# The dependence of the gravity effect in elliptic neutron guides on the source size

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**Abstract.**
Elliptic neutron guides are expected to be widely used for construction of long neutron beamlines at the future European Spallation Source and other facilities due to their superiour transmission properties compared to conventional straight guides. At the same time, neutrons traveling long distances are subject to the action of gravity that can significantly modify their flight paths. In this work, the influence of gravity on a neutron beam propagating through elliptic guides is studied for the first time in a systematic way with Monte-Carlo simulations. It is shown that gravity leads to significant distortions of the phase space during propagation through long elliptic guides, but this effect can be recovered by a sufficiently large source size. The results of this analysis should be taken into account during design of long neutron instruments at the ESS and other facilities.

## 1. Introduction

Flight paths of thermalised neutrons at reactor and spallation sources are modified by the action of gravity. Its influence increases with rising wavelength of the neutrons and longer flight paths. For example, a 10 Å neutron traveling a distance of $d = 100$ m is displaced by gravity by

$$\Delta h = 0.5 \times g \times (d/v(\lambda))^2 = 0.5 \times 9.81\,\mathrm{m/s}^2 \times \left(\frac{100\,\mathrm{m} \times 10\,\mathrm{Å}}{3956\,\mathrm{mÅ/s}}\right)^2 \approx 31\,\mathrm{cm}.$$

This effect is significant and needs to be taken into account when designing or operating long neutron beamlines.

The gravity problem has already received some attention in the past. A way to counteract the vertical displacement of long-wavelength neutrons for instruments not comprising neutron guides was found to be a modification of the vertical position of the (virtual) source with respect to the sample and detector position [1], [2]. The influence of gravity on neutrons propagating through a collimation system and a consequential distortion of reflectivity measurements on liquid interfaces was included in an elaborated resolution theory that was confirmed by Monte-Carlo (MC) simulations [3]. On the other hand, the treatment of the gravity effect in neutron guide tubes requires a numerical approach due to the occurrence of reflections. At a time when computing power was limited and thus extensive MC simulations were difficult to carry out, an analytical matrix formalism being less demanding in terms of calculation time was developed to trace phase space during its propagation through straight or curved guides, including the influence of gravity [4]. The calculation of neutron trajectories in and outside guides then became more accessible since the invention of MC software packages like VITESS [5].

At the future European Spallation Source (ESS) facility [6], gravity will play a significant role due to the length of planned instruments that often exceed 100 m. Such long beamlines will need to include ballistic neutron guides to efficiently transport the neutrons to the sample position [7]. In particular, elliptically shaped guides have lately received a significant attention regarding their transmission and focusing properties [8], [9]. Currently, it can be expected that several instruments at the ESS will comprise elliptic guides. However, the influence of gravity on the beam properties after transmission through an elliptic guide has not been studied so far in a systematic way, even though it was found that the focusing ability of elliptic guides might be severely disturbed [8]. For a very long instrument of 300 m using a quite narrow waveband of 0.8 Å around 6.66 Å it appears that incorporating the trajectory curvature into the shape of the elliptic guide allows to remove the direct line-of-sight (LoS) without suffering flux losses and preserve the instrument resolution [10]. The latter study, however, was carried out for a potential ESS backscattering instrument, for which the influence of the beam divergence distribution on the measured resolution is significantly reduced. Hence the present work aims at studying the influence of gravity on the phase space structure for a large neutron waveband after propagation in elliptic guides, in particular concerning the shape of the vertical divergence distribution. This is important for instruments where the divergence distribution has a direct impact on the illumination homogeneity of the sample/detector or on the shape of structures in the scattering spectrum (e.g. for diffraction).

