Fundamentals of neutron waveguides: a proposal for slow neutron beams confinement and applications

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ABSTRACT

Neutron optics is the branch of quantum physics devoted to the study of the optical properties of slow neutrons and their behavior as wave-particles. Slow neutrons beams (with typical energy the order of 0.025 eV, known as thermal neutrons, and also smaller) can propagate confined in guides of various transverse dimensions, longitude and geometries, under total internal reflection conditions, like in the case of classical optical waveguides. We study the properties and possible applications of neutron waveguides with small transverse dimensions. In particular, we have implemented a new algorithm to simulate neutron beams as they are confined in particular waveguides. The results, obtained from a new analytical formalism, are compared with standard numerical methods as the FDTD and, then, enhance the feasibility for recreating the beam structure as the later propagates inside the waveguide.

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1. INTRODUCTION

Neutron optics started since the very early work of Fermi and Zinn in 1946[1]. For comprehensive accounts, see Byrne[2] and Sears[3]. Neutrons have the dual wave-particle nature and, therefore, the associated de Broglie wavelength which is, for thermal neutrons: λ_B=1.8 Å. The neutron is electrically neutral and unstable, its average life time being the order of 15 min. The particular phenomenon of neutron confinement, studied here, takes place within time intervals smaller than the average life time.

In neutron optics, the wave function $\varphi\,(\boldsymbol{x},\,t)$ for a slow neutron propagating in a material medium (or vacuum) satisfies the stationary (time-independent) Schrödinger equation:

$$\left[\frac{-\hbar^2}{2m}\nabla^2 + V(\boldsymbol{x}) - E\right]\varphi(\boldsymbol{x}) = 0 \ . \tag{1}$$

In Eq. (1) m is the neutron mass ($m = 939.57$ MeV/c^2), $V(\boldsymbol{x})$ is the effective scalar potential due to the medium, depending on the spatial coordinates, $\hbar$ is Planck's constant and E is the total kinetic energy. For the current study we consider only thermal neutrons with E=0.025 eV. Eq. (1) is an equation, having analogies with scalar wave equations used for classical electromagnetic fields deduced from Maxwell's equations, which can be exploited for characterizing the behaviour of a slow neutron beam.

Neutron phenomena associated with total internal reflection in guides with macroscopic diameter (i.e.: centimeters) and neutron diffraction at shorter scales are well characterized provided that a constant potential be considered[2-3].

$$V = \frac{2\pi\hbar^2}{m}b\rho \qquad . \tag{2}$$

In Eq. (2), b is the coherent neutron-nucleus scattering amplitude (depending only on the material and isotope) and ρ is the density of nuclei per unit volume.

Those neutron phenomena (having in mind similarities with the refractive index for the corresponding optical phenomenon of total internal reflection) can also be described in terms of an effective refractive index:

$$n^2 = 1 - V/E_0 \, . \tag{3}$$

Where: E_0 is the energy of the neutron in the medium. The refractive index for neutrons plays a role in discussing confinement of neutron waves, under strict total internal reflection conditions. We remind here that for confined propagation in waveguides, the beam wavelength is close to characteristic length scales of the system through which the neutron wave propagates (say, transverse sizes of thin films or fibers). Eqs. (2)-(3) yield practical approximate descriptions provided that Bragg reflections do not occur and other scattering and absorption processes are negligible.

There are some antecedents on slow neutron beam confinement in waveguides with small transverse dimensions. In 1973 Wames and Sinha[4] proposed the coupling of neutrons in planar thin film waveguides. In 1984 and 1986, Álvarez-Estrada and Calvo studied theoretically the confinement of slow neutrons in cylindrical waveguides[5-6]. In 1994, Feng et al. demonstrated, experimentally, confined propagation of modes for slow neutrons in Ti films[7]. Important studies by Kumakhov et al.[8] and Chen et al.[9], both in 1992, established experimentally the focusing of slow neutrons by using polycapillary glass fibers. In all these studies, there are key parameters in the design of the guides, namely, dimensions, geometry, wavelength and energy of the neutron beam, materials to be used, values of the critical angle, in order to assure an effective confinement and low loss of energy. Since experiments with neutron beams require some special technologies, arranging neutron sources and transport to the required point for the study, it is quite necessary, previously, to develop theoretical models to implement numerical simulations. These theoretical models are not yet well developed, because of the necessity to deal with non-trivial wave phenomena in the framework of the Schrödinger equation. It has been discussed previously that the numerical solution of Schrödinger equation, for propagation in a medium with some specific potential and geometry, requires a carefully choice of the method. For example, Matlab is very popular these days but it requires time-consuming programs and has to be optimized. Moreover, the inclusion of boundary conditions is an added requirement since the waveguide has finite dimensions. These aspects are treated in the next section. We have designed[10] neutron devices, behaving as couplers, which could possibly be applied in Boron Neutron Capture Therapy (BNCT) and for other purposes.

