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Theory of a velocity focusing instrument for neutron small angle scattering

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Abstract

The theory of an instrument for small angle scattering of neutrons is discussed which uses velocity focusing by means of the gravitational field. It has a considerable intensity advantage compared to a conventional instrument. The advantage factor as a function of resolution is discussed together with different ways of using a multidetector system. The application of this method is provided for the small angle scattering instrument which is under construction for the very high flux reactor at the v. Laue-Langevin-Institut in Grenoble.

Zusammenfassung

Theorie einer Kleinwinkel-Streuapparatur mit Geschwindigkeitsfokussierung für Neutronen

Es wird die Theorie eines Instruments zur Messung der Kleinwinkelstreuung von Neutronen diskutiert, welches sich unter Benutzung der Schwerkraft einer Geschwindigkeitsfokussierung bedient. Die Anordnung besitzt einen ansehnlichen Intensitätsvorteil im Vergleich zu einem konventionellen Instrument. Der Gewinnfaktor wird als Funktion der instrumentellen Auflösung berechnet. Verschiedene Methoden der Verwendung von Multidetektoren werden diskutiert. Die Kleinwinkel-Streuapparatur, die sich für den Höchstfluß-Reaktor in Grenoble in Bau befindet, ist so ausgelegt, daß die Methode der Geschwindigkeitsfokussierung mittels Schwerkraft zur Anwendung gebracht werden kann.

EURATOM/INIS DESCRIPTORS

VELOCITY
FOCUSING
INSTRUMENTS
NEUTRONS
SMALL ANGLE SCATTERING
GRAVITATION
RESOLUTION

1. Introduction

Small angle scattering of neutrons and of x-rays is an important method to study structures and fluctuations of large period or of extended correlation range (30 ... 3000 Å). The main application of neutron small angle scattering concerns the investigation of magnetic systems. Many problems of this kind have been studied so far and are, at the same time, of further interest, for instance the study of critical magnetic scattering in ferromagnets, which has been performed by numerous authors [1], the study of vortex lines in supra conductors [2], the investigation of dislocation lines in cold worked ferromagnets [3; 4], and the investigation of periodic precipitation structures in hard ferromagnetic materials [5]. There are also cases where neutron small angle scattering is supplementary to x-ray scattering, as for the study of organic macro molecules [6], of large precipitations in metals, and of density or concentration fluctuations at the critical point of gases, of liquid mixtures, and of alloys. Furthermore, scattering on edge dislocations has not yet been successfully studied with x-ray scattering but with neutrons [7; 8] where double–Bragg scattering can be avoided by the choice of a sufficiently large wave-length.

The main draw-back of neutrons compared to x-rays is the relatively small luminosity of the available neutron sources. However, this can be compensated by the availability of larger sample and source areas, and by the greater flexibility concerning the choice of the neutron wave length and the wave length resolution which can be adapted to the special problem which is under investigation [9].

In the following we describe and discuss a new type of instrument for small angle scattering of slow neutrons which has a considerable intensity advantage compared to conventional instruments. It applies the principle of velocity focusing by means of the gravitational field. The basic ideas concerning focusing by means of gravitation have been discussed in a paper by *Maier-Leibnitz* [10] in connection with the development of the gravitation refractometer at the FRM reactor [11].

In the theoretical discussion of such an instrument we consider only scattering on static fluctuations and structures which means that the scattering process is purely elastic. Under these circumstances the quantity to be measured is the elastic differential scattering cross section $d\sigma/d\Omega$ which is only a function of the scattering vector $\varkappa = \boldsymbol{k}_0 - \boldsymbol{k}$ with

$$\varkappa = (4\pi/\lambda)\sin(\vartheta/2) \simeq 2\pi\vartheta/\lambda$$

(ϑ scattering angle, $k_0 = k = 2\pi/\lambda$ wave number; λ neutron wave length). $\hbar\varkappa$ is the momentum transfer during the scattering process.

2. Principle of the velocity focusing instrument

A conventional small angle scattering instrument where the momentum transfer is measured in the horizontal plane is shown in Fig. 1 a. The projection of the neutron paths before and after the scattering process in the sample are straight lines. If the momentum transfer is measured in the vertical y-direction (Fig. 1 b) the neutron path are curved in the (y, z)-

