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Systematic study on the performance of elliptic focusing neutron guides

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ABSTRACT

In neutron scattering experiments there is an increasing trend towards the study of smaller volume samples, which make the use of focusing optics more important. Focusing guide geometries based on conic-sections, such as those with parabolic and elliptic shapes, have been extensively used in both recently built neutron instruments and upgrades of existing hardware. A large fraction of proposed instruments at the European Spallation Source feature the requirement of good performance when measuring on small samples. The optimised design of a focusing system comes after time consuming Monte-Carlo (MC) simulations. Therefore, in order to help reduce the time needed to design such focusing systems, it is necessary to study systematically the performance of focusing guides. In the present work, we perform a theoretical analysis of the focusing properties of neutron beams, and validate them using a combination of Monte-Carlo simulations and Particle Swarm Optimisations (PSOs), where there is a close correspondence between the maximum divergence of the beam and the shape of the guide. The analytical results show that two limits can be considered, which bound a range of conic section shapes that provide optimum performance. Finally, we analyse a more realistic guide example and we give an assessment of the importance of the contribution from multiple reflections in different systems.

1. Introduction

In recent years, there has been significant use of conic section mirror geometries for focusing neutron optics. Elliptic and parabolic focusing guides have been used extensively in different instruments with very satisfactory results [1–3]. In theory, a parabolic mirror focuses perfectly collimated trajectories to a common focal point, whereas an elliptic mirror reflects trajectories from one point source at one focus to produce a 1:1 point image of the first focal point at the second focal point.

There are two reasons why these theoretically valid approaches deviate from their theoretical properties in the real world. For elliptic systems, real neutron beams are emitted from spatially extended sources, not point sources. For parabolic systems, there is no perfectly collimated beam because free neutron transport sacrifices performance $\propto 1/R^2$, so instruments are generally located close to their (virtual) sources. Typically, the off-axis rays (coming from the edges of the source) have a different focal point compared to those coming from the source near to the beam central axis. The effect of this aberration is to disperse the beam, which decreases the performance of such systems [4]. There are also advanced concepts that have been explored to overcome optical aberrations with neutrons. For example, solutions that have been successful in x-ray optics or astronomy, namely Kirkpatrick–Baez mirrors and Wolter optics [5,6], can be applied to neutron beams [7–9], or hybrid elliptic-parabolic systems [10]. These are ideal for creating optically excellent beams and focusing conditions, but at an increase in complexity and price compared to the simpler, traditional methods. They also take some time to fully optimise, generally via heavy use of Monte-Carlo (MC) simulations for various sample geometries and instrument scenarios. Whilst these advanced methods certainly have a place in the neutron optics toolbox, we also require an improved lower complexity option with good beam characteristics for the cases with less stringent requirements and based around *regular* guides where possible.

The usual way of adjusting the system is to start with the theoretical configuration of focal points on sources and sample positions, and then perform time-expensive exploration of the

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configuration for a realistic-sized sample using MC simulation codes like VITESS [11] and McStas [12]. Furthermore, it can be mentioned that while MC simulations are heavily used in practice, they often provide results to a user with little understanding of the underlying physics. One of the aims of this work is to derive analytical treatments of focusing systems which can provide additional insight into the important physics processes involved.

For these reasons, a systematic study on the focusing properties could give some hints on choosing the parameters close to the optimal solution. This would make it faster to design a focusing system and also lead to a deeper understanding of the physics involved. First, we develop the proper analytical tools that could be used for the evaluation of the performance of such a system. Then we use MC simulations and numeric optimisation methods in order to analyse the effect of the shape of the guide on its performance in ideal conditions. Finally, we investigate a more realistic case as an example of how to implement the design in practice.

2. Initial considerations

Strictly speaking, a converging elliptic mirror reflects trajectories emanating from one focal point and produces a sharp image at the second focal point. On the other hand, a converging parabolic mirror reflects parallel trajectories emanating from infinity and focuses them at a focal point. When examining a focusing guide end piece, the choice between a parabola or an ellipse becomes somewhat irrelevant once realistic neutron beams with finite spatial extent and divergence are considered and some amount of defocusing is used. We therefore, for simplicity, concentrate our efforts on an elliptic shape in this study, which also seems to be the most popular concept for scientists to understand and work with, despite the added complexity compared to a parabolic shape.

