambda_i \delta_{ij} . \tag{3.8}$$

If at least one of the eigenvalues of the matrix  $\hat{\Gamma}$  has a positive-definite real part, the paths diverge exponentially and the motion is unstable.

Over short time intervals, the matrix  $\hat{s}$  occurring in expression (3.7) can be regarded as independent of time (however,  $\hat{s}$  depends on the coordinate  $r_1$ ). The eigenvalues of the matrix  $\hat{\Gamma}$  define a local, i.e. that corresponding to given values of the coordinates, stability of motion.

The condition for determination of the eigenvalues of the matrix is

$$\det\left(\hat{\Gamma}-\lambda\right)=0. \tag{3.9}$$

Hence, we find the eigenvalues  $\lambda$ :

$$\lambda_{1,2,3,4} = \pm \left[ -b \pm (b^2 - 4c)^{1/2} \right]^{1/2}, \qquad (3.10)$$

where

$$b = \frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2}, \quad c = \frac{\partial^2 U}{\partial x^2} \frac{\partial^2 U}{\partial y^2} - \left(\frac{\partial^2 U}{\partial x \partial y}\right)^2$$

If b > 0, then for c > 0 all the eigenvalues  $\lambda_i$  are imaginary quantities and, consequently, the motion should be stable. If c < 0, one of the roots  $\lambda_i$  is real and positive. The motion is then unstable since it results in exponentially rapid divergence of the paths.

The sign of the quantity c is identical with the sign of the Gaussian curvature K(x, y) of the surface U(x, y):

$$K(x, y) = c \left[ 1 + \left( \frac{\partial U}{\partial x} \right)^2 + \left( \frac{\partial U}{\partial y} \right)^2 \right]^{-1} .$$
 (3.11)

The curvature is a local concept so that the above stability criterion is local. Therefore, stable motion corresponds to a situation in which it occurs in a region with a positive curvature K(x, y) of the surface. However, if the particle path reaches a region with a negative curvature of the same surface, the motion is unstable.

In the case of the Henon-Heiles potential the line corresponding to zero curvature of the  $U_{H-H}(x, y)$  surface is a circle (Fig. 5). This line separates regions with a positive curvature, which are inside the circle, and those with a negative curvature, which are outside the circle. At low energies a particle travels near the minimum value of the potential energy, where the curvature is positive. In this case

the motion is stable and is of regular quasiperiodic nature. An increase in the energy means that the particle path may pass through a region with a negative value of the curvature of the function  $U_{\rm H-H}(x, y)$ . In these regions the stability of motion is lost, i.e. the initially closed paths begin to diverge at a rate which is an exponential function of time. The longer the time that a particle spends in a region with a negative curvature of the potential energy, the stronger is the divergence of the paths. Therefore, the criterion of a negative curvature of the potential energy can be used to find the energy of a particle at which the transition from regular to chaotic motion could take place.

# **3.3 Instability of motion in multiple scattering by three centres**

In the preceding sections we have considered the finite motion of a particle in a two-dimensional potential well and we have shown that it can be both regular and chaotic. In chaotic motion a small change in the initial conditions leads to an exponentially rapid divergence of paths, which corresponds to an instability of motion. This instability is essentially related to the two-dimensional nature of the potential in which such motion takes place. We shall show that an instability does not necessarily appear during motion in a potential well, but that it can occur also in the course of scattering. At least three centres must participate in such scattering. The simplest scattering arises as a result of elastic reflection. Therefore, in order to illustrate the above statement, we shall consider the simplest problem of the scattering of a particle by elastic reflection from three disks lying in the same plane [55]. For simplicity, we shall assume that the disks are identical and that their centres form an equilateral triangle. We shall also assume that the particle moves in one plane and, therefore, it can experience (in principle) any number of collisions with the disks, but it can also escape from the triangle.

In a collision with a single disk a particle is reflected from it at an angle which is equal to the angle of incidence [i.e. the angle between the momentum of the particle and the normal to the disk tangent at the point of incidence (Fig. 7)]. The scattering angle is related to the impact parameter b by

$$\varphi(b) = \pi - 2 \arcsin \frac{b}{R} \,, \tag{3.12}$$

where R is the disk radius.

If there is a second disk, the particle reflected from the first disk may bypass the second disk or be reflected by it. In principle, a situation may arise in which the particle is reflected an infinite number of times from the first and second disks, i.e. the particle oscillates between them. Such oscillatory motion is however unstable because a small change in the initial conditions causes the particle to leave the area after several oscillations between the disks.

The situation is more complex when there are three disks. We can then expect multiple reflections from three disks in which the particle remains all the time in the space between them. The number of such particle paths is, in contrast to the case of two disks, infinitely large and all such paths are unstable. An example of a path of this kind is shown in Fig. 8.

The time that a particle spends in the space between three disks depends strongly on the initial conditions governing the particle path. We shall determine this time for the case when the particle is incident on the disks



Figure 7. Motion of a particle in the field of three disks located on a plane.



Figure 8. Multiple scattering of a particle by disks.

perpendicular to the line that joins the centres of disks I and 3 (Fig. 8). The delay time is defined as a function of the quantity  $y_0$ . The delay time  $\tau(y_0)$  is understood to be the time spent by the particle in the space defined by the circle which touches all three disks. The particle path is then a complex function of time and of the initial conditions. Therefore, a numerical method has to be used to find the delay time  $\tau(y_0)$ .

Fig. 9 gives the calculated dependences of  $\tau(y_0)$  on the impact parameter  $y_0$ . The ordinate gives the quantity  $F = \log[\tau(y_0)/T]$  and the abscissa represents  $y_0$ . Here,



Figure 9. Dependence of the time spent by a particle in the space between disks on the impact parameter  $y_0$ .

T = R/v (the disk radius R and the velocity v are assumed to be dimensionless, so that R = 1 and v = 1) and  $y_0$  is measured from the midpoint between the two disks. The graphs show that there is a range of values of  $y_0$  where the function  $\tau(y_0)$  changes very rapidly with  $y_0$ . At some values of  $y_0$  the delay time  $\tau(y_0)$  can be very long. In other words, for such values of  $y_0$  the particle can spend a long time in the region between the disks.

The question now is the finer structure of the functional dependence of the delay time on the impact parameter in the regions where  $\tau(y_0)$  changes rapidly. Calculations were therefore carried out in which the step of  $y_0$  was reduced. Stretching of the graph along the  $y_0$  axis revealed that the pattern obtained on an enlarged scale did not differ from the initial one (this can be judged by going over from Fig. 9a to Fig. 9b). This property of the function  $\tau(y_0)$ , i.e. the constancy of the pattern, is retained also after the next change in the scale of  $y_0$  (Fig. 9c). This behaviour of the function  $\tau(y_0)$  is called fractal [56]. The fractality means here that a change in the scale of  $y_0$  produces practically the same pattern of the scattering of a particle by three disks.

The problem of such scattering by three disks is discussed in detail in Refs [55, 57]. Some mathematical problems are also considered there and they include the stability of motion, entropy, the Hausdorff dimension, etc. This problem is also of considerable interest because it can be treated quantum-mechanically (see, for example, Refs [57-59]).

A similar problem for some other potentials that vary smoothly in space is considered in Refs [60-62].

Three disks can be regarded as an initial element from which a planar periodic structure can be built up. Such a periodic structure is analogous to the structure of atomic rows in a crystal. The scattering of a particle by a periodic structure consisting of three disks is in many respects similar to the scattering on the periodic field of atomic rows in a crystal. Therefore, a two-dimensional periodic structure of three disks is a good model for the investigation of the nature of motion of a charged particle in a crystal.

# 4. Regular and chaotic motion of fast charged particles in crystals

### 4.1 Channelling of positive particles

We have considered the motion of fast charged particles in a crystal at a small angle  $\psi$  to one of the crystallographic axes and we have shown that at high energies such motion is governed primarily by the continuum potential of atomic rows in a crystal described by expression (2.34). If  $\psi \leq \psi_c$ , the motion of a particle in such a field can be finite or infinite relative to the atomic rows. The potential in which such motion occurs is a complex nonlinear function of two coordinates. Therefore, the description of motion of a particle in a crystal reduces in fact to the problem of motion in a two-dimensional periodic nonlinear field. The motion of a particle in such a field (Section 3) may be both regular or chaotic. A similar situation occurs also when a charged particle is moving in a crystal. We shall consider the possibility of realisation of a particular type of motion of a particle in a crystal in the case of channelling and above-barrier mechanisms. We shall begin with the motion of a positive high-energy particle in a crystal.

The continuum potential in which a particle moves inside a crystal depends strongly on the crystallographic axis along which such motion is directed (Section 2.4). If a particle travels in a silicon crystal along the  $\langle 111 \rangle$  axis, the equipotential surfaces of the continuum potential of atomic rows are of the kind shown in Fig. 3. This potential forms a well at large distances from the rows and the shape of the well resembles the Henon-Heiles potential. In fact, at large distances from the row the potential can be expanded as a Taylor series relative to the central point of the well. Summation of the potentials of the adjacent chains of atoms, which in fact determine the potential well, and retention of the cubic terms in the expansion leads us to the problem of motion in the Henon-Heiles potential. The energy of a particle is governed by the energy of transverse motion  $\varepsilon_{\perp}$ . We have seen earlier that the motion of a particle in the Henon-Heiles potential can be both regular and chaotic, depending on its energy and on the initial conditions.

Therefore, channelling of a positive high-energy particle in a potential well in a silicon crystal along the  $\langle 111 \rangle$  axis can be either regular or chaotic. On increase in the transverse-motion energy, as  $\varepsilon_{\perp}$  approaches the energy at



Figure 10. Same as in Fig. 3, but for the (100) crystallographic axis.

a saddle point, the range of the initial conditions leading to chaotic motion widens rapidly.