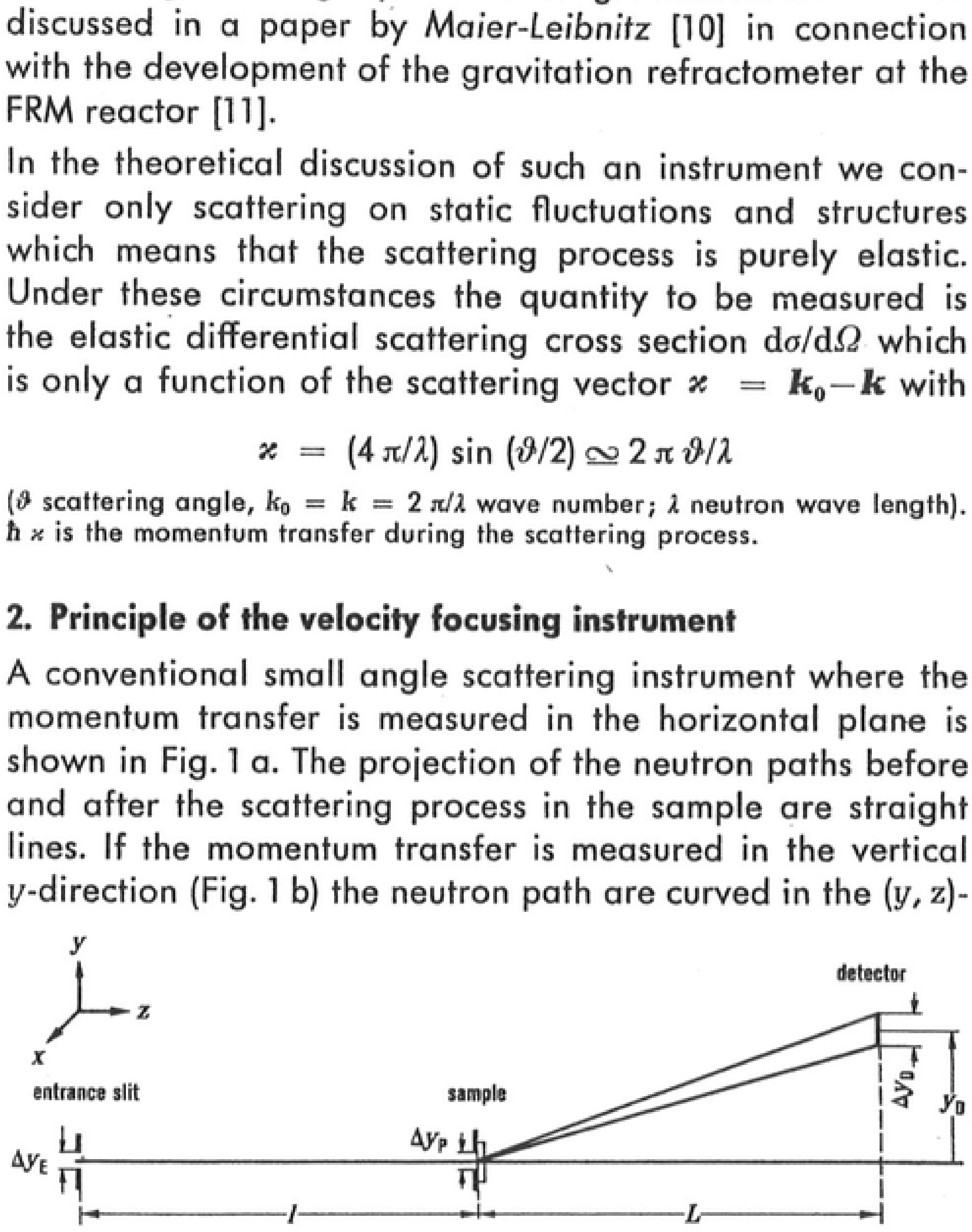

Fig. 1 a: Schematic view of a conventional neutron small angle scattering instrument. The gravitational force is perpendicular to the (y, z)-plane.

Fig. 1 a: Schematische Ansicht einer konventionellen Neutronen-Kleinwinkel-Streuapparatur. Die Schwerkraft liegt senkrecht zur (y, z)-Ebene