## 2. Analysis and results

The gravity effect is studied using a simple instrument layout, see Fig 1. A source emitting a constant spectrum as a function of wavelength is followed by an elliptic neutron guide with a square cross section, of which the semi-axes are $a = 75$ m along the instrument axis and $b = 0.15$ m in both directions perpendicular to it. The reflectivity of the guide coating $R(\tilde{m})$ is 0.99 for $\tilde{m} < 1$ (with $\tilde{m} = 10 \times \theta\,[^\circ]/\lambda\,[\AA]$, where $\theta$ is the reflection angle), decreases linearly to $R(\tilde{m} = 5.7) = 0.52$ and then drops quickly [11]. The guide is followed by a 1 $cm^2$ sample. Both the source and the sample are located in the focal points of the ellipse. This study utilises the new elliptic guide module available in the VITESS software from version 3.0, which handles neutron propagation through a perfect ellipse, thus avoiding effects connected with guide segmentation [8], since in such a study the gravity effect should be considered separately from other imperfections. The distance $D_0$ between the source and the guide entry and between the guide exit and the sample is the same and the total length of the instrument is fixed to 150 m. $D_0$ is varied between 20 cm and 5 m, thus varying the entry/exit width $W_0$ between 2.2 cm and 10.8 cm. The source is a square with the edge length $X_0$, which is varied between $1 \times 1$ $cm^2$ and $12 \times 12$ $cm^2$. All input parameters are summarized in Tab. 1. **The coordinate system follows the convention used in VITESS, i.e. the x-axis corresponds to the instrument axis, while the y- and z-axis are completing a right-handed coordinate system in horizontal and vertical directions, respectively.**

The goal of the performed simulations is to monitor the beam characteristics at the sample position with regard to gravitational effects. Since it can be expected that gravity modifies the vertical divergence distribution (and thus the distribution in real space at the detector), an asymmetry parameter $\Delta\gamma$ is introduced in order to describe this effect:

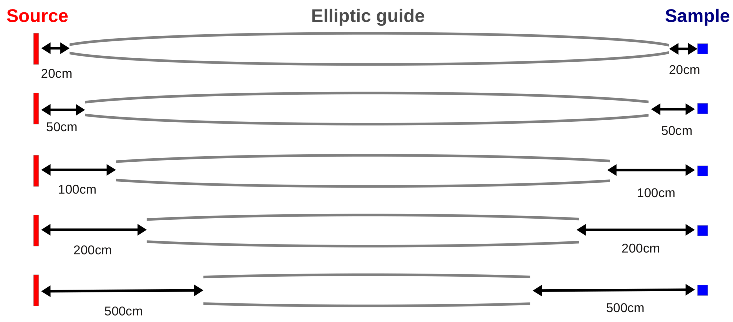


**Figure 1.** A sketch of the instrument layout used in the present study. The distance between the source and the sample is kept constant at 150 m, whereas the distance between the source and the guide entry (the guide exit and the sample) is varied between 20 cm and 500 cm. The source edge length is varied between 1 cm and 12 cm. See text for further details.

**Table 1.** Summary of input parameters used in the simulations.

| | |
|---|---|
| **Source** | Spectrum: $I(\lambda) = const$<br>Continuous wavelengths: 1 Å – 12 Å<br>Discrete wavelengths: 2 Å, 6 Å, 10 Å<br>Edge length $X_0$: 1 cm, 2 cm, 4 cm, 6 cm, 8 cm, 10 cm, 12 cm |
| **Guide** | Elliptic guide, a = 75 m, b = 15 cm, m=6 coating<br>Source-to-guide (guide-to-sample) distance $D_0$:<br>0.2 m, 0.5 m, 1 m, 2 m, 5 m<br>Guide entry (exit) $W_0$: 2.2 cm, 3.5 cm, 4.9 cm, 6.9 cm, 10.8 cm<br>Source and sample at focal points |
| **Sample** | Size: $1 \times 1$ cm$^2$ |

$$\Delta\gamma = \left| \frac{I(\gamma)_+ - I(\gamma)_-}{I(\gamma)_+ + I(\gamma)_-} \right| = \left| \frac{\int_0^{+\infty} [I(\gamma) - I(-\gamma)] d\gamma}{\int_0^{+\infty} [I(\gamma) - I(-\gamma)] d\gamma} \right|, \quad (1)$$

where $I(\gamma)$ is the beam intensity as a function of divergence $\gamma$ either in vertical or horizontal direction. The simulations are carried out for the waveband ranging from 1 Å to 12 Å and for discrete wavelengths 2 Å, 6 Å and 10 Å to illustrate the different behaviour of short- and long-wavelength neutrons.