Let us now consider the motion of a particle in a silicon crystal along the  $\langle 100 \rangle$  axis. As in the preceding case, the potentials of adjacent atomic chains form a potential well (Fig. 10), but its shape is different from that of the potential well for the motion along the  $\langle 111 \rangle$  axis. Expansion of the potentials of the adjacent atomic rows relative to the central point of the well, in terms of a small displacement from this point, and retention of the first nonlinear term in the expansion leads us to the problem of motion in a potential<sup>†</sup> described in Ref. [31]:

$$U(x, y) = 4U_{\rm H} \left( \tilde{x}^2 + \tilde{y}^2 - \tilde{x}^4 - \tilde{y}^4 + 14\tilde{x}^2 \tilde{y}^2 \right), \qquad (4.1)$$

where  $\tilde{x} = 4x/a$ ;  $\tilde{y} = 4y/a$ ; *a* is the lattice constant;  $U_{\rm H}$  is the potential energy at a saddle point. In view of the symmetry of the potential applicable to this case, the terms containing the cubic terms of the expansion are missing and the first nonlinear term contains the fourth powers of the coordinates.

The nature of motion of a particle is determined by the curvature of the potential-energy surface. In the field under discussion the presence of the fourth powers of the coordinates means that the curvature of the potentialenergy surface can be both positive and negative in a potential well. Expansion (4.1) readily yields the following equation for a line on which the curvature of the potentialenergy surface is zero:

$$1 + 8(\tilde{x}^2 + \tilde{y}^2) - 84(\tilde{x}^4 + \tilde{y}^4) - 552\tilde{x}^2\tilde{y}^2 = 0.$$
 (4.2)

Lines of this type are represented by dashed curves in Fig. 10.

Depending on the value of  $\varepsilon_{\perp}$ , the motion of a particle in the field described by expansion (4.1) can take place either entirely within the region with the positive curvature of the

Regular and chaotic motion of a positively charged particle along the  $\langle 100 \rangle$  axis in a silicon crystal has been investigated also elsewhere [30] without recourse to expansion (4.1).



Figure 11. Poincare sections and corresponding paths of particles in finite motion in a field described by expression (4.1), calculated for  $\varepsilon_{\perp} = 1 \text{ eV}$  (a),  $\varepsilon_{\perp} = 2 \text{ eV}$  (b), and  $\varepsilon_{\perp} = 3 \text{ eV}$  (c).

potential energy surface or partly in a region with a positive curvature and partly in that with a negative curvature. In other words, the motion of a particle in such a field can be regular and/or chaotic.

Fig. 11 shows typical paths of a particle in a field described by expansion (4.1) and the corresponding Poincare sections for different values of the transverse energy. We can see that at low values of this energy  $\varepsilon_{\perp}$ , when the particle path lies entirely in a region with a positive curvature of the potential-energy surface, the motion is regular. An increase in the value of  $\varepsilon_{\perp}$ , when the particle path begins to enter a region with a negative value of the curvature of the potential energy U(x, y), both regular and chaotic motion of the particle in the investigated well become possible. An increase in  $\varepsilon_{\perp}$ , when the transverse energy approaches the energy at a saddle point, increases the range of the initial conditions that make the motion chaotic.

A similar situation occurs also in the case of finite motion of a particle in a potential well along the  $\langle 110 \rangle$  axis. The potential well has a more complex structure than for the motion of a particle along the  $\langle 111 \rangle$  or  $\langle 100 \rangle$  axes, and we shall not discuss this case in detail.

#### 4.2 Axial channelling of negative particles

We shall now consider axial channelling of negative particles in crystals. The potential energy of a particle then has the opposite sign to the potential energy of a positive particle and finite motion occurs in potential wells close to atomic rows. These potential wells differ from the wells for positively charged particles by a greater depth and by different shapes (see Figs 3, 4, and 10, in which the equipotential surfaces should be taken with the opposite sign).

In the case of motion along the  $\langle 111 \rangle$  and  $\langle 100 \rangle$  axes in a silicon crystal the potential energies in the region of the wells can be approximated quite accurately by a function which has the cylindrical symmetry (this follows directly from Figs 3 and 10), and we then face the problem of finite motion of a particle in a field  $U(\rho)$  which depends only on the modulus of the distance between the particle and the chain axis. It is obvious that in a field of this kind both the transverse motion energy  $\varepsilon_{\perp}$  and the angular momentum M are conserved. In terms of cylindrical coordinates  $(\rho, \phi)$ , these integrals are given by the following formulas:

$$\varepsilon_{\perp} = \frac{1}{2} \varepsilon \dot{\rho}^2 + \frac{M^2}{2\varepsilon \rho^2} + U(\rho), \quad M = \varepsilon \rho^2 \dot{\phi} , \qquad (4.3)$$

where  $\varphi$  is the azimuthal angle in the (x, y) plane.

The set of relationships (4.3) readily yields the dependences  $\rho(t)$  and  $\varphi(t)$ . In the case of finite motion, the dependence  $\rho(t)$  is a periodic function and its period is

$$T = 2 \int_{\rho_{\min}}^{\rho_{\max}} \frac{\mathrm{d}\rho}{\dot{\rho}} , \qquad (4.4)$$

where  $\rho_{\min}$  and  $\rho_{\max}$  are the minimum and maximum distances from a particle to the axis of a row, found from the equation

$$\varepsilon_{\perp} = rac{M^2}{2 \varepsilon 
ho^2} + U(
ho) \; .$$

In general, the particle precesses and then during a time T the radius vector rotates by the angle

$$\Delta \varphi = 2 \int_{\rho_{\min}}^{\rho_{\max}} \frac{M \,\mathrm{d}\rho}{\epsilon \rho^2 \dot{\rho}} \,. \tag{4.5}$$

It is worth noting that the lines corresponding to zero curvature of the potential-energy surfaces for negatively charged particles, plotted in Figs 3, 4, and 10, are located close to the potential well minima. This means that, in a wide range of transverse energies  $\varepsilon_{\perp}$ , the path of an axially channelled particle is in a region with a negative curvature of the potential-energy surface and it would seem that its motion should always be chaotic. However, we have seen already that this is not true. The potential of each row of atoms at short distances from its axis has the cylindrical symmetry, so that the motion of a particle in the field of this potential should be regular and quasiperiodic. The apparent conflict between the criterion of the Gaussian curvature for chaotic motion of a particle in an external field and regular motion in a cylindrically symmetric field is due to the following. The Gaussian curvature criterion for determination of the nature of the motion of a particle in an external field is derived on the assumption that the matrix  $s_{ii} = \partial^2 U / \partial r_i \partial r_i$  depends weakly on time intervals  $\Delta t \sim \lambda_i^{-1}$  during which the initially close paths become divergent. In other words, the potential energy U(x, y)should vary slowly with the coordinates. This condition is not satisfied near atomic rows and, consequently, in such regions we cannot apply the Gaussian curvature criterion to determine the nature of the motion of a particle in the field of an atomic row.

Therefore, in general, the finite motion of a particle in the field of a potential  $U(\rho)$  is regular and quasiperiodic. This situation occurs when a particle traverses a silicon crystal along the  $\langle 111 \rangle$  or  $\langle 100 \rangle$  axis and the continuum potential in the region of a potential well may be approximated by a cylindrically symmetric function. Such a situation cannot occur when the motion occurs along other crystallographic axes. For example, when a negative particle crosses a silicon crystal along the  $\langle 110 \rangle$  axis, the potential well is formed by two atomic rows located close to one another. The potential energy does not then have cylindrical symmetry: the function U(x, y) has deep minima at coordinates governing the positions of these rows and a saddle point on the line joining these rows (Fig. 12). A negative particle channelling in such a field may be affected by one or two atomic rows, depending on  $\varepsilon_{\perp}$ .



Figure 12. Potential well for a channelled negative particle, moving in a silicon crystal along the  $\langle 110 \rangle$  axis.



Figure 13. Poincare sections and corresponding paths of particles moving in a potential well shown in Fig. 12, calculated for  $\varepsilon_{\perp} = 1.1U_s$  (a) and  $\varepsilon_{\perp} = 0.4U_s$  (b).

The case when the energy of transverse motion is close to the potential energy at a saddle point is of special interest. This is because the particle path can then pass through a region with a negative curvature of the potentialenergy surface near a saddle point. Consequently, we may expect the motion of such a particle to be unstable against small changes in the initial conditions. We shall therefore consider in detail the motion of a negative particle when  $\varepsilon_{\perp} \sim U_s$ , where  $U_s \approx -25$  eV is the potential energy at a saddle point, and the particle may reach the region of such a point [28, 63].

The Poincare sections corresponding to the values  $\varepsilon_{\perp} = 1.1U_s$  and  $\varepsilon_{\perp} = 0.4U_s$  are plotted in Fig. 13. If  $\varepsilon_{\perp} = 1.1U_s$ , a particle can move only in one of the two parts (halves) of the potential well formed by two atomic rows (Fig. 12). Depending on the initial conditions, this particle can move in a regular or chaotic manner in one of the halves of the shared potential well. The paths corresponding to regular and chaotic motion are shown in Fig. 13a for  $\varepsilon_{\perp} = 1.1U_s$ .

If  $\varepsilon_{\perp} = 0.4U_{\rm s}$ , the particle moving in this potential well can switch from one atomic row to another. The particle then moves chaotically in the potential well under almost all the initial conditions. One of such paths is shown in Fig. 13b.

We thus can see that, as in the case of a positive particle, the motion of a negative particle in the field of the continuum potential of atomic rows in a crystal can be both regular and chaotic. However, the shapes and depths of the potential wells are very different for positively and negatively charged particles.

## 4.3 Dynamic chaos in above-barrier motion of particles in a crystal

We have considered so far the finite motion of a fast charged particle in a field of the continuum potential of atomic rows in a crystal and we have shown that such motion can be regular or chaotic. We shall now discuss the case when a particle is in infinite (above-barrier) motion relative to the atomic rows. This situation occurs if the energy of transverse motion exceeds the potential energy at saddle points (Section 2.4).