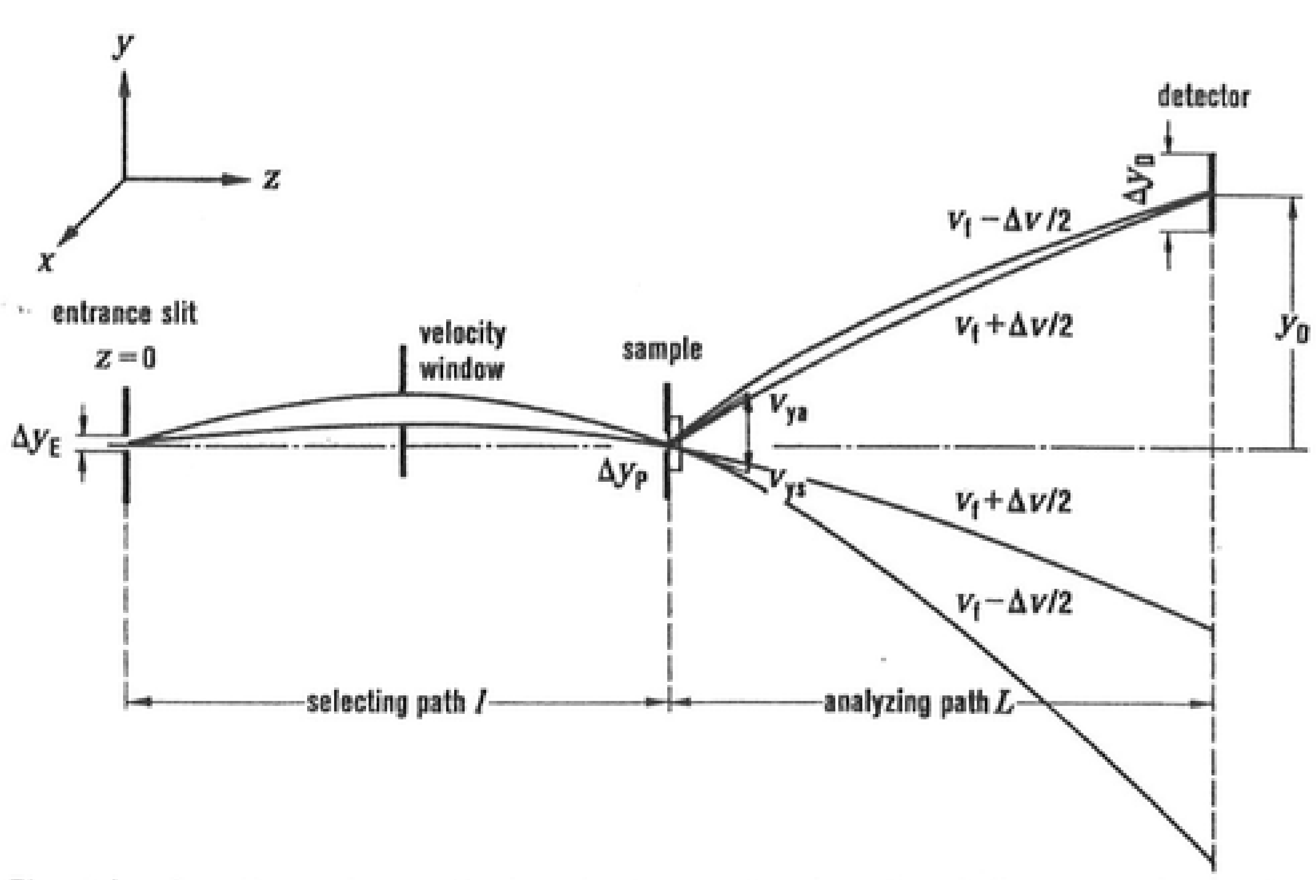

Fig. 1 b: Small angle scattering instrument using the influence of gravity. Gravitational force parallel to y-direction.

Fig. 1 b: Kleinwinkel-Streuapparatur, welche den Einfluß der Schwerkraft ausnützt. Schwerkraft parallel zur y-Richtung plane due to the gravitational field. The system works in the following way: Neutrons which originate from a neutron conducting tube pass through the selection path (length l), and then, between sample and detector, through the analyzing path (length L). The widths of the entrance slit, of the sample aperture and of the detector are Δy_E, Δy_P, and Δy_D, respectively. The paths of the neutrons are ballistic parables (the Coriolis force can be neglected). The apertures between the entrance slit and the sample are provided for a rough selection of a certain interval of neutron velocities. A velocity selection of this kind is not sufficient for high resolution work, and a mechanical selector with helical slits should be used.

The vertical distance of the detectors from the instrumental axis is called y_D. The velocity components in the vertical direction at the sample position are $\check{v}_{ys}$ and $\check{v}_{ya}$ before and after scattering, respectively. The momentum transfer for elastic scattering, $\hbar\varkappa$, is then

$$\hbar\varkappa = m(\check{v}_{ya} - \check{v}_{ys})$$

if we assume that the scattering angle and the divergency of the incident beam is small compared to unity. For simplification we introduce the momentum transfer in units of the velocity

$$K = \check{v}_{ya} - \check{v}_{ys} \tag{1}$$

(1 m/s corresponds to $1{,}59 \cdot 10^{-3}$ Å^{-1}). For neutrons which are crossing the entrance slit ($z = 0$) at $y = y_E$ and the sample ($z = l$) at y_P the following equation holds

$$\check{v}_{ys} = (y_P - y_E)\, v/l - g\, l/2\, v \tag{2}$$

(g gravitational acceleration constant). Neutrons which hit the detector at y_D fulfil the relation

$$\check{v}_{ya} = (y_D - y_P)\, v/L + gL/2\, v \tag{3}$$

Therefore, for a scattering process with a momentum transfer K one finds from Eqs. (1), (2) and (3)

$$K = v\left(\frac{y_D - y_P}{L} - \frac{y_P - y_E}{l}\right) + \frac{g(L + l)}{2v} \tag{4}$$

$K(v)$ has a flat minimum for a certain velocity $v = v_f$. At this velocity the width of K is determined by the width of the velocity spectrum only by second order. This fact has been called "velocity focusing" in Sec. 1. From $\partial K/\partial v = 0$ one obtains an equation to determine v_f:

$$\left(\frac{y_D - y_P}{L} - \frac{y_P - y_E}{l}\right) v_f = \frac{g(L + l)}{2\, v_f} \tag{5}$$

From (4) and (5) one finds the corresponding K-values as a function of L

$$K_f = g(L + l)/v_f \tag{6}$$

With Eqs. (4), (5) and (6) one has

$$\frac{K}{K_f} = \frac{1}{2}\left(\frac{v}{v_f} + \frac{v_f}{v}\right) \tag{7}$$