The equation of the ellipse we use is the following one:

$$y = b\sqrt{1-\left(\frac{x}{a}\right)^2} \tag{1}$$

where x is the direction of neutron propagation, y the perpendicular direction, and a and b are the semi-major and semi-minor axes of the ellipse respectively.

It is also useful to consider the derivative of the ellipse as it represents the angle of the tangent at the ellipse surface, which is given by:

$$\beta(x) = \left|\frac{dy}{dx}(x)\right| = \frac{bx}{a^2\sqrt{1-\left(\frac{x}{a}\right)^2}} \tag{2}$$

We consider that the focusing guide starts at $x=0$. This is convenient in the case of the neutron beam coming from a straight guide where the gaps in the phase space will be smaller due to an abrupt change in the incident angle of a given neutron. The second reason is that this condition reduces the complexity of the equations.

Fig. 1 shows a sketch of the system we are considering, where the most important parameters are defined. There are some parameters that are fixed. For example, the distance between the guide end and the sample D and the sample size S are usually defined by the requirements of the instrument. The reader will notice that the focal point of the ellipse (from now on we refer it to as *geometrical focal point*) and the sample position are not the same. The geometrical focal point only depends on the guide geometry. We define the *effective focal point* of the guide where the neutron flux is highest, which due to coma is slightly offset from the geometric focal point. The difference between the geometric focal point and the effective focal point is the amount of *defocus* that was discussed previously.

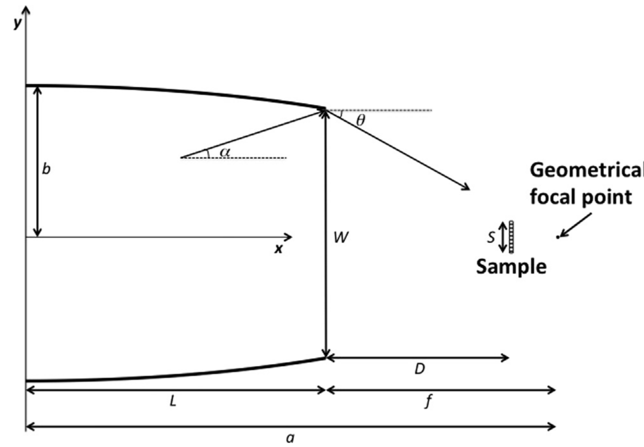

Fig. 1. A sketch of the simulated system, indicating the variables as described in the text.

We also define a parameter which is related to the eccentricity of the ellipse, i.e., the shape of the ellipse and is given as follows:

$$\gamma = \frac{b}{a} \tag{3}$$

For the guide geometry definition, we consider a number of approximations. First, the neutron grazing angles are set to be small and therefore $\tan(\alpha) = \alpha$ in all cases. The second approximation is that the distance between the two foci of the ellipse will be $2a$. This is taken due to the fact that ellipses suitable for neutron transport will have a very small γ in order to have small reflection angles. Therefore, the foci will be very close to the ellipse ends. The third condition is that we consider a two-dimensional system, which is equivalent to a three-dimensional system in which the transverse direction to the beam has rotational symmetry.

Another important consideration is the nature of the incoming beam, which has to be simple to treat in analytic calculations but also realistic enough at the same time. We expect that the beam comes from a guide and after several bounces inside the guide the beam is in equilibrium such that the divergence distribution can be considered to be independent of transverse position. It is also important to bear in mind that the divergence distribution depends on the neutron wavelength because the critical reflection angles in the coatings are wavelength-dependent. The maximum divergence, α_{max}, increases linearly with the wavelength but is however limited by the beam extraction system. This means that it reaches a maximum divergence at a certain value of the wavelength while for higher values of the wavelength the divergence distribution is constant. Furthermore, in ballistic guides where the extraction system is a defocusing guide, the phase space can be transformed in a way in which the divergence of the beam coming from the source decreases. Therefore, for the sake of simplicity in the analytical study, we do not consider the dependency of the divergence with the neutron wavelength. However, we introduce this dependence at a further stage in this work and analyse it with MC simulations.

3. Analytical limits in the parameter space

In the design of a focusing guide it is necessary to notice that the focused beam has three different contributions. The first one is the contribution with zero reflections, and it depends on the size of the exit aperture, the divergence of the beam, and on the distance between the guide end and the sample position. This contribution is always present. The second contribution comes from the neutrons that have been reflected once. Finally, the third