In the above-barrier motion a particle collides successively with different atomic rows which are parallel to the z axis near which the particle is travelling. There may be a correlation or none between successive collisions. The existence of correlations corresponds to regular motion of a particle in the field of atomic rows. However, its absence corresponds to irregular, i.e. chaotic, motion in the periodic field of atomic rows. If we consider a positive particle, we face a problem similar to that of a particle in a periodic field of disks discussed in Section 3.3. The analogy is particularly close if the motion occurs along the  $\langle 111 \rangle$  crystallographic axis in silicon which has a periodic structure resembling that formed by periodically distributed disk triads (Section 3.3).

Important changes in the particle path occur at distances of its closest approach to the rows of atoms where the gradients of the potential are maximal and the potential can be regarded as cylindrically symmetric. Therefore, in the description of the motion of an abovebarrier particle in the field of the continuum potential of atomic rows we can assume, in the first approximation, that the potentials of the adjacent rows are cylindrically symmetric in a region  $\rho \leq \bar{a}/2$ , where  $\bar{a}$  is the distance between the rows, and the potential elsewhere between the rows is zero. We then have a problem similar to that discussed in Section 3.3, of the scattering in a periodic field of disks and the reflection from disks which corresponds to the scattering of a particle by atomic rows. It is worth noting that a long time spent by a positive particle in the region between disk triads in fact corresponds to the

phenomenon of axial channelling of positively charged particles in a crystal.

However, although the problems are similar, there are still some differences. The scattering by disks appears to be 'hard', i.e. at all energies the angle of incidence is equal to the angle of reflection, and the particle cannot enter the region bounded by the disks. Consequently, the motion of a particle in such a system is extremely unstable: close paths rapidly diverge under all initial conditions. Regular periodic motion of a particle in a field of disks is possible only for some selected paths (Section 3.3).

However, when the motion takes place in the periodic field of atomic rows in a crystal, a particle can enter a region where the potential of a row differs from zero. This has the effect that, apart from the ranges of the initial conditions in which the motion is chaotic, there are also ranges of such conditions when the motion is regular and stable (for example, the motion along crystallographic planes).

As in the finite motion in a potential well, the nature of the motion of a particle in the periodic field of atomic rows in a crystal can be determined by the Poincare section method. In view of the periodicity of a crystal, we can reduce the problem of the motion of a particle in the field of many atomic rows to the motion in one cell [63]. One should take account of the reflection of a particle from the cell edges. This means that the problem is similar to that of the motion of particles in billiards, when the billiard table is in an external field (see Refs [31, 64, 65]).

The procedure of constructing the Poincare sections is the simplest when the motion occurs in a silicon crystal along the  $\langle 100 \rangle$  axis and the atomic chains form a periodic structure with a square cell in a transverse plane (Fig. 10) [31, 63]. Such sections are shown in Fig. 14a for positive particles with  $\varepsilon_{\perp} = 2Ze^2/d$ . A unit cell in the (x, y) plane is then a square with its centre on the axis of one of the atomic rows and the sides of the square are parallel to the (011) and (011) crystallographic planes. It is assumed that a particle crossing the cell edges is reflected elastically. The Poincare sections plotted for this case correspond to the points of intersection of the phase path of a particle and one of the sides of the cell.

Similar sections can easily be constructed also for the reflection of a particle from disks distributed periodically in

the (x, y) plane and characterised by a square unit cell (Fig. 14b). We can see that in the scattering by atomic rows, we can expect not only irregular, but also regular particle motion. The latter corresponds to the motion along crystallographic planes formed by atomic rows. However, in the reflection from disks the motion is chaotic for practically all the initial conditions. There are only a few isolated points in the phase space at which the paths are regular.

As  $\varepsilon_{\perp}$  increases, so does the size of the regions in the phase space of a Poincare section when the motion of a particle is regular. New regions also appear and they correspond to regular motion of a particle along other crystallographic planes characterised by less close packing of the atomic rows than that exhibited by the (011) plane. When disks reflect particles, then at all energies the motion of positive particles is chaotic.

Let us now consider above-barrier motion of negative charged particles in the field of atomic rows in a crystal. In contrast to positive particles, these negative particles are attracted to the atomic rows and, therefore, at all transverse energy values they can approach closely atomic rows where the gradients of the potential are high. This results in strong stochastisation of their motion in the periodic field of atomic rows, compared with positively charged particles. This is illustrated by the Poincare section (Fig. 14c) for negatively charged particles travelling in a silicon crystal near the (100) axis. (The method of constructing this section is the same as for positive particles.) This section shows that for  $\varepsilon_{\perp} = 2Ze^2/d$  the motion of negative particles in the periodic field of atomic rows in a crystal is chaotic for almost all the initial conditions. This situation is retained up to very high values of  $\varepsilon_{\perp}$  ( $\varepsilon_{\perp} \sim 10 Ze^2/d$ ).

We can see that the chaotic motion of negative particles in the periodic field of atomic rows in a crystal is closer to the nature of particle motion in the periodic field of disks on a plane (Section 3.3). However, particles are reflected by such disks, whereas negative particles are attracted by the atoms in a row.

It follows that both positive and negative particles may be in chaotic motion in the periodic field of atomic rows. The motion of negative particles is more chaotic: the chaotic regime is realised for a wider range of the initial conditions than in the case of positive particles.



Figure 14. Poincare sections for positive (a) and negative (c) particles in above-barrier motion in a silicon crystal near the  $\langle 100 \rangle$  axis; (b) corresponding sections for particles reflected by disks forming a square cell in a plane.

## 4.4 Nature of motion of particles in multiple scattering by atomic rows in a crystal and the possibility of describing it

In the preceding sections we have demonstrated that, in order to determine the nature of motion of a particle, it is necessary to know its path in the periodic field of atomic rows. Therefore, we may have given an impression that if the path itself is known, then determination of the nature of the motion of a particle is of no special interest. However, this is not true, because knowledge of the nature of motion and determination of the regions in the phase space corresponding to different types of motion makes it possible to simplify greatly the description of the physical processes associated with the nature of motion (for example, multiple scattering of particles by atomic rows and the emission of bremsstrahlung radiation).

In fact, if it is known that a particle is in regular motion along one of the crystallographic planes, for example the (y, x) plane, then for small angles  $\psi$  between the particle momentum and the axis of the atomic rows forming the plane, its path can be found in the first approximation by assuming that the plane is continuous, i.e. by using the lattice potential averaged over the coordinates in this plane [19]:

$$U_p(x) = \frac{1}{L_y} \int_{-\infty}^{\infty} \mathrm{d}y \, U(\boldsymbol{\rho}) , \qquad (4.6)$$

where  $L_y$  is the linear size of the plane along the y axis and  $U(\boldsymbol{\rho})$  is the continuum potential of the atomic rows forming the plane.

In the field described by expression (4.6) the particle momentum components  $p_z$  and  $p_y$ , parallel to the (y, z)plane, are conserved. This means that the situation can be reduced to the one-dimensional problem of the motion of a particle in the periodic field  $U_p(x)$  of crystalline planes. The path of a particle along the x axis, orthogonal to a crystal plane, is then described by equations [14, 19-21]

$$\ddot{x} = -\frac{1}{\varepsilon} \frac{\partial}{\partial x} U_p(x) , \qquad (4.7)$$

the solution of which can be expressed in terms of the integral of the energy of transverse motion with respect to the crystallographic planes:

$$\varepsilon_{\perp p} = \frac{1}{2} \, \varepsilon \dot{x}^2 + U_p(x) \ . \tag{4.8}$$

Depending on the value of  $\varepsilon_{\perp p}$ , a particle in the field  $U_p(x)$  can be in finite motion (planar channelling) or in infinite motion relative to the crystallographic planes. The latter situation is possible for positive and negative particles. If we know the particle path in the field  $U_p(x)$ , we can find — for example—the characteristics of the radiation emitted by the particle in this field, the probabilities of its collisions with nuclei, and other characteristics of the interaction of the particle with the lattice atoms.

However, the validity of the continuum potential approximation of crystalline planes, described by expression (4.6), is governed by the conditions ensuring regular motion of a particle in the periodic field of atomic rows. In some cases (for example, when  $\psi \ge \psi_c$ ) such conditions can be derived by analytic estimates from the requirement of the existence of correlations between successive collisions of a particle with atomic rows [31, 66]. However, in general (in particular, if  $\psi \le \psi_c$ ), a numerical analysis of the problem by the Poincare section method is required. Such an

analysis shows that the approximation of a continuous plane can be used for positive particles in order to describe the motion of these particles along certain crystallographic planes even when  $\psi \leq \psi_c$ , but in a limited region of the phase space (Fig. 14a). Such a description is not possible (Fig. 14c) for negative particles when  $\psi \leq \psi_c$ .

However, if a particle moves chaotically in the periodic field of atomic rows, then its collisions with different rows can be regarded as random. We are speaking here of multiple scattering of a particle by atomic rows. If it is known that this scattering process is random, it is easy to write down the equation for the angular distribution function of the scattered particles. Since the scattering involving collisions with different atomic rows occurs along an azimuthal angle  $\varphi$  in a plane orthogonal to the axis of the rows, we can derive the following equation for the distribution function of the particles in terms of the angle  $\varphi$  at a depth z from the crystal surface<sup>†</sup>:

$$\frac{\mathrm{d}}{\mathrm{d}z}f(\varphi,z) = nd\psi \int_{-\infty}^{\infty} \mathrm{d}b \left[f\left(\varphi + \varphi(b), z\right) - f\left(\varphi, z\right)\right], \quad (4.9)$$

where  $\varphi(b)$  is the function representing the deflection of a particle in the field of a single atomic row in a crystal, given by expression (2.21) and governed by the impact parameter of a row b, and n is atomic density in the crystal.