This function is shown in Fig. 2. The detector positions which fulfil the condition of focusing for a given $v = v_f$ and for a fixed l are situated on a parabola. This is shown in Fig. 3 where also possible arrangements of detectors for simultaneously registration are indicated (Sect. 4). Obviously, the effect of focusing acts only on the component of the scattering vector K parallel to the direction of gravity. Consequently, it is appropriate to use slit-shaped apertures

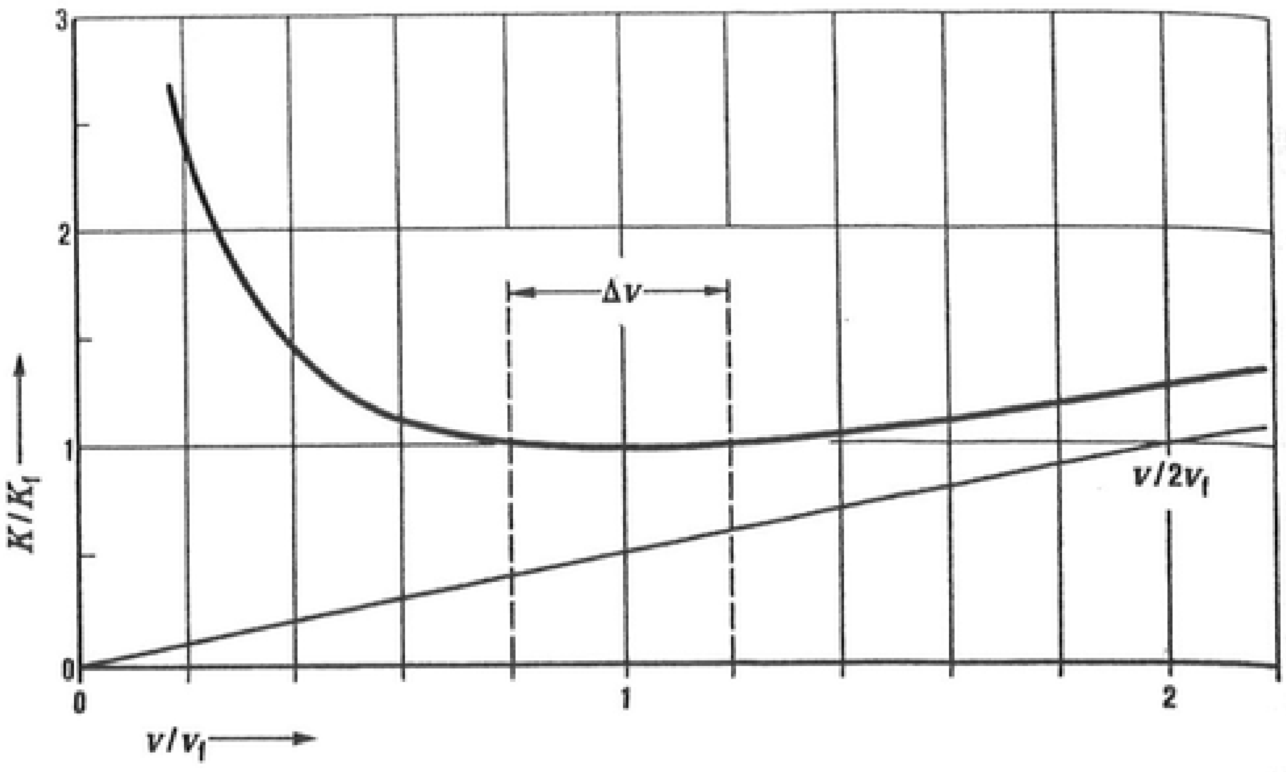

Fig. 2: Momentum transfer K as a function of the velocity v of the incident neutrons. K and v are given in dimensionless units (v_f = velocity where the focusing condition holds). Δv indicates the width of the incident spectrum which is centered at v_f. The asymptotic line concerns the nonfocusing case

Fig. 2: Impulsübertrag K als Funktion der Geschwindigkeit v der einfallenden Neutronen. K und v in dimensionslosen Einheiten (v_f ist die Geschwindigkeit, welche die Fokussierungsbedingung erfüllt). Δv bedeutet die Breite des einfallenden Spektrums, dessen Schwerpunkt bei v_f liegt. Die Asymptote betrifft den Fall ohne Fokussierung

with their long axis in the horizontal direction and to analyze the K-component only perpendicular to the slit axis.

The resolution width of the momentum transfer K contains geometrical contributions which are due to the vertical width of the detector, Δy_D, the width of the entrance slit, Δy_E, and the width of the sample, Δy_P. Furthermore, there is a contribution from the width of the velocity spectrum Δv, which is proportional to Δv^2 if the focusing condition (5) is fulfilled. A Taylor expansion of Eq. (4) gives

$$\begin{aligned}\delta K = {} & \delta y (v/L) + \delta y_E (v/l) + \delta y_P (v/L + v/l) + \\ & + \delta v\left[\frac{y_D - y_P}{L} - \frac{y_P - y_E}{l} - \frac{g(L + l)}{2\, v^2}\right] + \\ & + \frac{\delta v^2\, g(L + l)}{2\, v^3} + \text{mixed terms}\end{aligned} \tag{8}$$

where δ are small deviations from the nominal values y and v. The geometrical terms in the first line are the same as for an instrument without gravity influence.

