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Phase Space and Phase Space Transformations

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Abstract

The large advantage of a pulsed neutron flux consists in the applicability of time dependent phase space transformations. A large number of neutrons are wasted, if the same transformations are applied at a steady state source. Three typical examples of phase space transformations at a pulsed neutron source will be discussed. The first example is the well known time of flight technique. Neutron bunching is an example of a phase space transformation performed by time and by forces (moving crystal). In the last example, the Doppler instrument, only a force is used to transform a phase space volume. The shape is time independent. The last two techniques have not been used on steady state sources, however, they may become very attractive on pulsed sources because in addition to the gain of the peak flux an extra gain of about 10 for the bunching spectrometer and 20 for the Doppler instrument have been estimated as compared to conventional techniques like chopper and rotating crystal instruments (IN5 and IN4 at the ILL in Grenoble).

Introduction

The phase space concept was first applied by Maier-Leibnitz to intensity and resolution considerations of neutron scattering instruments and experiments /1/. One advantage is the fact that the natural quantity "momentum", which plays a superior role in neutron scattering theory, is used in this formalism. In contrast, intensity and resolution considerations with quantities like wavelength, energy and solid angle are very cumbersome. As has been pointed out by Maier-Leibnitz and Springer, another great advantage of the phase space concept is the direct application of Liouville's theorem to a "neutron gas" /2/. This theorem tells us, that the phase space density remains unchanged during the free propagation of a neutron beam or in a transformation of the coordinate system (e.g. Bragg reflection, mirror reflection) and under the influence of conservative forces (such as gravity, magnetic field gradients or moving crystals). The behaviour of a phase space volume can be compared with an incompressible liquid /3/. This means that the shape of the phase space volume can easily by changed, but not the density. For neutron scattering instrumentation Liouville's theorem plays a similar role as the second law of thermodynamics at least in the sense that from time to time "ingenious" devices are discussed seriously, which are meant to increase the phase space density, these devices are analogous to a perpetuum mobile of the second kind.

Phase Space and Neutron Intensity

The phase space density is defined as

$$\frac{\Delta^6 n}{\Delta V_p} = \frac{\Delta^6 n}{\Delta k_x \Delta k_y \Delta k_z \Delta x \Delta y \Delta z \cdot \hbar^3}$$

n is the number of neutrons in the phase space volume.

For a Maxwellian distribution one obtains

$$\frac{\Delta^6 n}{\Delta V_p} = \frac{\Phi m}{2\pi \hbar^4 k_T^4} e^{-k^2/k_T^2}$$

$$\text{with } k_T = \sqrt{2mk_B T}/\hbar$$

It is important to note that for a fixed k there is one moderator temperature for which the phase space density has a maximum. The intensity of a neutron beam in z-direction through an area ΔF(sample area) is proportional to the phase space density in the moderator

$$\Delta^5 J = \frac{\Phi k_z}{2\pi k_T^4} e^{-k_z^2/k_T^2} \Delta k_x \Delta k_y \Delta k_z \Delta F$$

The most important task for a neutron scattering experiment is the optimization of the intensity and the resolution. With respect to k, the best what has been achieved up to now is the installation of three different moderators, a hot, a thermal and a cold moderator (ILL). What remains to be done is the selection and shaping of the momentum space volume $\Delta k_x \Delta k_y \Delta k_z$. In the following it will be shown that the phase space concept is very useful to treat this problem, expecially for a pulsed neutron source.

Phase Space Transformations

a) Time dependence of the phase space volume of a short neutron pulse

We consider the most important case of a phase space transformation at a pulsed neutron source, the development in time of the phase space volume of a short polychromatic neutron pulse. To simplify the discussion, it is assumed that the neutron pulse is propagating within a neutron guide tube in z-direction. In this case the time dependent phase space volume is two-dimensional, because the x- and y-componets and their conjugate components are conserved.The abscissa in Fig. 1 represents the z-coordinate on the ordinate the conjugate variable k_z is shown. The phase space volume at