It is assumed in Eqn (4.9) that an elementary event, governing the interaction of a particle in the lattice, is the collision of a particle with a single row of atoms in a crystal.

The function  $f(\varphi, z)$  is normalised by the condition

$$\int_{0}^{2\pi} \mathrm{d}\varphi f(\varphi, z) = 1 \ . \tag{4.10}$$

The solution of Eqn (4.9) satisfying the condition  $f(\varphi, 0) = \delta(\varphi)$ , where  $\delta(\varphi)$  is the delta function, is described by [26]

$$f(\varphi, z) = \frac{1}{2\pi} \sum_{k=-\infty}^{\infty} \cos(k\varphi)$$
$$\times \exp\left\{-nd\psi z \int_{-\infty}^{\infty} db \left[1 - \cos[k\varphi(b)]\right]\right\} . (4.11)$$

We can readily use the solution described by expression (4.11) to find the average square of the angle of multiple scattering of a particle by atomic rows in a crystal:

$$\overline{\theta^2} = \int_0^{2\pi} \mathrm{d}\varphi f(\varphi, z) \, 4\psi^2 \sin^2 \frac{\varphi}{2} \,. \tag{4.12}$$

This quantity can be rewritten in the form

$$\overline{\theta^2} = 2\psi^2 \left\{ 1 - \exp\left[-2nd\psi z \int_{-\infty}^{\infty} db \sin^2 \frac{1}{2} \,\varphi(b)\right] \right\} . (4.13)$$

Some limiting cases of formulas (4.11) and (4.13) are discussed in Refs [66–69]. Here we shall draw attention solely to the conditions of validity of these formulas.

Formulas (4.11) and (4.13) are valid if the collisions of a particle with rows of atoms in a crystal can be regarded as random. This is true if the whole phase space in a Poincare section corresponds to chaotic motion. If a Poincare section includes extended regions corresponding to regular motion,

<sup>†</sup>Eqn (4.9) was used in Refs [67, 68] to describe the scattering of positive particles in a crystal when  $\psi \lesssim \psi_c$ . It is shown in Ref. [69] that at high energies this equation can be used to describe the scattering of positive and negative particles in a crystal when  $\psi \gtrsim \psi_c$ .

the distribution function of the particles in terms of the angles  $f(\varphi, z)$  may deviate from the distribution described by formula (4.11). The methods for numerical simulation of particle motion are particularly important in determination of  $f(\varphi, z)$ .

By way of example, let us compare the average squares of the angle of multiple scattering of a particle by atomic rows in a crystal,  $\theta^2$ , obtained by partial simulation of particle motion in the periodic field of atomic rows and on the basis of formula (4.11), valid if the collisions of a particle with different rows can be regarded as random (random row approximation). This comparison is made in Fig. 15 for the scattering of positive and negative particles in a <u>crystal</u> [31]. The <u>ordinate</u> in this figure represents  $f = (\theta^2/\theta_{am}^2)^{1/2}$ , where  $\theta_{am}^2 = \varepsilon_s^2 L/\varepsilon^2 L_{rad}$  is the average square of the angle of multiple scattering of particles in an amorphous medium,  $\varepsilon_s^2 = 4\pi m^2/e^2$ , *m* is the mass of an electron,  $L_{rad}$  is the radiation length [12, 14], and the abscissa gives the value of  $\psi/\psi_c$ .

The continuous curves in Fig. 15 represent the results of a calculation of  $\theta^2$  from formula (4.13) for particles of  $\varepsilon = 30$  GeV energy, travelling in a silicon crystal L = 50 µm thick close to the  $\langle 100 \rangle$  axis.

The simulation was based on the formula

$$\overline{\theta^2} = \frac{1}{N} \sum_{i=1}^{N} 4\psi^2 \sin^2 \frac{\varphi_i}{2}, \qquad (4.14)$$



Figure 15. Orientational dependences of the average square of the angle of multiple scattering of positive (a) and negative (b) particles by rows of atoms in a silicon crystal, when these particles are travelling close to the  $\langle 100 \rangle$  axis.

where N is the number of particles whose motion is being simulated (N = 200) and  $\varphi_i$  is the azimuthal scattering angle of the *i*th particle after its escape from a crystal. This angle is found by a numerical solution of Eqn (2.35) and the index *i* refers to different initial conditions (different values of the impact parameter in the first collision of a particle with a row of atoms).

The open circles an<u>d</u> triangles in Fig. 15 represent the results of simulation of  $\theta^2$  for different orientations of the x and y crystallographic axes relative to the projection  $p_{\perp}$  of the momentum of the incident particle onto an (x, y) plane orthogonal to the z crystallographic axis near which the motion takes place. The black squares are the results of simulation when the adjacent atomic rows are shifted in the (x, y) plane in a random manner relative to one another.

The results obtained show that  $\theta^2 \ge \theta_{am}^2$  is obeyed in a wide range of the angle  $\psi$  and if the collisions of a particle with different atomic rows are random, the results of simulation agree with analytic calculations of the quantity f. However, if the motion occurs in the periodic field of atomic rows in a crystal, the results of simulation agree with analytic calculations of the function f, carried out on the basis of formula (4.13), only in the angular range  $\psi \le \psi_c$ . For negative particles the agreement is observed in a wider range of the angles  $\psi$  than for positively charged particles. This is related to the stronger stochastisation of the motion of negative particles in the periodic field of atomic rows, compared with positive particles.

A considerable difference between the simulation results (open circles and triangles) and analytically calculated values of f in the range  $\psi \gg \psi_c$  is due to the influence, on the scattering, of a regular motion of a particle in the periodic field of atomic rows.

We shall conclude this section by noting that the reported results are obtained ignoring noncoherent particle scattering by inhomogeneities of the crystal potential, associated with the thermal scatter of the positions of atoms in the lattice and also with the scattering by the electron subsystem of the lattice. When these three effects are taken into account, the regions in the phase space associated with the regular motion become smaller. There is a corresponding increase in the regions of the phase space where the multiple scattering can be described by the model of random rows [see Eqn (4.9)]. Inclusion of the non-coherent scattering effects also shows that particles may be scattered not only along the azimuthal angle  $\varphi$ , but also along the polar angle.

Inclusion of the noncoherent effects in the scattering complicates the motion of a particle in a crystal, so that computer simulation methods become particularly useful in solving this problem.

# 5. Passage of high-energy charged particles through a bent crystal

# 5.1 Bending of the paths of positive particles during planar channelling in a bent crystal

It is shown in the preceding section that if a fast charged particle moves in a regular manner along one of the crystallographic planes, its motion is governed primarily by a one-dimensional continuum potential  $U_p(x)$  of crystallographic planes, described by expression (4.6); here, x is the coordinate of a particle orthogonal to the crystallographic planes. The particle in the field of the continuum potential of crystallographic planes can be either in finite motion (channelling) or in infinite (above-barrier) motion relative to the planes.

Let us assume that the planes are bent, but remain parallel to one another (Fig. 16). Then, bending of the channel should also result in bending of the particle path. This can be used for extraction of high-energy chargedparticle beams from cyclic accelerators if a bent crystal is attached in a suitable manner to an accelerator. This effect was pointed out in Ref. [39].



Figure 16. Bending of a positively charged particle in planar channelling in the field of bent crystallographic planes.

Since the average crystal fields exceed greatly the external magnetic fields that are employed in beam bending, it follows that the dimensions of a bent crystal used in beam extraction will be considerably smaller than the dimensions of the devices employed in beam extraction by means of external fields (see, for example, Refs [40-43]). This opens up also other opportunities for the control of beams and of their parameters. They include the possibility of splitting a beam into several components [70], removal of the beam halo [71], beam focusing [43], etc. It would be therefore of major interest to study the passage of high-energy charged-particle beams through bent crystals. This will now be discussed in detail.

Let us begin with the derivation of the equations of motion for a bent path of a particle moving in a field formed by bent crystallographic planes. For simplicity, we shall assume that the radius of curvature  $\mathcal{R}$  of bent crystallographic planes is the same at all points on a bent plane and it is sufficiently large, so that the motion takes place in spatial regions whose dimensions are small compared with  $\mathcal{R}$ . The motion occurs in a cylindrically symmetric field  $U_p(r)$ , where r is the distance from the centre of curvature, which can be written in the form

$$r = \mathcal{R} + x \ . \tag{5.1}$$

Here, x is a small deflection of a particle from the crystallographic planes in the direction of the normal to the surface:  $|x| \ll \mathcal{R}$ .