To obtain an estimation of the total resolution width of K, we assume that the distributions of all quantities contribut-

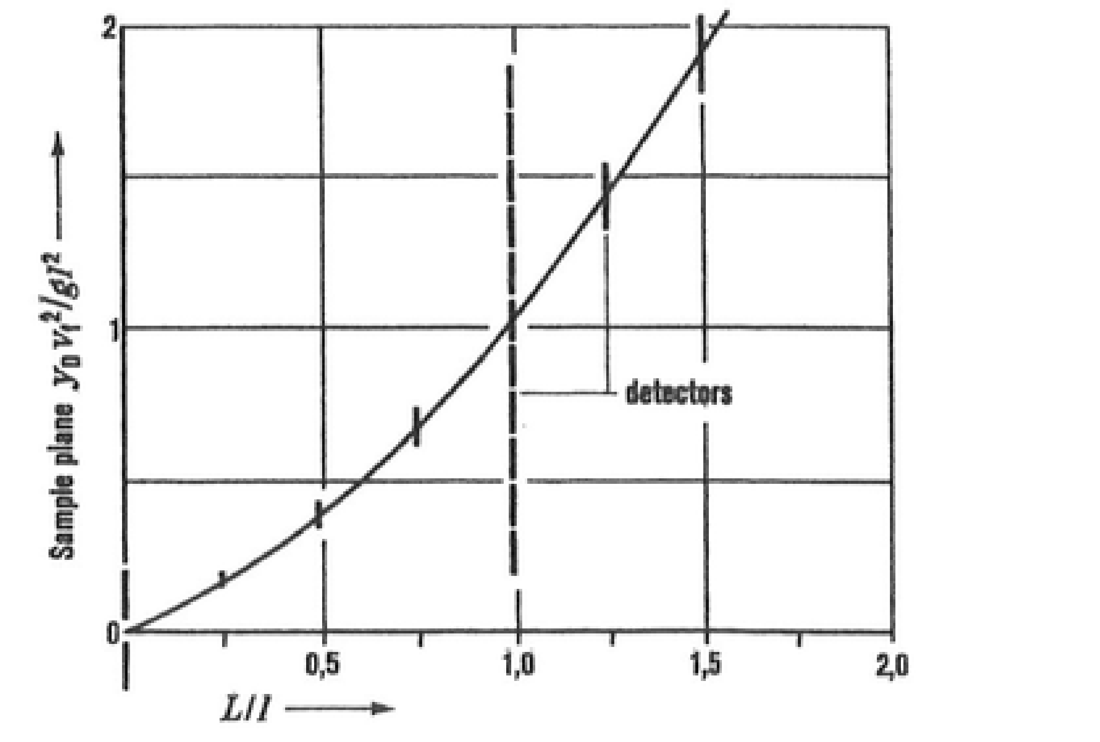

Fig. 3: The parabel at which the condition of focusing holds. Detector position y_D in dimensionless units. K_{f0} is K_f at $L = l$. The detectors are indicated for two possible arrangements (multidetector of the "ladder" type and of the "plane" type)

Fig. 3: Parabel, auf welcher die Fokussierungsbedingung erfüllt ist. Detektorposition y_D in dimensionslosen Einheiten. K_{f0} ist K_f für $L = l$. Die Detektoren sind für zwei mögliche Anordnungen gezeichnet (Multidetektor vom »Leiter«-Typ und in ebener Anordnung)

ing to δK are not correlated among each other. Then we can write

$$\langle(\delta K-\langle\delta K\rangle)^2\rangle = \langle\delta y_D^2\rangle(v/L)^2+\langle\delta y_E^2\rangle(v/l)^2+\delta y_P(v/L+v/l)^2+$$
$$+\langle\delta v^2\rangle\left[\frac{y_D-y_P}{L}-\frac{y_P-y_E}{l}-\frac{g(L+l)}{2v^2}\right]^2+$$
$$+(\langle\delta v^4\rangle-\langle\delta v^2\rangle^2)\,g^2(L+l)^2/4v^6+\text{ mixed therms} \quad (9)$$

If the velocity focusing condition holds, the term proportional to $\langle\delta v^2\rangle$ vanishes. Assuming that the probabilities for a neutron crossing the entrance slit, the sample and the detector are constant within the limits $-\Delta y/2 \leq \delta y \leq /2$, and zero otherwise, one finds

$$\langle\delta y^2\rangle = \Delta y^2/12 \quad (10)$$

with indices E, P and D. Correspondingly one obtains

$$\langle\delta v^2\rangle = \Delta v^2/12 \quad (11)$$

and

$$\langle\delta v^4\rangle - \langle\delta v^2\rangle^2 = \Delta v^4/180 \quad (12)$$

The mixed terms proportional to $\delta v\,\delta y$ vanish because of the independence of the velocity and the space coordinates.