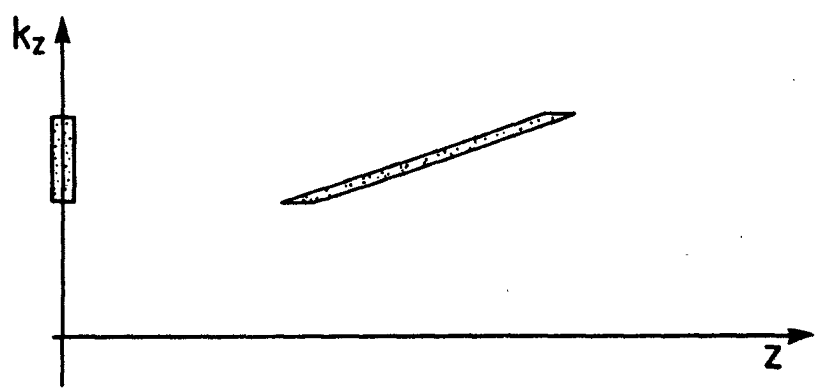

Fig. 1: The time dependence of a twodimensional phase space volume of a short neutron pulse propagating in a neutron guide tube. In this case the four other dimensions of the phase space volume are time independent.

t = 0 is represented by a rectangular area at z = 0. This area is homogeniously filled with neutrons. Due to the fact that the neutrons in the upper part of the area move faster than the neutrons in the lower part, the area will be elongated in z-direction after a time t_1. The area and hence the phase space density is conserved. The elongation of the area in z-direction is proportional to the flight path. This kind of phase space transformation serves to separate neutrons of different velocities in space or at a fixed point z in time. This is the fundamental technique in all time of flight methods to separate neutron velocities. It is obvious that this technique is especially useful for pulsed sources, because all the neutrons, which are produced in the moderator, are contained in th phase space volume (at least in the ideal case), whereas on a steady state source short pulses have to be cut out of the continous beam, leading to a loss factor of neutrons given by t_n/T, where t_n is the pulse length and T is the repetition rate.

b) Neutron bunching

A high resolution time focussing spectrometer, also called bunching spectrometer, was proposed by Maier-Leibnitz fifteen years ago /4/. This type of instrument never was built on a continous source. But on a pulsed source, this instrument may become very attractive. Its principle is based on a phase space transformation inverse to the one described in section a. In Fig. 2 again a twodimensional phase space is shown. At z = 0 a space volume of which $\Delta z = v_0 t_n$ is produced in the moderator. The width Δk_z can be produced with choppers. One special transformation is shown for a distance far outside the shielding of the neutron source. From now on we consider only those neutrons which are contained in the dashed perpendicular stripe. After an additional length L_B (bunching length) the elongated dashed stripe is selected and transformed into the stripe below. After the distance L_B backwards on the z-axis this phase space volume is focused in space and time. The realization of this phase space transformation can be performed with a moving crystal which slows down the neutrons which are faster and speeds up those neutrons which are slower than the mean velocity v_0. The time dependence of the neutron velocity in the dashed area at L_B is given by

$$v(t) = v_o - \frac{v_o^2}{L_B} t$$

(Neutrons with the velocity v_0 arrive at the crystal at t = 0). If the crystal at rest reflects a velocity v_0 then it has to be moved with a velocity

$$v_D(t) = -\frac{v_o^2}{L_B} t$$

because the relative velocity between the neutrons and the moving crystal has to be v_0. First the crystal has to be moved in the direction of the neutron beam (away from the source), at the arrival time of v_0 the direction is turned (v_D = 0) and then it moves against the beam. It follows that the neutron velocity are shifted from

$$v(t) = v_0 + \frac{v_0^2}{L_B}t \quad \text{to} \quad -v_0 - \frac{v_0^2}{L_B}t$$

which gives the transformation shown in Fig. 2. After this velocity transformation the phase space volume is transformed by time of flight into the perpendicular stripe. It should be mentioned that this bunching technique is very similar to that applied in accelerators /5/. A rather detailed