The results of the simulations are illustrated in Figs. 2 - 6. A careful consideration of the obtained distributions reveals **the** following major findings:

- Gravity can strongly affect the vertical divergence distribution in long elliptic guides, as opposed to propagation through a straight neutron guide of comparable dimensions, see Fig. 2.
- The magnitude of distortion of the divergence distribution due to gravity depends on two parameters:
  - (i) Wavelength: As it could be expected, the divergence distribution is more distorted with increasing wavelength, see Fig. 3. For short wavelengths (and small sources/samples

[8]), the final divergence distribution is more affected by propagation through an ellipse than by gravity [8].

(ii) Source and guide entry size: The **asymmetry** decreases with increasing source size (Fig. 2 (b), Fig. 3 (b) and (c)) or with decreasing entry width $W_0$/source-to-guide distance $D_0$ (Fig. 4).

- Despite the asymmetry in the divergence distributions, elliptic guides still provide a reasonable focusing in space, i.e. the flux is the largest at the sample position. At the same time, the focusing is more strongly reduced for larger $X_0$ distances in vertical than in horizontal direction (if the source size $W_0$ is kept constant), see Fig. 5.
- To minimize the distortion of the divergence distribution, the source needs to be of the same size or larger than the guide entrance, see Fig. 6 (a). But – not surprisingly – the actual ratio needed of the source size $X_0$ to the guide entrance size $W_0$ is wavelength dependent, see Fig. 6 (b) for a (rough) quantification[1].
- When a symmetric and featureless divergence distribution is reached, a further increase of the source size does not increase the flux at the sample, see Fig. 2 (a), (b) and Fig. 3.

In particular the last two points are important findings. It can be observed that for a given elliptical guide there is a certain (virtual) source size that completely smears out the gravity distortion and features characteristic **for** transmission through elliptic guides. At the same time, the source of this size provides the maximum flux on the sample, a fact deserving serious attention when designing a neutron beamline. This is confirmed by an additional set of simulations using an elliptic guide with the semi-axes $a = 37.5$ m, $b_1 = 0.15$ m and $b_2 = 0.075$ m, a fixed distance between the source and the guide of 1 m and varying the size of the source again between $1 \times 1$ cm$^2$ and $12 \times 12$ cm$^2$. Here it was again observed that the divergence distribution obtains a symmetric shape around zero every time the source is larger than the guide entry, see Fig. 7. The conclusion is that the recovering of a symmetric divergence distribution happens by mixing the neutron trajectories through multiple reflections, which are by far the most dominant transmission regime in elliptic guides [8], such that all inhomogeneities are smeared out. This process is more efficient if the source injects more phase space into the guide.

## 3. Discussion and conclusions

The simulation results described in the last section clearly show that gravity can play an important role in neutron transport in long elliptic guides, in particular for small sources and long wavelengths. At the same time, it has been shown that these effects can be removed by increasing the size of the (virtual) source such that it exceeds the guide entry dimensions. Such a source is able to smear out the features in the divergence distribution at the sample position coming both from gravity influence and transmission effects. Hence in principle, elliptic guides are able to transport neutrons over long distances and provide a smooth phase space at the sample position, if provided with an adequate input beam. This should be kept in mind for design of instruments that are in need of a smooth phase space at sample/detector position.