The equations of motion for x(t) can be derived conveniently with the aid of the relativistic Hamiltonian-Jacobi equations for the action  $S(\mathbf{r}, t)$  of a particle moving in the field  $U_p(\mathbf{r})$  [46]:

$$\left[\frac{\partial}{\partial t}S + U_{\rm p}(r)\right]^2 = (\nabla S)^2 + m^2 .$$
(5.2)

Since the potential energy is a cylindrically symmetric function of r, the action S should be sought in the form

$$S(\mathbf{r}, t) = -Et + M\varphi + f(r) , \qquad (5.3)$$

where E is the particle energy, M is its angular momentum,  $\varphi$  is the angle of bending of the particle path, and f(r) is some function of r. It follows from expression (5.3) that f(r) can be described by the following equation:

$$\left(\frac{\mathrm{d}f}{\mathrm{d}r}\right)^2 + \frac{M^2}{r^2} + m^2 = \left[E - U_\mathrm{p}(r)\right]^2,$$

which yields

$$f(r) = \int dr \left\{ \left[ E - U_{\rm p}(r) \right]^2 - \frac{M^2}{r^2} - m^2 \right\}^{1/2} \,. \tag{5.4}$$

The relationship  $\partial S / \partial E = \text{const}$  gives the following equation for the particle path r(t):

$$\left(\frac{\mathrm{d}r}{\mathrm{d}t}\right)^2 = \frac{\left[E - U_{\mathrm{p}}(r)\right]^2 - M^2/r^2 - m^2}{\left[E - U_{\mathrm{p}}(r)\right]^2} \,. \tag{5.5}$$

The quantity E in the above equation represents the total energy of a particle in a crystal. It is related to the energy  $\varepsilon$  of the particle incident on a crystal by  $\varepsilon = E + U_p(r_0)$ , where  $r_0$  is the value of the coordinate r at which the particle enters the crystal. Since for a fast particle, we have  $\varepsilon \ge U_p$ , it follows that Eqn (5.5) can be simplified to

$$\left(\frac{\mathrm{d}r}{\mathrm{d}t}\right)^2 \approx \left(\frac{p^2}{\varepsilon^2} - \frac{M^2}{\varepsilon^2 r^2}\right) \left[1 + 2 \frac{U_{\mathrm{p}}(r) + U_{\mathrm{p}}(r_0)}{\varepsilon}\right] -2 \frac{U_{\mathrm{p}}(r) + U_{\mathrm{p}}(r_0)}{\varepsilon} \,.$$

We note now that M = pb, where p is the particle momentum and b is the impact parameter  $(b = r_0)$ , and that  $r = \mathcal{R} + x$  and  $b = \mathcal{R} + x_0$ , where  $x_0$  is the point at which the particle enters the crystal (Fig. 17),  $|x| \leq \mathcal{R}$  and  $|x_0| \leq \mathcal{R}$ . Then, in the first approximation in terms of the parameters  $x/\mathcal{R}$  and  $U_p/\varepsilon$ , we obtain the following equation for x(t):

$$\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)^2 \approx 2 \, \frac{x - x_0}{\mathcal{R}} - 2 \, \frac{u(x) + u(x_0)}{\varepsilon} \,. \tag{5.6}$$

Here,  $u(x) = u_p(\mathcal{R} + x)$ .

In principle, Eqn (5.6) describes the particle path x(t) as a function of time t. It can be interpreted in a clear manner if we differentiate the above equation with respect to time:

$$\frac{\mathrm{d}^2 x}{\mathrm{d}t^2} = -\frac{1}{\varepsilon} \frac{\partial}{\partial x} \ U_{\mathrm{eff}}(x) , \qquad (5.7)$$

where

$$U_{\rm eff}(x) = u(x) - x \,\frac{\varepsilon}{\mathcal{R}} \,. \tag{5.8}$$

Therefore, the quantity  $U_{\text{eff}}(x)$  can be regarded as the effective potential energy of a particle moving in a bent crystal.

Eqn (5.7) is identical with the corresponding result obtained in Ref. [72] by another method.

The quantity u(x) in expression (5.8) is the potential energy of the interaction of a particle with the continuum potential of crystallographic planes and  $-x\varepsilon/\mathcal{R}$  represents



Figure 17. Effective potential energy, described by expression (5.8), of the interaction of a particle with the continuum potential of bent crystallographic planes, calculated for different bending radii: (1)  $\mathcal{R} \to \infty$ ; (2)  $\mathcal{R} > \mathcal{R}_c$ ; (3)  $\mathcal{R} < \mathcal{R}_c$ .

the centrifugal energy. Fig. 17 shows graphs of the function  $U_{\rm eff}(x)$  for positively charged particles moving in a bent crystal. These paths are plotted for different values of the radius of curvature.

In the limit  $\mathcal{R} \to \infty$ , a particle moves in a periodic field of the crystallographic planes of a straight crystal. The motion in such a field can be both finite or infinite relative to the crystallographic planes (this is shown in Section 4.4). The finite motion is realised if the energy of transverse motion  $\varepsilon_{\perp p} = \frac{1}{2}\varepsilon\theta^2$  is small compared with the maximum potential energy  $U_{p, max}$ , where  $\theta$  is the angle between the momentum of a particle incident on a crystal and a crystallographic plane. If  $\varepsilon_{\perp p} > U_{p, max}$ , such a particle follows an infinite path relative to the planes.

However, if the motion occurs in a bent crystal and the bending radius is sufficiently large, then  $U_{\text{eff}}(x)$  contains a negative correction to the potential energy, and this correction increases linearly with x. The result is a modification of the potential well formed by the continuum potential of the crystallographic planes. One of the edges of the new potential well is depressed relative to the minimum value of the function  $U_{\rm eff}(x)$  in the region of the well (curve 2 in Fig. 17). A particle in such a field can, as in the case of a straight crystal  $(\mathcal{R} \to \infty)$ , be in finite motion relative to the crystallographic planes. Such motion is possible if the potential energy  $\varepsilon_{\perp p}$  is less than the potential barrier in a given problem. A particle then moves periodically in a channel formed by the potential of the adjacent planes and it follows the bending of the crystal planes. If the noncoherent scattering effects are ignored, such motion occurs over the whole length of the crystal and this bends the particle path by an angle  $\theta = L/\mathcal{R}$ , where L is the crystal thickness. It is clear that at high values of L this angle can be considerably greater than the critical angle for planar channelling  $\theta_p = (2U_{p,max}/\epsilon)^{1/2}$ . In other words, a beam may be bent by an angle exceeding considerably the critical planar channelling angle.

The depth of the potential well formed by  $U_{\text{eff}}(x)$  decreases with reduction in  $\mathcal{R}$  and at some value of  $\mathcal{R}$ 

the well disappears completely (curve 3 in Fig. 17). The radius  $\mathcal{R} = \mathcal{R}_c$  at which the potential well  $U_{\text{eff}}(x)$  disappears is well known as the critical bending radius. If  $\mathcal{R} < \mathcal{R}_c$ , finite motion is impossible in the field  $U_{\text{eff}}(x)$  and, consequently, bending of a beam by a bent crystal is also impossible.

If the interplanar potential is assumed to be that described by a harmonic oscillator [21]  $u(x) = U_p(4x^2/d_p^2)$ , where  $|x| \leq \frac{1}{2} d_p$  and  $d_p$  is the distance between the planes located at  $x = \pm \frac{1}{2} d_p$ , it then follows (which can easily be checked) that

$$\mathcal{R}_{\rm c} = d_{\rm p} \, \frac{\varepsilon}{4U_{\rm p}} \,. \tag{5.9}$$

For example, in the case of protons of  $\varepsilon = 100$  GeV energy, moving in a bent silicon crystal along (110) crystallographic planes, we have  $U_{\rm p} \approx 22$  eV,  $d_{\rm p} \approx 2$  Å, and, consequently,  $\mathcal{R}_{\rm c} \approx 25$  cm. We then have  $\theta_{\rm p} = 10^{-5}$  rad. Then, if  $\mathcal{R} > \mathcal{R}_{\rm c}$ , the particles in a beam can be bent by an angle  $\theta = L/\mathcal{R} \gg \theta_{p}$ . It should be stressed once again that the average fields acting on a particle in a crystal are several orders of magnitude higher than the static macroscopic external fields, which can be created by physical equipment. Therefore, the dimensions of a bent crystal can be small compared with the dimensions of the devices used to bend the beams by magnetic fields. For example, bending of heavy positive particles of energy  $\varepsilon = 800$  GeV through an angle  $\theta \sim 10^{-3}$  rad requires a bent silicon crystal whose thickness is L = 10 cm and the bending radius is  $\mathcal{R} = 100$  m, whereas in magnets creating a field B = 1 kG, such bending can be achieved in a system which is 60 m long.

Bending of beams of heavy negative particles is also possible in a bent crystal because such a crystal should have a potential well. However, in contrast to positive particles, there are important noncoherent scattering effects in the case of negative particles and these effects are associated with the fact that a particle of this kind can approach quite closely the nuclei of the atoms forming the crystallographic planes. Therefore, the efficiency of bending a beam of negative particles is considerably less than for a beam of positive particles. So far, bending of a beam of negative particles in bent crystals has not been observed experimentally, whereas bending of positive particles has not only been confirmed in many experiments [41, 42, 73-86], but has found practical use in tackling a number of tasks such as extraction of a beam from an accelerator, measurement of the magnetic moment of the  $\Sigma^+$  hyperon [87, 88], etc. (for reviews, see Refs [40, 43]).

# 5.2 Motion of fast particles in the field of atomic rows in a bent crystal

We have considered above the motion of a positive particle under planar channelling conditions in a bent crystal and we have shown that if the bending of the crystal is small, it is possible to bend the paths of the particles which are in finite motion. A similar situation arises in the case of axial channelling, but it is much more complicated than in the planar case. This is due to the fact that in the planar case the problem is one-dimensional, but it is two-dimensional for axial channelling. Moreover, the role of the abovebarrier motion of particles complicates further the problem of axial channelling. In planar channelling such abovebarrier particles are not deflected in a bent crystal, whereas in axial channelling they are deflected (as shown below) in the same way as the particles in finite motion in the field of atomic rows. It is then found that the majority of the beam particles deflected in a bent crystal are in infinite motion.

In this section we shall consider above-barrier motion of a fast charged particle (irrespective of its charge) in the field of atomic rows in a bent crystal. We shall assume that the potential of atomic rows is continuous and depends only on the distance between the particle and the nearest row. (In the next section we shall discuss a more realistic problem in which infinite motion should be accompanied by finite motion in the field of atomic rows and, moreover, we shall take account of the noncoherent scattering effects.)

We shall begin by demonstrating that when particles are in above-barrier motion in the field of atomic rows, they may be deflected not only in a bent crystal, but also in a straight one.