3. Optimization of Intensity

For a given K-resolution a broader width of the incident velocity spectrum is allowed in the focusing case than for a conventional instrument. In the following we calculate the corresponding intensity gain for an instrument which is optimized for a given resolution width. The number of neutrons per unit time which hit a surface element $dx_p\,dy_p$ of the sample within an element in momentum space $m^3 dv_{xs}\,dv_{ys}\,dv_z$ is given by [12]

$$dJ_P = \left(\frac{\Phi}{2\pi}\right)e^{-v^2/v_T^2}\frac{v\,dv_{xs}\,dv_{ys}\,dv}{v_T^4}\,dx_P\,dy_P \quad (13)$$

with $dv_z \cong dv$. Φ is the total thermal neutron flux. The velocity distribution is assumed to be Maxwellian with an average velocity $v_T = (2\,k_B\,T/m)^{1/2}$. T is the neutron temperature. The number of neutrons scattered from this sample element into a solid angle $d\,\Omega$ of the detector is then

$$dJ_D = dJ_P\,\frac{d\Sigma(\varkappa)}{d\Omega}\,D\,e^{-D\,\Sigma_t(v)}\,d\Omega \quad (14)$$

$d\Sigma/d\Omega = N\,d\sigma/d\Omega$ is the macroscopic scattering cross section for small angle scattering (N = particle density). D is the sample thickness. Σ_t is the total macroscopic cross section of the sample. We assume a slit geometry and detectors being sufficiently long in the x-direction. Then one has to introduce a cross-section which is integrated to infinity with respect to the x-component of K

$$S(K_y) = \int_{-\infty}^{+\infty}\frac{d\Sigma(K_x,K_y)}{d\Omega}\,dK_x \quad (15)$$

For a sufficiently small width of the apertures and of the spectrum the total number of neutrons hitting the detector per unit time can be approximated as[1]

$$\Delta J_D = (\Phi/2\pi)\,e^{-v^2/v_T^2}(v^2\Delta v/v_T^3)\,\Delta x_P\,\Delta x_E(\Delta y_E\,\Delta y_P\,\Delta y_D/Ll^2)\cdot$$
$$\cdot\frac{D\,S(K_y)}{v_T}\,e^{-D\,\Sigma_t} \quad (16)$$

[1] The width of the incident spectrum is necessarily large. In spite of this it can be shown that the error in replacing $\int\ldots dv$ by Δv can be neglected.

where we have used

$$\Delta v_{xs} = \Delta x_E\,v/l;\ \Delta v_{ys} = \Delta y_E\,v/l;\ \Delta v_{ya} = \Delta y_D\,v/L$$

We introduce a dimensionless resolution

$$b^2 = b_g^2 + b_v^2 = \langle(\delta K-\langle\delta K\rangle)^2\rangle/K^2 \quad (17)$$

where b_g is the geometrical component of the total resolution width, and b_v is due to the width of the velocity spectrum. From (9) to (12) one has

$$b_g^2 = (v^2/12\,K^2)\left[\Delta y_D^2/L^2+\Delta y_E^2/l^2+\Delta y_P^2(1/L+1/l)^2\right] \quad (18)$$

and

$$b_v^2 = (\Delta v/v)^4/720 \quad (19)$$

if the focusing condition is fulfilled, and

$$b_v^2 = (\Delta v/v)^2/12 \quad (20)$$

in the case of an instrument without influence of gravity on resolution (Fig. 1 a). The rate ΔJ_D is now differentiated with respect to Δy_E, Δy_p, Δy_D, Δv, and put equal to zero. Combining these equations with the condition that the resolution b^2 in Eq. (17) has a fixed value, one obtains the optimum choice of the experimental parameters, which should be applied, namely:

$$\Delta y_E/\Delta y_P = 1+(l/L) \quad (21)$$

$$\Delta y_D/\Delta y_P = 1+(L/l) \quad (22)$$

$$\Delta v/v = \Delta y_P\,(v/K)\,(1/L+1/l) \quad \text{(non-focusing)} \quad (23)$$

$$\Delta v/v = \left[\Delta y_P(v/K)\sqrt{30}\,(1/L+1/l)\right]^{1/2} \quad \text{(focusing)} \quad (24)$$