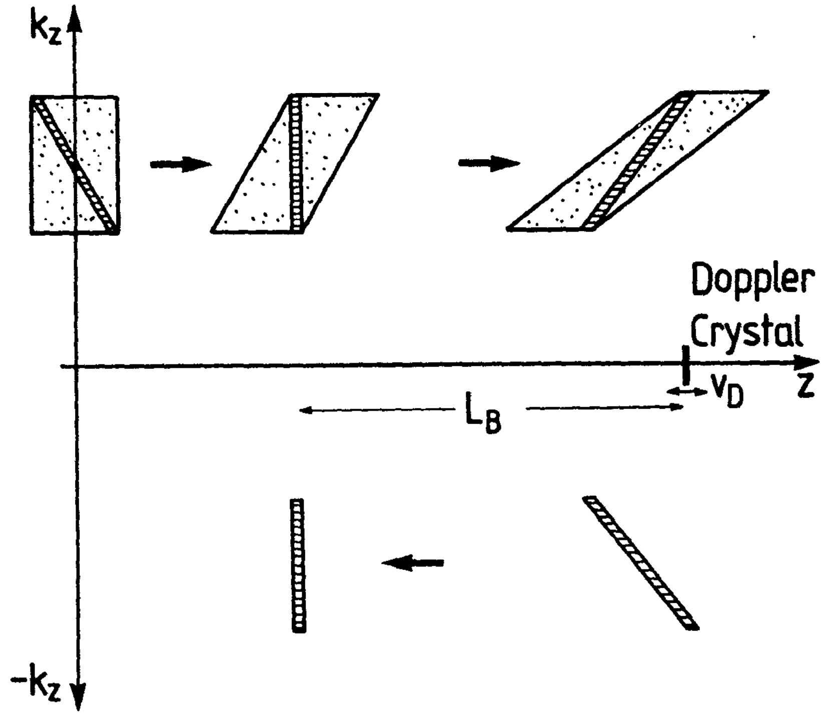

Fig. 2: Phase space transformation of the bunching instrument. The hatched part of the whole neutron pulse near the moderator (z = 0) is first transformed by time of flight, then it is backscattered by a moving crystal and transformed into the lower part of the (k_z, z)-plane. This phase space volume is refocussed after the distance L_B.

discussion on the realization of a bunching spectrometer at a pulsed source has been given by RICHTER and ALEFELD /6/. It was shown that in addition to the gain of the peak flux of a pulsed source a factor of about 10 is gained as compared to a nonfocusing spectrometer with the same resolution of about $\Delta E/E = 10^3$.

c) The increase of the phase space density by a fast moving crystal at thermal energies.

It has been shown above that the phase space density of a neutron spectrum in thermal equilibrium with the moderator is given by

$$\frac{\Delta^6 n}{\Delta V_p} = \frac{\Phi m}{2\pi \hbar^4 k_T^4} e^{-k_z^2/k_T^2}$$

Fig. 3 shows the phase space density of a cold moderator with a temperature of 50 K and of a thermal moderator with a temperatur of 350 K. If it is possible to shift the phase space density of the cold moderator to a higher k_z value one obtains a phase space density which is higher than available from the source. In Fig. 3 it was assumed that the phase space density for a wave vector k_z can be shifted to a wave vector $(k_z + 1.59)$ Å^{-1} which is equivalent to a shift from the velocity v_z to the velocity $(v_z + 1000)$ m/s. The highest gain factor of 28 is obtained by shifting neutrons with $k = 1.4$ Å^{-1} to a wave vector $k = 3$ Å^{-1}. This corresponds to a shift from 889 m/s to 1889 m/s. In Fig. 4 this phase space transformation is again shown in the twodimensional phase space of a neutron guide tube. We assume that the pulse length of the source is 350 μs for all velocities. The twodimensional phase space volume of the neutron pulse near to the moderator is shown at z = 0. A nearly monochromatic region around the velocity 889 m/s is labeled with the letter a. The whole phase space volume moves to the right and at a distance of about 20 m a crystal in back reflection is moved with a velocity of 500 m/s against the neutron beam. The lattice spacing of the crystal is chosen in such a way that it would reflect neutrons with a velocity of 1389 m/s if it were at rest. The moving crystal picks up the neutrons around the velocity 889 m/s (labeled with b) and after the reflection the neutrons are transformed to the velocity $-(889 + 2v_D) = -1889$ m/s, this part is labeled with c. First of all we see that the pulse length of the original neutrons of 350 μs is compressed to a pulse length of 164 μs. For most applications, this pulse length still is too long. A simple possibility to shorten the pulse length is to rotate the crystal during the reflection time. In this case the condition for back reflections is time dependent. If the crystal is out of back reflection by an angle α the angle of the reflected neutrons relative to the neutron guide is changed by 2 α. A pulse length of $t_n = \Delta\alpha/\omega$ is expected, where $\Delta\alpha$ is the divergence for neutrons with the velocity 1389 m/s. This value is 10^{-2} rad for a nickel