In fact, a fast charged particle incident on a crystal at a small angle  $\psi$  to one of its crystallographic axes (z axis) collides successively with different rows of atoms oriented parallel to this axis. The scattering by collision with each atomic row occurs mainly along the azimuthal angle  $\varphi$  in a plane orthogonal to the z axis. Multiple scattering by different atomic rows results in a redistribution of the particles in terms of the angles  $\varphi$ . If the angle  $\psi$  between the particle momentum and the crystallographic z axis is sufficiently small ( $\psi \leq \psi_c$ ), a uniform distribution of the particles in respect of the angles  $\varphi$  is established very rapidly (as demonstrated by the results of numerical simulation of the passage of fast charged particles through a crystal when  $\psi \sim \psi_c$  [86]). As a result, the centre of the scattered beam is directed along the crystallographic z axis, i.e. if multiple scattering by atomic rows takes place, the beam axis is bent through an angle equal to  $\psi$ . Such beam bending is possible for both positive and negative particles [86].

A redistribution of the particles in a bent crystal occurs both in respect of the azimuthal angle  $\varphi$  relative to the running direction of the crystallographic axis and in respect of the polar angle  $\psi$  relative to this axis. Some special features of such scattering are worth noting.

We shall consider the simplest case when during the interaction of a particle with a single row of atoms the change in the angle  $\psi$  between the particle momentum and the row axis is small. This condition is satisfied if the bending radius of a crystal is large. Then the scattering by each row of atoms can be regarded in the  $\psi = \text{const}$  approximation. The angular coordinates of a particle then change on going over from one row of atoms to another and the changes can be described by the following recurrent relationships:

$$\theta_{x,i+1} = \theta_{x,i} \cos \varphi_i + (\theta_{y,i} - \theta_i) \sin \varphi_i , \theta_{y,i+1} = (\theta_{y,i} - \theta_i) \cos \varphi_i - \theta_{x,i} \sin \varphi_i + \theta_i ,$$
(5.10)

where  $\theta_{x,i}$  and  $\theta_{y,i}$  are the angular coordinates of the particle in a plane orthogonal to the initial direction of the crystallographic axis, before the *i*th collision with a row of atoms;  $\varphi_i$  is the azimuthal scattering angle of the particle in the *i*th collision [according to expression (2.21),  $\varphi_i$  is governed by the polar angle  $\psi_i$  and by the impact parameter of a row  $b_i$ ];  $\theta_i = L_i/\mathcal{R}$  is the running direction of the crystallographic axis;  $L_i$  is the path travelled by the particle in the crystal before the *i*th collision;  $\mathcal{R}$  is the bending radius of the crystal (it is assumed that the bending



Figure 18. Changes in the angular coordinates of a particle during successive collisions with rows of atoms in a bent crystal.

is along the y axis). Such recurrent relationships are illustrated in Fig. 18.

If in the set of relationships (5.10) we go over to variables  $\theta'_{y,i} = \theta_{y,i} - \theta_i$ ,  $\theta'_{x,i} = \theta_{x,i}$ , the result is in the form of recurrent relationships for the quantities  $\theta'_{y,i}$  and  $\theta'_{x,i}$ , which determine the angular coordinates of a particle relative to the running direction of the crystallographic axis [89, 90]:

$$\begin{aligned} \theta'_{x,i+1} &= \theta'_{x,i} \cos \varphi_i + \theta'_{y,i} \sin \varphi_i ,\\ \theta'_{y,i+1} &= \theta'_{y,i} \cos \varphi_i - \theta'_{x,i} \sin \varphi_i - \frac{l_i}{\mathcal{R}} ,\\ \psi_i &= \left( \theta'^{2}_{x,i} + \theta'^{2}_{y,i} \right)^{1/2} . \end{aligned}$$
(5.11)

The above set of relationships gives also one for  $\psi_i$  which links the value of the angle  $\psi_i$  between the particle momentum and the crystallographic axis in the case of the *i*th collision to the angular coordinates of the particles  $\theta'_{x,i}$  and  $\theta'_{y,i}$ . The quantity  $l_i$  in one of the above relationships is the path travelled by the particle between the *i*th and (i + 1)th collisions with rows of atoms:  $l_i = L_{i+1} - L_i$ .

The set of relationships (5.11) can be used in a study of the dynamics of a particle in a bent crystal and in numerical simulation of the passage of a particle through a crystal. The motion of fast particles in a periodic field of atomic rows in a crystal can be regular or chaotic. Therefore, in general, the pattern of the passage of particles through a crystal is fairly complex and requires numerical simulation in which the real geometry of the distribution of atomic rows in a crystal is taken into account. Before we consider the numerical simulation results, let us examine some analytic relationships which follow from the main recurrent formulas (5.11) that describe the scattering of particles by atomic rows in a bent crystal [94].

Let us assume that each collision with an atomic row establishes a uniform distribution of particles over the angles  $\varphi_i$ , i.e. that the function representing the distribution of particles over angles  $\varphi_i$  is independent of  $\varphi_i$ . Averaging of the set of relationships (5.10) over such a distribution yields self-evident relationships

$$\overline{\theta_{x,i+1}} = 0, \quad \overline{\theta_{y,i+1}} = \frac{L_i}{\mathcal{R}},$$
(5.12)

where the bar denotes averaging over  $\varphi_i$ . These relationships show that when the conditions for a uniform distribution of particles over the angles  $\varphi_i$  are satisfied, the beam centre is displaced along a bent crystallographic axis. The numerical simulation results obtained in a model of binary collisions demonstrate [86] that this approximation is qualitatively correct if the angle  $\psi$  between the particle momentum and the crystallographic axis is small compared with the critical axial channelling angle  $\psi_c$ .

We shall now find the average values of the angles of scattering of particles by atomic rows  $\theta_{x,i+1}^{\prime 2}$  and  $\theta_{y,i+1}^{\prime 2}$ , relative to the running direction of the crystallographic axis when the distribution of the particles over the angles  $\varphi_i$  is uniform. Squaring the first relationship in the set (5.11) and averaging it over  $\varphi_i$ , we find that

$$\overline{\theta_{x,i+1}^{\prime 2}} - \overline{\theta_{x,i}^{\prime 2}} = \frac{1}{2} \left( \overline{\theta_{y,i}^{\prime 2}} - \overline{\theta_{x,i}^{\prime 2}} \right) .$$
(5.13)

If we assume that in going over from one cell to the other the quantities  $\theta_{x,i+1}^{\prime 2}$  change only slightly, we can write down the following equation for  $\theta_{x,i}^{\prime 2}$ :

$$\frac{\mathrm{d}}{\mathrm{d}i} \,\overline{\theta_{x,i}^{\prime 2}} = \frac{1}{2} \left( \overline{\theta_{y,i}^{\prime 2}} - \overline{\theta_{x,i}^{\prime 2}} \right) \,. \tag{5.14a}$$

Similar procedures apply to the second relationship in the set (5.11) and yield the following equation for  $\theta_{v,i}^{/2}$ :

$$\frac{\mathrm{d}}{\mathrm{d}i} \ \overline{\theta_{y,i}^{\prime 2}} = -\frac{1}{2} \left( \overline{\theta_{y,i}^{\prime 2}} - \overline{\theta_{x,i}^{\prime 2}} \right) + \left( \frac{l_i}{\mathcal{R}} \right)^2.$$
(5.14b)

Adding and subtracting Eqns (5.14a) and (5.14b), we find that

$$\frac{\mathrm{d}}{\mathrm{d}i} \overline{\psi_i^2} = \left(\frac{l_i}{\mathcal{R}}\right)^2,$$

$$\frac{\mathrm{d}}{\mathrm{d}i} \left(\overline{\theta_{y,i}'^2} - \overline{\theta_{x,i}'^2}\right) = -\left(\overline{\theta_{y,i}'^2} - \overline{\theta_{x,i}'^2}\right) + \left(\frac{l_i}{\mathcal{R}}\right)^2,$$

where  $\overline{\psi_i^2} = \overline{\theta_{x,i}'^2} + \overline{\theta_{y,i}'^2}$ . We shall now replace  $l_i$  with the average distance l travelled by a particle between consecutive collisions with atomic rows. This distance is given by [19]

$$\frac{1}{l} = nd \int_{-\infty}^{\infty} db \left[ 1 - \cos \varphi \left( b \right) \right] \,, \tag{5.15}$$

so that if we note that  $di \approx dz/l$ , we obtain the following equations for  $\theta_x^{\prime 2}(z)$  and  $\theta_y^{\prime 2}(z)$ :

$$\frac{\mathrm{d}}{\mathrm{d}z} \,\overline{\psi^2} = \frac{l}{\mathcal{R}^2} \,; \, l \,\frac{\mathrm{d}}{\mathrm{d}z} \left(\overline{\theta_y^{\prime 2}} - \overline{\theta_x^{\prime 2}}\right) = -\left(\overline{\theta_y^{\prime 2}} - \overline{\theta_x^{\prime 2}}\right) + \left(\frac{l}{\mathcal{R}}\right)^2 \,.$$
(5.16)

If the order of magnitude of this distance is given by  $l \approx a^2/R \psi_c$ , where *a* is the distance between the rows of atoms and *R* is the screening radius of the atomic potential, we find that

$$\overline{\psi^2} \approx \frac{lL}{\mathcal{R}^2} \,, \tag{5.17a}$$

$$\overline{\theta_y'^2} \approx \overline{\theta_x'^2} + \left(\frac{l}{\mathcal{R}}\right)^2$$
. (5.17b)

It <u>follows</u> from the above relationships that if  $l \ll \mathcal{R}\psi_c$ , then  $\theta_{y,i}^{\prime 2} \approx \theta_{x,i}^{\prime 2}$  and for  $L \gg l$  the average square of the particle bending angle relative to the final direction of the bent crystallographic axis, given by relationship (5.17a), is much less than the square of the angle of the crystal bending of the beam  $\theta^2 = (L/\mathcal{R})^2$ . In other words, in this case the beam bending is along the bending of the crystallographic axis when fluctuations of the scattering angles of the beam particles are small compared with the angle of bending of the beam by the bent crystal:

$$\theta^2 \gg \psi^2 \ . \tag{5.18}$$

It should be stressed that the beam bending applies in this case to the particles which are in infinite motion relative to the atomic rows. Both positive and negative particles may be bent. This bending requires that the condition of uniform distribution of the particles over the angles  $\varphi$  be satisfied, which—as pointed out above—is possible if  $\psi \leq \psi_c$ . Since at the exit from the crystal we have  $\psi^2 = \theta_x'^2 + \theta_y'^2$ , the condition  $\psi \leq \psi_c$  can be written in the form

$$\frac{lL}{\mathcal{R}^2} \leqslant \psi_c^2 . \tag{5.19}$$

This condition determines the relationship between L,  $\mathcal{R}$  and  $\varepsilon$  when the bending of a particle beam is possible in the course of their multiple scattering by atomic rows in a bent crystal.