## Acknowledgments

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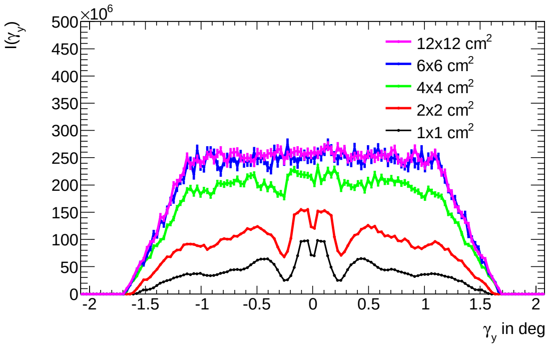
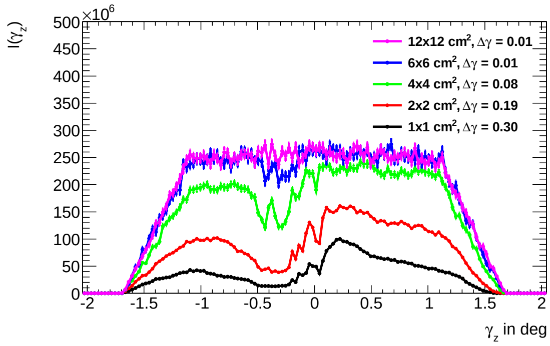
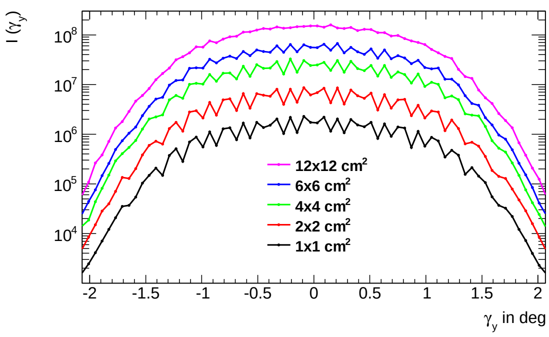
[1] **For each wavelength, this ratio was determined by simply averaging the smallest source-to-entrance size ratios that still led to an asymmetry smaller than 1% and 5% thresholds, respectively, for all source sizes under study.**



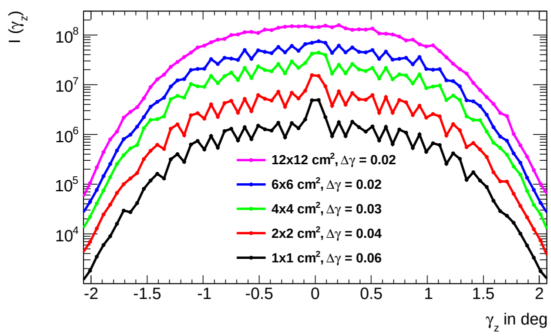

(a) Horizontal divergence distribution at sample position for an elliptic guide




(b) Vertical divergence distribution at sample position for an elliptic guide for varying source size $X_0$