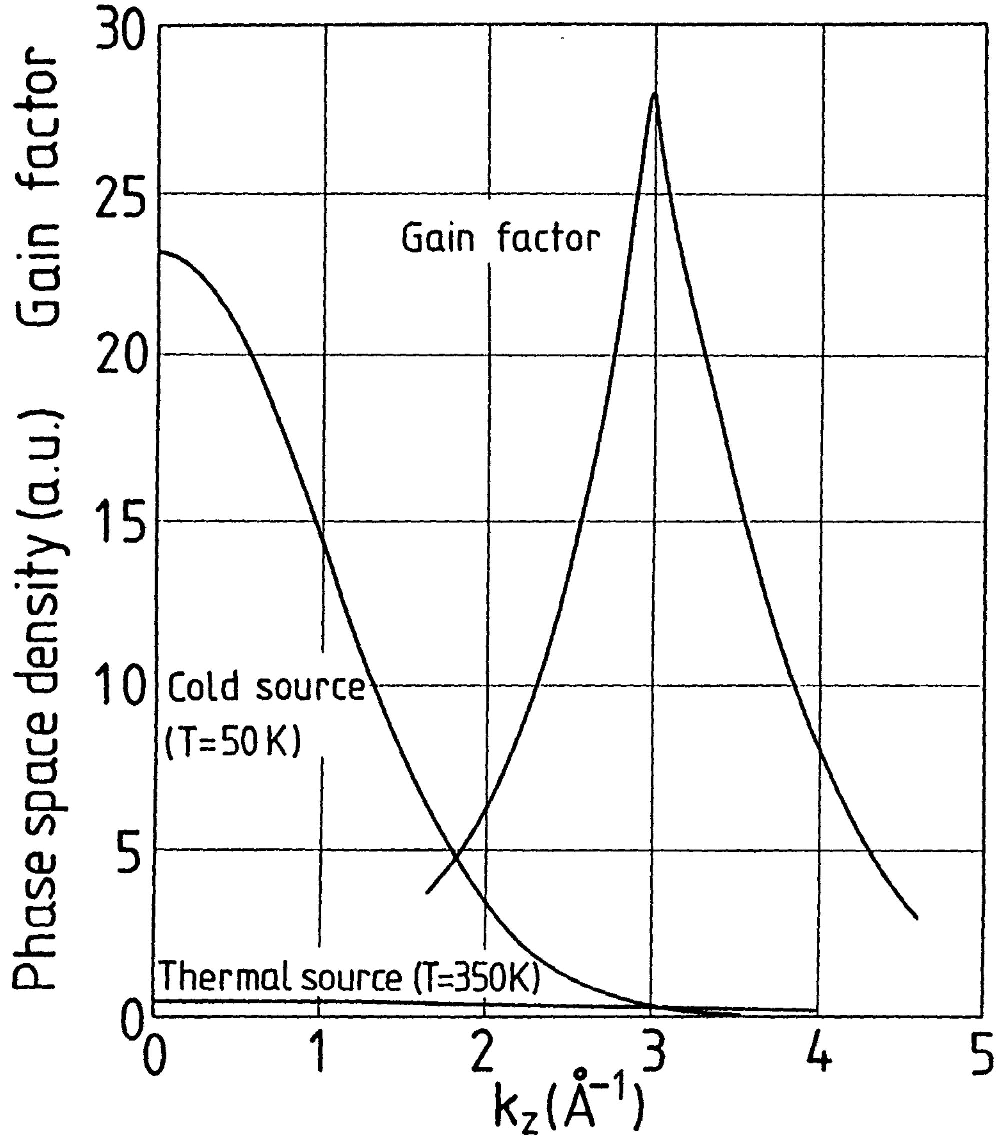

Fig. 3: The phase space density $\Delta^6 n/\Delta^6 V_p$ of a cold moderator (T = 50 K) and a thermal moderator (T = 350 K). The gain is obtained by shifting neutrons from k_z to $(k_z + 1.59)$ Å^{-1} which is equivalent to a shift from v_z to $(v_z + 1000)$ m/s. For $k_z < 3$ Å^{-1} the gain factor is defined as the ration between $\exp-(k_z-1.59)^2/k^2_{T=50}$ and $\exp-k_z^2/k^2_{T=50}$. For $4.59 > k_z > 3$ the gain is defined as the ratio between $k^{-4}_{T=50}\exp-(k_z-1.59)^2/k^2_{T=50}$ and $k^{-4}_{T=350}\exp-k_z^2/k^2_{T=350}$.

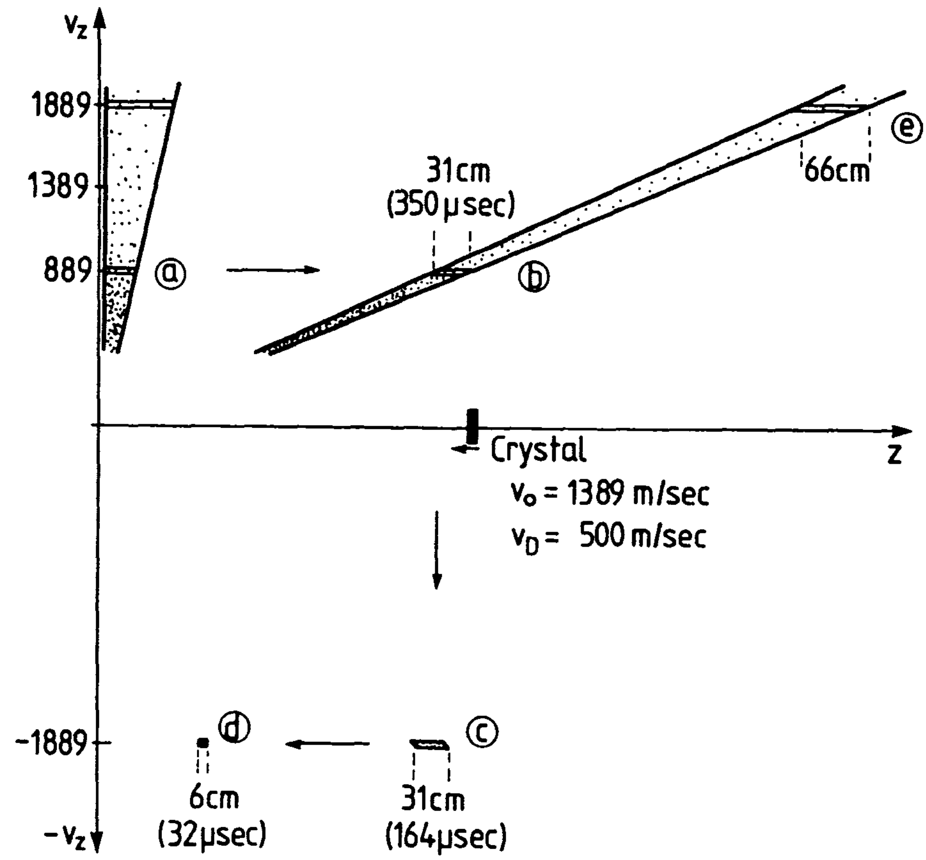

Fig. 4: Phase space transformation of a Doppler instrument. The phase space volume at z = 0 (near to the moderator) moves for some time, till the hatched nearly monochromatic region around 889 m/s, (labeled by a) is impinging onto a crystal which is moved against the neutron beam. The phase space volume labeled by b is only slightly deformed. After the reflection the phase space volume is shifted to a region where the original phase space density was much lower. Compare region c with region e. The cutting down of the pulse length of 156μs to 32μs is achieved by a simultanious rotation of the Doppler crystal.

coated neutron guide tube. Putting $\omega = 314\ s^{-1}$ we finally obtain for the pulse length the value $t_n = 32\ \mu s$. This part of the phase space volume in Fig. 4 is labeled with d. The most important point however is the fact that the phase space density in the part d is by a factor of 28 (see Fig. 3) larger than in the conventional case by taking the original phase space volume at v = 1889 m/s (labeled with e in figure 4) and cutting it down with choppers to the length of 32 µs. It should be noted, that the peak flux at the cold source of the SNQ is expected to be about a factor of 2 lower than at the thermal source /7/. From Fig. 3 it can be seen that in this case a maximum gain factor of about 10 is obtained for $k = 2.8\ Å^{-1}$.