Relationships (5.12) - (5.19) are derived without specifying the law governing the distribution of atomic rows in a plane orthogonal to the crystallographic z axis. Therefore, relationships (5.12) - (5.19) can be applied to the motion of a particle in a periodic field of the atomic rows and also when the positions of rows in a plane transverse to the z axis can be regarded as random. The only necessary condition is a uniform distribution of particles between the angles  $\varphi$  in collisions with atomic rows. Such a distribution is qualitatively correct if  $\psi \ll \psi_c$ . Since  $\psi \leqslant \psi_c$ , the bulk of the beam particles is in chaotic motion in the periodic field of such atomic rows and the actual law governing the distribution of the rows in a transverse plane is unimportant from the point of view of the scattering.

The condition given by formula (5.19) is identical with that obtained in Ref. [42] for the dechannelling length of fast particles in a bent crystal. However, the solution of the system of equations (5.17) has been obtained employing the relationship  $l \approx a^2/R\psi_c$ . According to Eqn (5.15), the quantity *l* is generally a function of  $\psi^2$ . Therefore, Eqn (5.17a) is a nonlinear differential equation for  $\psi^2(z)$ . The case when  $l \approx a^2/R\psi_c$  applies to the potential of a row of atoms described by  $U(\rho) = U_0(R/\rho)^2$ . However, for other functions  $U(\rho)$ , this solution is different. For example, if the potential is  $U(\rho) = U_0 \pi R/2\rho$ , which is frequently used in the theory of channelling, we then have  $l = l_0 \psi/\psi_c$ ,  $l_0 = 4/\pi^2(1/ndR\psi_c)$  [19] and the equation for  $\psi^2(z)$  becomes

$$\frac{\mathrm{d}}{\mathrm{d}z}\,\overline{\psi}^2 = \frac{l_0}{\mathcal{R}^2}\,\frac{(\overline{\psi}^2)^{1/2}}{\psi_\mathrm{c}}\,,$$

where  $\psi$  in the expression for  $l(\psi)$  is replaced with  $(\psi^2)^{1/2}$ . The solution is then

$$\overline{\psi^2} = \frac{4}{\psi_c^2} \left(\frac{l_0 L}{\mathcal{R}^2}\right)^2 \,.$$

It is easily demonstrated that in the case under discussion as well as when  $l \approx a^2/R \psi_c$ , there are such values of  $\varepsilon$ , L, and  $\mathcal{R}$  for which the relationships  $\theta^2 \gg \overline{\psi^2}$  and  $\overline{\psi^2} \leqslant \psi_c^2$  are obeyed, i.e. a beam of particles undergoing multiple scattering by atomic rows may be bent in a bent crystal.

We shall now consider some characteristics of the motion of fast charged particles in a bent crystal due to the periodicity of the distribution of atomic rows. With this in mind we shall show that when particles are in regular motion along the crystallographic plane, the recurrent relationships (5.10) are transformed into the corresponding results obtained in the theory of motion of particles in the field of the continuum potential of bent crystallographic planes obtained in the preceding section. As before, we shall assume that atomic rows form a square cell in the (x, y) plane and the sides of this cell are directed along the x and y axes.

We note first of all that for  $\psi \ge \psi_c$  the characteristic values of the azimuthal angles of the scattering of a particle by a row of atoms, described by expression (2.25), are small compared with unity:  $\varphi_{i, \text{eff}} \sim (\psi_c/\psi_i)^2$ . Then, if the initial angles  $\theta_{x,0}$  and  $\theta_{y,0}$  are such that  $\theta_{x,0} = \psi \ge \psi_c$  and  $\theta_{y,0} \le \psi_c$ , there is a correlation in the successive collisions of a particle with atomic rows distributed periodically in planes parallel to the (x, z) crystallographic plane. Expansion of the recurrent relationships (5.10) in terms of small values  $\varphi_i \ll 1$  gives, in the first approximation,

$$\theta_{x,i+1} \approx \theta_{x,i} \approx \psi ,$$

$$\theta_{y,i+1} \approx \theta_{y,i} - \psi \varphi_i - \frac{l_i}{\mathcal{R}} ,$$
(5.20)

where  $l_i = a/\psi$ ,  $\psi \ge \psi_c$ , and *a* is the distance between the rows of atoms in the (x, z) plane.

It therefore follows that in the case under discussion the component of the particle velocity along the x axis is conserved and the motion in a transverse direction is described by

$$\theta_{y,i+1} - \theta_{y,i} \approx -\psi \varphi_i - \frac{a}{\psi \mathcal{R}}$$
 (5.21)

The values of  $\varphi_i$  and  $\psi \ge \psi_c$  are given by formula (2.25). The integral with respect of x, which occurs in this formula, can be related to the continuum potential  $U_p(b_i)$  in a crystallographic plane by

$$\frac{1}{a} \int_{-\infty}^{\infty} \mathrm{d}x \; U_R \left( x^2 + b_i^2 \right)^{1/2} = U_p(b_i) \; .$$

Since quantities  $\theta_{y,i}$  vary slowly with *i* and are proportional to the particle velocity component  $v_{y,i}$  along the *y* axis, the following equation is obtained for  $v_{y,i}$ :

$$\frac{\psi}{a} \frac{\mathrm{d}}{\mathrm{d}i} v_{y,i} = -\frac{1}{\varepsilon} \frac{\partial}{\partial y_i} U_p(y_i) - \frac{1}{\mathcal{R}} \,.$$

The variable  $b_i$  is replaced here with  $y_i = b_i$ . Finally, subject to the relationship  $(a/\psi) di = d\tau_i$ , we obtain

$$\frac{\mathrm{d}^2 y}{\mathrm{d}\tau^2} = -\frac{1}{\varepsilon} \frac{\partial}{\partial y} U_p(y) - \frac{1}{\mathcal{R}}, \qquad (5.22)$$

which in fact is identical with the corresponding Eqn (5.7) for a particle moving in the continuum potential of bent crystallographic planes. The difference between these equations is only this: in Eqn (5.7) the bending is in the direction of smaller values of x, while in Eqn (5.22) it is in the direction of higher values of y. This results in the

opposite sign in front of the centrifugal term (which is proportional to  $1/\mathcal{R}$ ).

It therefore follows that if a particle is in regular motion along a crystallographic plane, the recurrent relationships (5.10) go over to the corresponding Eqn (5.7) in the theory of motion of particles in a periodic field of bent crystallographic planes.

# 5.3 Simulation of the passage of high-energy charged particles through a bent crystal

The recurrent relationships (5.11), which link the angular coordinates of a particle as it goes over from one row of atoms to another, are analysed above on the assumption that there is a uniform distribution of the particles over the azimuthal angle arphi in a plane orthogonal to that crystallographic axis near which a particle is moving. However, this assumption of a uniform distribution of particles over the angles  $\varphi$  should be regarded only as qualitative. If no assumption is made of a uniform distribution of particles in terms of the angles  $\varphi$ , the recurrent relationships (5.11) have to be investigated by numerical simulation. We shall give some results of such a numerical simulation and the results of a study of the influence of noncoherent effects on the passage of fast particles through a bent crystal. These effects are associated mainly with multiple scattering of the transmitted particles by the thermal vibrations of atoms in the lattice.

In numerical calculations one needs not only the recurrent relationships (5.10), but also those linking the impact parameters  $b_{i+1}$  and  $b_i$  for successive collisions of a particle with rows of atoms. We can readily see (Fig. 19) that these quantities are related by

$$b_{i+1} = b_i + \left(\frac{\theta_{x,i+1}}{\psi_{i+1}} c_y - \frac{\theta_{y,i+1}}{\psi_{i+1}} c_x\right),$$
(5.23)

where  $c_x$  and  $c_y$  are the coordinates of the centres of an adjacent row of atoms (relative to a row of atoms with the index *i*) which a particle reaches after crossing the *i*th cell. Within the limits of a unit cell, the continuum potential of a row of atoms is assumed to be radially symmetric.



**Figure 19.** Impact parameters  $b_i$  and  $b_{i+1}$  for successive collisions of a particle with rows of atoms  $(\xi_{i+1} = \theta_{x,i+1}/\psi_{i+1})$ 

Since the parameters  $b_i$  are related in a definite way to the angles  $\varphi_i$  [see relationship (2.19)], it follows that formula (5.23) makes it in fact possible to establish a relationship between the angles  $\varphi_i$  and  $\varphi_{i+1}$ . The recurrent relationships (5.11) can then help in solving the problem of the motion of a particle in the periodic field of atomic rows in a bent crystal. Strictly speaking, formulas of the (5.23) type apply to a straight crystal. However, since the bending is slow, they can be applied also to a bent crystal.

In the problem under discussion, an elementary event of the interaction of a particle with a crystal is its scattering by a row of atoms and not by a single atom as in the binary collision model (see, for example, Ref. [86]). Therefore, the method employed can be used to study the passage of particles through a fairly thick crystal.