From practical arguments, a reasonable choice would be

$$\Delta y_E \cong \Delta y_D \cong 2\,\Delta y_P \quad \text{or} \quad L = l.$$

It is clear that the focusing case permits a velocity width which is considerably larger than in the case without focusing. Introducing (21) to (24) into (16) one obtains the optimum value of the rate

$$\Delta J_D^{opt} = \left(\frac{\Phi}{2\pi}\right)e^{-v^2/v_T^2}\,\Delta x_P\,\Delta x_E\,\frac{DS}{v_T}\,e^{-1}\,\frac{L}{(L+l)}\cdot$$
$$\cdot\begin{cases}9\,(b\,K)^4/v_T^3K & \text{(non-foc.)}\\ \alpha(b\,K)^{7/2}/v_T^3\,K^{1/2} & \text{(foc.)}\end{cases} \quad (25)$$

with $\alpha = (720/7)^{1/4}\,(24/7)^{3/2} \cong 20$. In (25) it has been used that the optimum choice of the sample thickness D is $D = 1/\Sigma_t$. For a sample where Σ_t is proportional to $1/v$, the optimum neutron velocity v_0 can be shown to be $v_0 = v_T/\sqrt{2}$. One concludes that, for an instrument with an optimum lay-out of all its parameters the intensity is proportional to the power 4 or 3,5 of the K-resolution. Because of the K-dependence of ΔJ_D the optimization is only possible for a selected value of K. From Eq. (25) the ratio of the intensities at the detector for a focusing (F) and a non-focusing (N) system is then

$$\frac{\Delta J_D^{opt(F)}}{\Delta J_D^{opt(N)}} = \frac{\alpha}{9\sqrt{b}} \simeq \frac{2{,}2}{\sqrt{b}} \quad (26)$$

For a resolution of $b = 0{,}05$ the "gain" is about 10.

4. Simultaneous measurements

It is desirable to investigate the scattering law for various K-values at the same time. In this case two multidetector arrangements are to be considered (see Fig. 3): (I) The axis of the detectors is situated on a parabola (like the rungs of a curved ladder) such that the focusing condition holds for each of them *("ladder system")*. (II) The detectors are arranged within a *plane* which is perpendicular to the axis of the instrument. In this case, the focusing condition can be fulfilled approximately only for a certain region of the detector system.

In Fig. 4, the resolution b is plotted for the ladder system as a function of K, i.e. of the distances L between the sample and the detectors. The various resolution contributions with respect to the space coordinates and the velocity have been chosen accordingly to the conditions of optimization as given in Sec. 3 (applied for a selected detector position $l = L$). The detector width has been assumed to vary with increasing distance L as $\Delta y_D = \Delta y_E(L/l)$. The resolution b is given in units of its value at $l = L$, $b_0 = \Delta y_P(v_F/K_f L) \cdot \sqrt{7/6}$. The strong increase of the resolution at small L or K is due to the geometrical contributions. The contribution $b_v = b_0/\sqrt{7}$ is constant over the whole range (thin line).

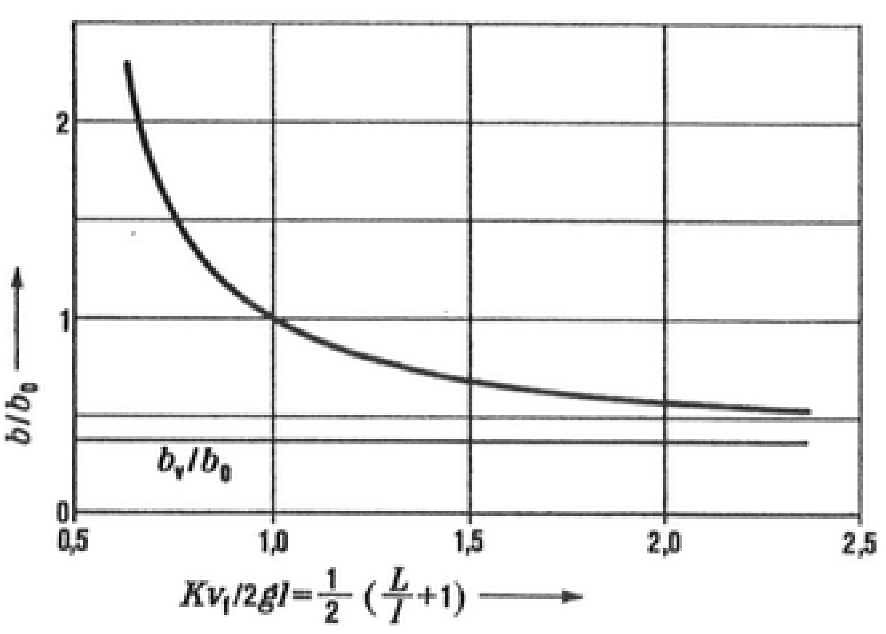

Fig. 4: Resolution b for a multidetector of the "ladder" type as a function of K, i.e. of the detector position L

Fig. 4: Auflösung b für einen Multidetektor vom »Leiter«-Typ als Funktion von K, d. h. von der Detektorposition L

Fig. 5 shows the resolution for the plane detector system with $L = l$. The optimization has been applied for the detector position where b_v has its minimum. In this case it is not possible to give a general resolution curve b/b_0 as in Fig. 4. b_g has been chosen as 0,05 $\sqrt{6/7}$ and b_v accordingly to Eqs. (18), (19), (24) as $0{,}05/\sqrt{7}$.