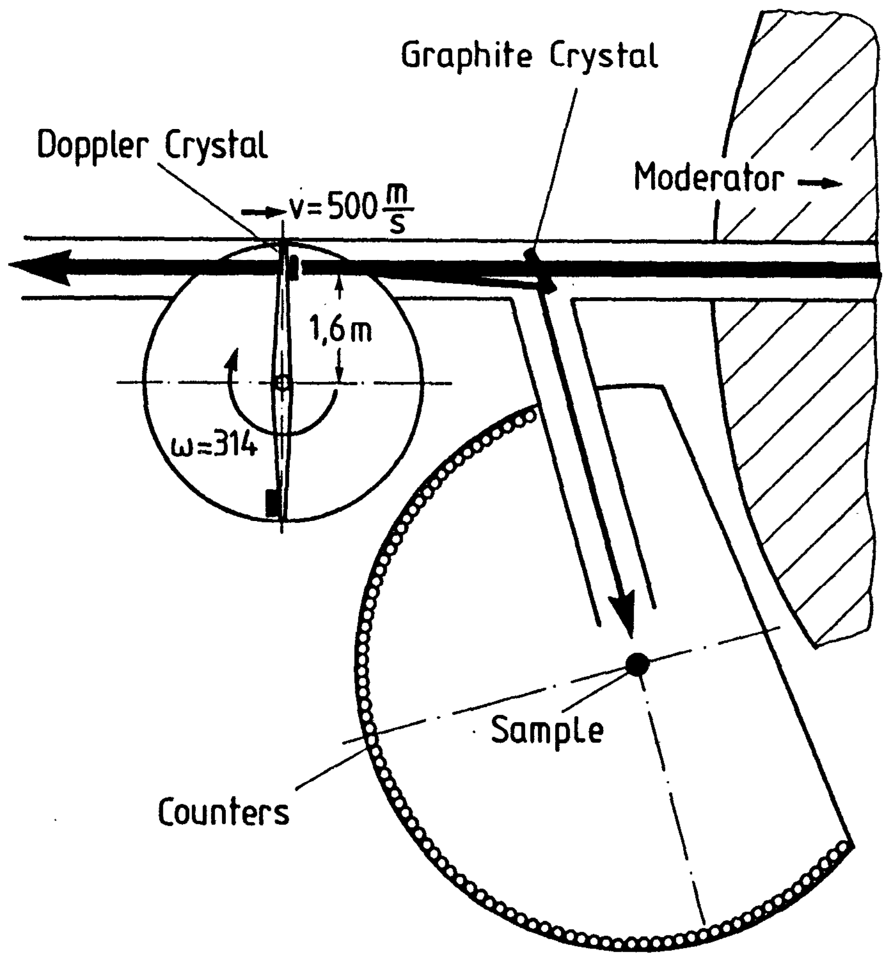

Fig. 5 Schematic drawing of a Doppler instrument. A white neutron beam passes the graphite crystal and hits the Doppler crystal which is mounted on a two-armed wheel. The wheel rotates with a frequency of 50 Hz and is synchronized to the source. The back reflected neutrons are deflected by the graphite crystal to the sample. The rest of the spectrometer is conventional.

Fig. 5 shows a schematic drawing of the Doppler instrument (BALDI). A white neutron beam passes the graphite crystal and hits the Doppler crystal which is mounted on a wheel with two arms. The wheel is synchronized to the pulsed source and rotates with $\omega = 314\ s^{-1}$. The reflected neutrons are deflected by the graphite crystal to the sample. The rest of the spectrometer is conventional.

Finally it should be mentioned that there are a number of other techniques of phase space transformations, which have been proposed to utilize the neutron flux of a pulsed source in a more efficient way than is possible on a steady state source /7,8,9/.

Acknowledgement

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