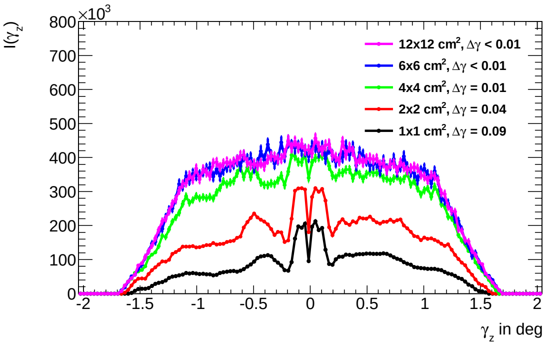



(c) Horizontal divergence distribution at sample position for a straight guide

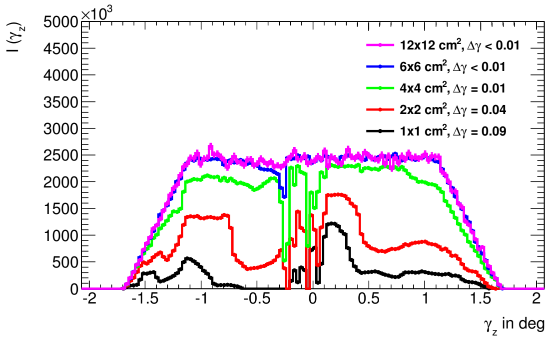



(d) Vertical divergence distribution at sample position for a straight guide

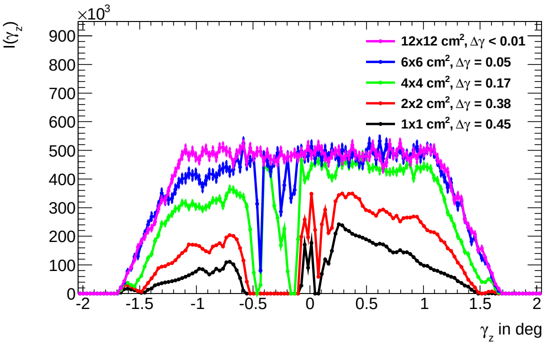
**Figure 2.** (a) and (b): Divergence distribution at sample position for $W_0 = 4.9$ cm ($D_0 = 1$ m) for an elliptically shaped guide, see Tab. 1, using source sizes from $1 \times 1$ cm$^2$ to $12 \times 12$ cm$^2$ and the full spectrum between 1 Å and 12 Å. (c) and (d): Horizontal and vertical divergence distributions at sample position for a 148 m long guide with a constant $10 \times 10$ cm$^2$ cross section having the same source-to-guide and guide-to-sample distance $D_0 = 1$ m. The y-axis is logarithmic to fit in distributions for small source sizes. The zig-zag structures, which are particularly visible for small source sizes, are a systematic effect and arise due to fractions of the total phase space missing the 1 cm$^2$ sample, since straight guides lack focusing abilities. Here and in other plots the error bars (mostly too small to be visible) represent the statistical uncertainty due to the number of simulated trajectories.




(a) Vertical divergence distribution at sample position for 2 Å neutrons




(b) Vertical divergence distribution at sample position for 6 Å neutrons




(c) Vertical divergence distribution at sample position for 10 Å neutrons

**Figure 3.** Vertical divergence distribution at sample position using $W_0 = 4.9$ cm ($D_0 = 1$ m) for 2 Å, 6 Å and 10 Å neutrons. Gravity leads to a modification and an asymmetry $\Delta\gamma$ of the vertical divergence distribution in particular for long wavelengths.

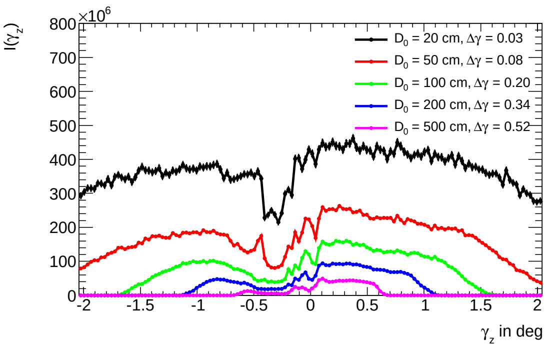
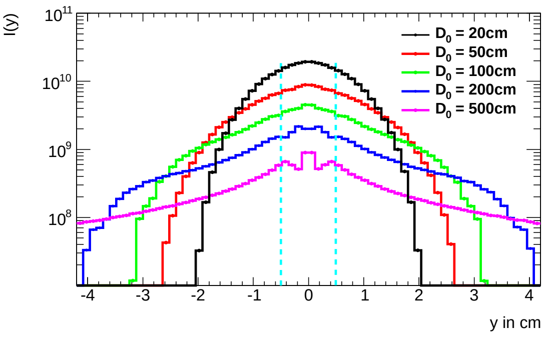
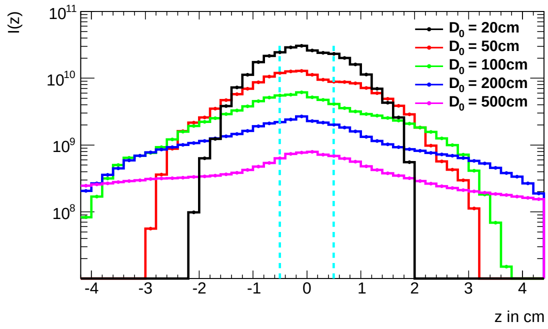



**Figure 4.** Vertical divergence distribution at sample position for an elliptically shaped guide using a source with $X_0 = 2$ cm and $W_0$ between 2.2 cm and 10 cm ($D_0$ between 20 cm and 5 m).