We conclude that for a simultaneous measurement of the scattered intensity the multidetector of the *"ladder"* type has the advantage that the K-width due to the spectral range is small by second order at all K-values. At small K-values, however, the sample-detector distance has to be small (eq. 6) and the geometrical contribution to the resolution becomes large. This restricts the accessible range at small K-values, especially if large samples are to be used. If samples of a large width are available, a *plane* multidetector is preferable because a great sample-detector distance can be chosen which is the same at all K-values. Of course, in this case the focusing condition is fulfilled only for one detector position and the full advantage of focusing holds only there.

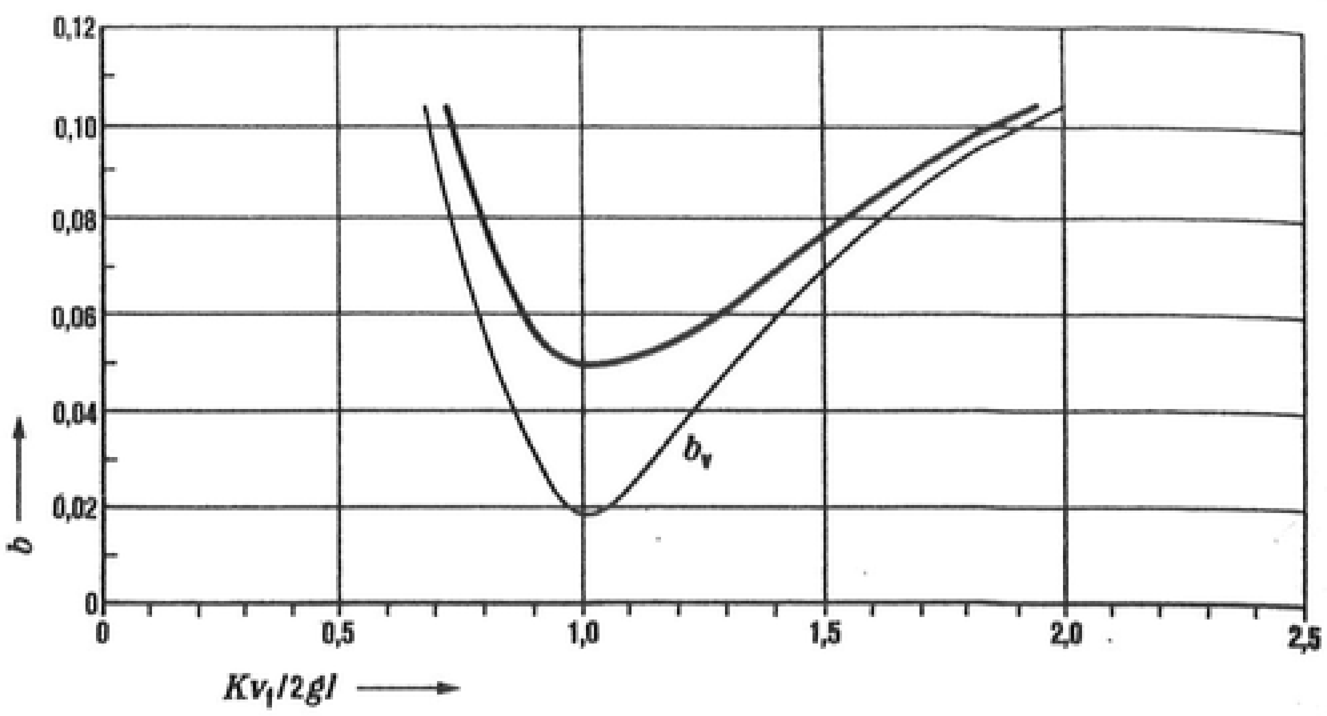

Fig. 5: Resolution b as a function of $K\check{v}_f/2\,gl$ for a plane multidetector system. The condition of velocity focusing holds at $Kv_f/2\,gl = 1$. The parameters have been optimized for this point and chosen in such a way that $b = 0{,}05$

Fig. 5: Auflösung b als Funktion von $K\check{v}_f/2\,gl$ für einen ebenen Multidetektor. Die Bedingung für Geschwindigkeitsfokussierung gilt für $Kv_f/2\,gl$. Die Parameter sind für diesen Wert optimalisiert und so gewählt, daß $b = 0{,}05$

Assumming a sample width of 0,5 cm, a detector width of 1,0 cm, and a velocity width of $\Delta v/v = 0{,}47$ at $v = 400$ m/s, a plane multidetector with a diameter of 64 cm covers a K-range from about $0{,}17 \cdot 10^{-3}$ to $1{,}2 \cdot 10^{-3}$ Å^{-1}, where b changes between 0,03 and 0,1. For a multidetector of the *ladder* type with a maximum length of 80 meters, and with the data as given before, the K-values cannot be higher than $0{,}3 \cdot 10^{-3}$ Å^{-1}.

The instrument which is under construction at the very high flux reactor at the v. Laue-Langevin-Institut in Grenoble uses a plane detector with 64×64 channels, 1×1 cm^2 each. L and l are variable between 2,5 and 40 meters. It will be possible to use vertical as well as horizontal slits to apply the principle of focusing as described in this article.

(Received on 10. 9. 1970)

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