We shall now give some results of the numerical calculations. Fig. 20 shows the angular distributions of positive and negative particles whose energy is  $\varepsilon = 300 \text{ GeV}$  and which cross a silicon crystal bent to a radius  $\mathcal{R} = 10^4$  cm. The results are plotted for several crystal thicknesses. The simulation was carried out for particles entering this crystal at a small angle ( $\psi \leq 0.1 \psi_c$ ) relative to the  $\langle 111 \rangle$  crystallographic axis. This was done for various values of the impact parameter *b*. The points in Fig. 20 represent the results of stimulation for 100 particles. A crystal was assumed to be bent along the *y* axis.



**Figure 20.** Angular distributions of negative (a, b) and positive (c, d) particles of  $\varepsilon = 300$  GeV energy passing through a silicon crystal bent to a radius  $\mathcal{R} = 10^4$  cm near the  $\langle 111 \rangle$  axis; the coordinates of the beam incident on the crystal are  $(\theta_x, \theta_y) = (0, 0)$ .

The results obtained demonstrate that, if the crystal bending radius is large, a beam can follow a crystallographic axis in a bent crystal and such beam bending is possible for both positive and negative particles. The average squares of the particle bending angles, measured relative to the running direction of the crystallographic axis, are in this case small compared with the square of the angle of beam bending. Therefore, in accordance with relationships (5.10), the whole beam is displaced in the direction of a crystallographic axis in a bent crystal if  $\mathcal{R}$  is large and L is small. It should be stressed once again that bending applies to particles in infinite motion relative to atomic rows and that it is due to characteristic features of the multiple scattering of particles by these rows.

The results of such simulation also demonstrate that the angular distributions of positive and negative particles are different. This is due to the difference of the motion of above-particles which have opposite signs. For example, if  $\psi \leq \psi_c$ , a fraction of positive particles may be in regular motion along crystallographic planes (see Fig. 14). These particles are represented in Fig. 20 by a distribution of some of the beam particles along the lines. If  $\psi \leq \psi_c$ , regular motion is not realised for negative particles and, therefore, there is no 'trapping' of such particles in crystallographic planes (Fig. 14c). However, the bulk of the positive particles moves chaotically in the field of atomic rows in a crystal if  $\psi \leq \psi_c$ . The mechanism of bending of this fraction of the beam particles is exactly the same as that which applies to negative particles.

It is worth noting that if the passage from one cell to another results in a random scatter of the target parameters (when the adjacent rows are shifted relative to one another in a random manner), collisions of a particle with different rows of atoms can be regarded as random. This model corresponds to what is known as the approximation of random collisions with atomic rows. The first calculations of the passage of high-energy particles through a crystal carried out on the basis of this model [89] have shown that positive and negative particles may be bent by a bent crystal when the bending radius is large. This result was confirmed when the real geometry of the distribution of atomic chains in a crystal was simulated [90]. Moreover, the simulation showed that it is important to take account of the real geometry of the distribution of atomic rows in a crystal when dealing with the motion of positive particles because the trapping of these particles in planar channels is possible.

The results discussed above are derived ignoring axial channelling (finite motion) of particles in the field of atomic rows and also ignoring noncoherent scattering of these particles in a crystal. We shall now consider the influence of these processes on the passage of high-energy particles through a bent crystal.

This problem was solved by an improved numerical model of the passage of particles through a crystal. This model takes account of the real geometry of the positions of atomic rows in a crystal and it can be used to consider in a unified manner the main dynamic and kinetic effects [91]. In this model the interaction of a particle with a crystal is investigated by dividing the particle path into a set of rectilinear sections within which the changes in the particle velocity associated with noncoherent scattering effects and with the continuum potential of atomic rows in a crystal are taken into account. The program of numerical calculations based on this model can be used to simulate the passage of high-energy ( $\epsilon \gtrsim 1 \text{ GeV}$ ) particles through a crystal of thickness up to several tens of centimetres.

Fig. 21 gives some of the results of such simulation of beams of positive and negative particles with energies  $\varepsilon = 300 \text{ GeV}$  and  $\varepsilon = 10^4 \text{ GeV}$  moving in a silicon crystal bent to a radius  $\mathcal{R} = 10^4 \text{ cm}$  and  $\mathcal{R} = 3 \times 10^5 \text{ cm}$  along the (111) axis. The simulation was carried out for a set of 100 particles. The ordinate and the abscissa of Fig. 21 give the angular coordinates of the particles at the exit from the crystal. The simulation was made for the particles entering the crystal along the (111) crystallographic axis. The



**Figure 21.** Angular distributions of negative (a, b) and positive (c, d) particles of energy  $\varepsilon = 300$  GeV (a, c) and  $\varepsilon = 10^4$  GeV (b, d) passing through a silicon crystal bent to a radius  $\mathcal{R} = 10^4$  cm (a, c), and  $\mathcal{R} = 3 \times 10^5$  cm near the  $\langle 111 \rangle$  axis.

distribution of the incident particles along  $x_0$  and  $y_0$  on the entry face of the crystal was assumed to be uniform.

It follows from these results that inclusion of the noncoherent effects in the scattering and axial channelling does not affect greatly the passage of particles through a bent crystal if the average values of the square of the angle of multiple noncoherent particle scattering in a crystal are small compared with the average square of fluctuations of the scattering angles, described by expression (5.16), due to the crystal bending. These results also demonstrate that when a beam is incident along a crystallographic axis of a bent crystal, large fractions of negative and positive particles in the beam may be deflected following the bending of the axis and the bending angle may exceed considerably the critical angle for axial channelling (for example,  $\theta_y \sim 8\psi_c$  in the case illustrated in Fig. 21b).

Fig. 22 shows the dependence, on the crystal thickness, of the fraction of negative particles in a beam moving along a bent crystallographic axis under axial channelling conditions (finite motion in a field of one of the atomic rows), and of the particles bent into the angular interval  $\Delta \theta \lesssim \psi_c$  relative to the running direction of the crystallographic axis. A comparison of these two curves shows that the dominant mechanism of bending of negative particles by bent atomic rows in a crystal is not axial channelling, but multiple azimuthal scattering of above-barrier particles by atomic rows in the crystal.

The exit angular distributions of positive and negative particles of energy  $\varepsilon = 300$  GeV are given in Ref. [70] for a beam of particles incident on a bent silicon crystal at the angle  $\psi_{in} = \theta_{x,0} = \psi_c$ ,  $\theta_{y,0} = 0$  relative to the (111) axis. The simulation results given in Ref. [70] show that the situation is as follows: some positive particles in the beam follow the bent crystallographic axis, but there are also several beam fractions which are trapped into planar channels and are bent following the shape of the relevant planes. Consequently, the incident beam splits into several beams along different angles. Such splitting does not occur in the case of negative particles.

It follows that the periodicity of the distribution of atomic rows in a crystal influences the passage of positive



**Figure 22.** Dependence, on the crystal thickness *L*, of the fraction of negative particles moving along bent rows of atoms in a silicon crystal under axial channelling conditions (1) and of particles deflected to the angular interval  $\Delta \psi \leq \psi_c$  relative to the running direction of the axis (2);  $\varepsilon = 10^4$  GeV,  $\mathcal{R} = 3 \times 10^5$  cm (Fig. 21b).

particles through a bent crystal, but does not affect significantly the passage of negative particles when the angle of incidence  $\psi = \psi_{in}$  is equal to several critical axial channelling angles  $\psi_c$ .

The results obtained suggest new opportunities for the control of the parameters of high-energy particle beams in accelerators, such as beam extraction from accelerators, splitting of a beam into several components, etc. We shall conclude that there have been as yet no experimental investigations of bending of beams of high-energy charged particles moving along a crystallographic axis in a bent crystal.

### 6. Conclusions

This review deals with the dynamics of high-energy charged particles in straight and bent crystals. It is shown that if motion occurs at small angles to one of the crystallographic axes, it is then governed mainly by the continuum potential of atomic rows in a crystal oriented along this axis. The continuum potential appears in a natural manner in motion investigated employing the Born approximation within the framework of quantum electrodynamics or classical electrodynamics. The continuum potential of rows of atoms in a crystal represents a complex periodic nonlinear function of two coordinates. Therefore, the task of investigating the motion of a particle in such a field belongs to the theory of nonlinear systems in which both regular and chaotic motion is possible. An important aspect is the stability of such motion. All these problems are encountered both in the finite motion of particles (channelling) and in the infinite (above-barrier) motion, relative to atomic rows in a crystal. The problem of abovebarrier motion of a particle in the periodic field of atomic rows in a crystal can be linked to the 'billiards' motion of a particle in an external field or to the elastic scattering of a particle by three disks located in one plane.

The nature of the motion of particles in a crystal and the conditions under which various types of motion take place are very important aspects in the selection of approximate analytic methods for the description of the interaction of particles with the lattice, particularly with a bent crystal. These approximations include the continuum potential of crystallographic planes and that of random collisions of a particle with atomic rows.

Analytic estimates and the results of numerical simulation of the passage of high-energy particles through a bent crystal given in this review demonstrate that under certain conditions a large fraction of beam particles may follow the bending of the crystallographic axis along which a beam is incident on the crystal. This mechanism of beam bending applies to both positive and negative particles and it is in the main due to the characteristics of multiple scattering of particles by atomic rows in a bent crystal. Detailed experimental investigations of the capabilities of this beam bending mechanism are still lacking.

Unfortunately, for lack of space, we have been unable to deal with many other manifestations of the different types of motion in the physical processes that accompany the passage of high-energy particles through a bent crystal, which include emission of coherent radiation under the conditions of real particle dynamics in a crystal [92], the influence of multiple scattering on the process of coherent emission of radiation from thin and thick crystals [66], resonant dechannelling [93], etc. Moreover, this review does not deal with general theoretical problems that belong to the theory of dynamic chaos, such as chaos in quantum systems, measure of chaos, and entropy. These concepts undoubtedly apply to the characteristics of particle beams moving in a crystal.

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