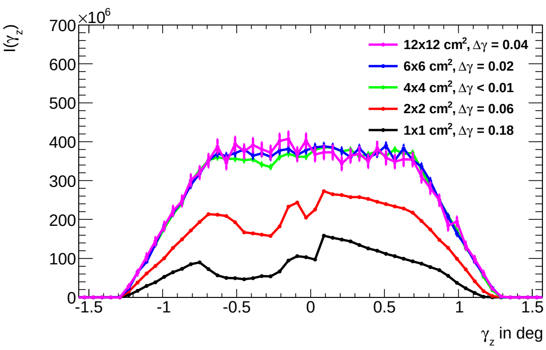



(a) Horizontal position distribution at sample position

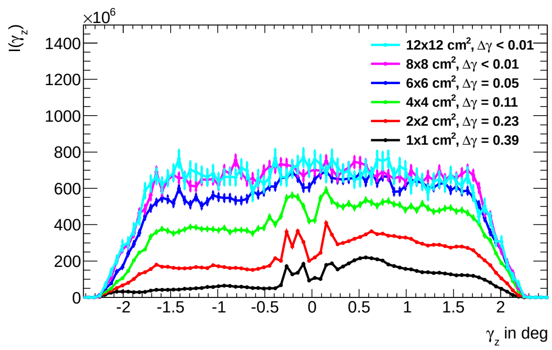



(b) Vertical position distribution at sample position

**Figure 5.** Distribution of neutrons in space for a $2 \times 2$ cm$^2$ source. The $1 \times 1$ cm$^2$ sample indicated by dotted lines is located at the guide symmetry axis that coincides with the location of the highest flux even for a 5 m distance between guide and sample (corresponding to $\approx 11$ cm guide exit width).

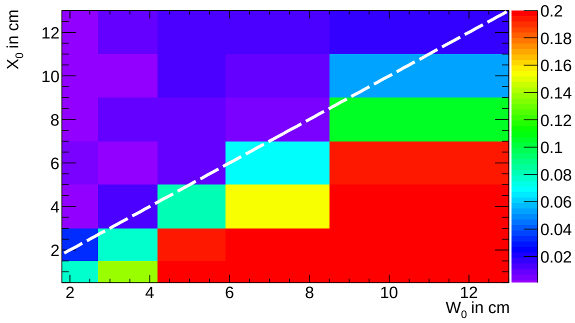



(a) a = 37.5 m, b = 0.075 m

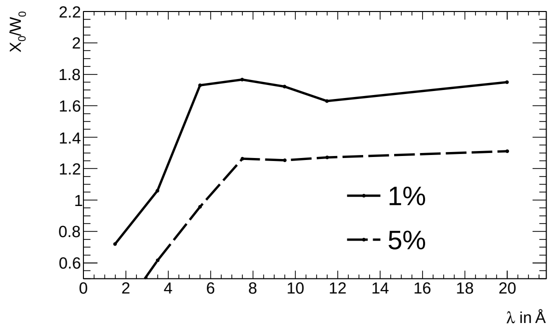



(b) a = 37.5 m, b = 0.15 m

**Figure 6.** Vertical divergence distribution at the $1 \times 1$ cm$^2$ sample being in the focal point of two different elliptic guides with given parameters. The distance $D_0$ is 1 m. The guide entry width is 3.44 cm for b = 0.075 m and 6.88 cm for b = 0.15 m, respectively. The divergence distribution saturates for source sizes being larger than the guide entry and the asymmetry parameter $\Delta\gamma$ becomes negligible.




(a) Vertical divergence asymmetry as a function of $W_0$ and $X_0$




(b) Size ratio of source to guide entry as a function of $\lambda$

**Figure 7.** (a) The vertical asymmetry parameter $\Delta\gamma$ defined in Eq. 1 as a function of the source edge length $X_0$ and the entry width $W_0$ of the elliptic guide for all neutrons. The colour plot is saturated at 0.2, with the maximum asymmetry at $X_0 = 1$ cm and $W_0 = 10.8$ cm. The white line corresponds to the relation $X_0 = W_0$. It is well visible that the gravity effect dominates for $X_0 < W_0$, i.e. for sources being smaller than the guide entrance. (b) The ratio of the source edge length $X_0$ to the entry width $W_0$ as a function of the neutron wavelength $\lambda$ that is needed to achieve a vertical divergence distribution at sample position, which exhibits an asymmetry of less than 5% or 1%, respectively. As expected, larger source sizes are needed for larger wavelengths.

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