2. THEORETICAL MODEL

We introduce a waveguide model that we have considered for the purpose of the numerical simulation of the thermal neutron beam confinement.
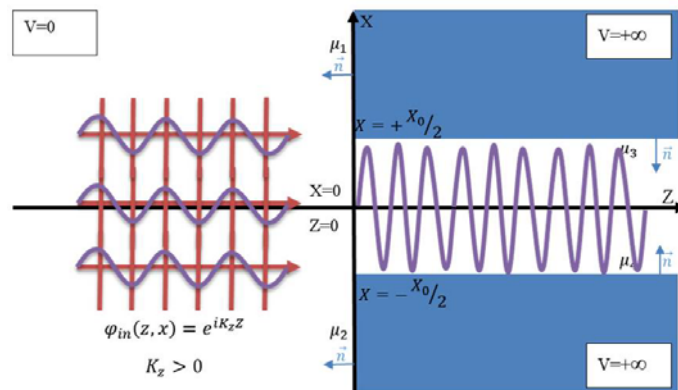

Figure 1. Schematic diagram of the neutron waveguide considered for the purpose of the numerical simulation.

Figure 1 displays the schematic representation for the neutron waveguide geometry considered in our study. An incoming neutron plane wave propagates, with $V=0$ in the air, at $Z<0$ and strikes a semi-infinite two-dimensional planar

waveguide. The neutron beam propagates confined along the waveguide. The waveguide has aperture dimension x_0, and confined modes are formed and propagate along the Z-axis (Z>0). The number of modes will depend on the particular geometry, transverse dimensions of the planar waveguide (say, aperture value) and incidence conditions. For suitably large incoming neutron energy, a high number of modes are formed (the neutron waveguide being a multimodal one). For simplicity, we have considered that the scalar repulsive potential (in the so-called clad) has an infinite value: $V = +\infty$. Although, this is far from a real case, however, this approach is quite convenient in order to obtain and to interpret approximate results for the modes formation. An integral representation is obtained for the neutron wave function by using the formalism of the two-dimensional Green's function. That integral representation includes four functions, namely, μ_1 and μ_2, defined at the walls of the entrance aperture of the guide, and μ_3 and μ_4, defined at the internal upper and lower walls of the waveguide, respectively.

We omit here for brevity the mathematical equations derived from the theoretical model. We state that the four μ's functions are uniquely determined by imposing the so-called Dirichlet boundary conditions (namely, the vanishing of the neutron wave function) at the four walls of the waveguide indicated above. Based upon them, approximate methods are applied to arrive to analytical solutions for odd and even propagation modes, respectively:

$$\varphi(z,x) = -i \sin\left(\frac{2n\pi x}{x_0}\right) e^{iz\sqrt{\frac{2mE}{\hbar^2} - \left(\frac{2n\pi}{x_0}\right)^2}} . \tag{4}$$

Eq. (4) denotes the representation for the odd modes. For even modes:

$$\varphi(z,x) = \cos\left(\frac{(2n+1)\pi x}{x_0}\right) e^{iz\sqrt{\frac{2mE}{\hbar^2} - \left(\frac{(2n+1)\pi}{x_0}\right)^2}} . \tag{5}$$

Eqs. (4)-(5) imply a semi-quantitative description of the wavenumber of those incoming neutrons which give rise to propagation modes. Both, odd and even modes are allowed into the waveguide.

Figure 2 shows the results of the maximum number of modes allowed in these waveguides as a function of the neutron incoming energy for different values of the aperture of the guide:
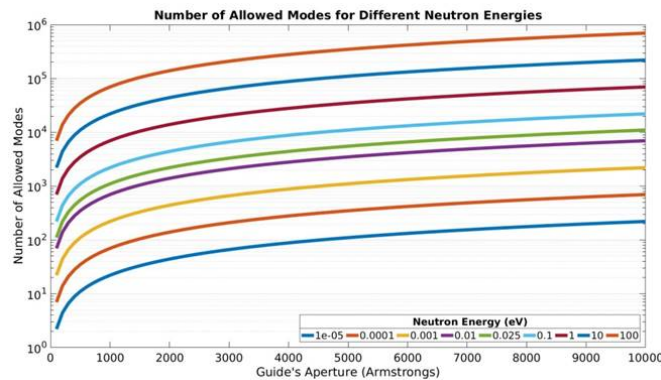

Figure 2. Number of allowed modes in neutron waveguides having clad with an infinite repulsive potential, as a function of the incoming wave energy, for different values of the aperture size.

In the present study, since we are supposing an ideal waveguide with infinite repulsive potential in the clad (Dirichlet boundary conditions), one finds that the critical angle is the order of $\pi/2$. Thus, the waveguide allows almost any angle of incidence.

3. NUMERICAL SIMULATION

We have developed an algorithm based upon the mentioned Green's functions formalism and Dirichlet boundary conditions. Approximate analytical results are obtained by applying the analogies with classical optical diffraction and the Sommerfeld-Rayleigh integral as well as its Fourier transform. Moreover, we have implemented an approximate iterative method for obtaining μ_3 and μ_4, which are more important to account for the confined beam within the waveguide. Results are displayed in Fig. 3 (a) compared with FDTD results in Fig.3 (b).
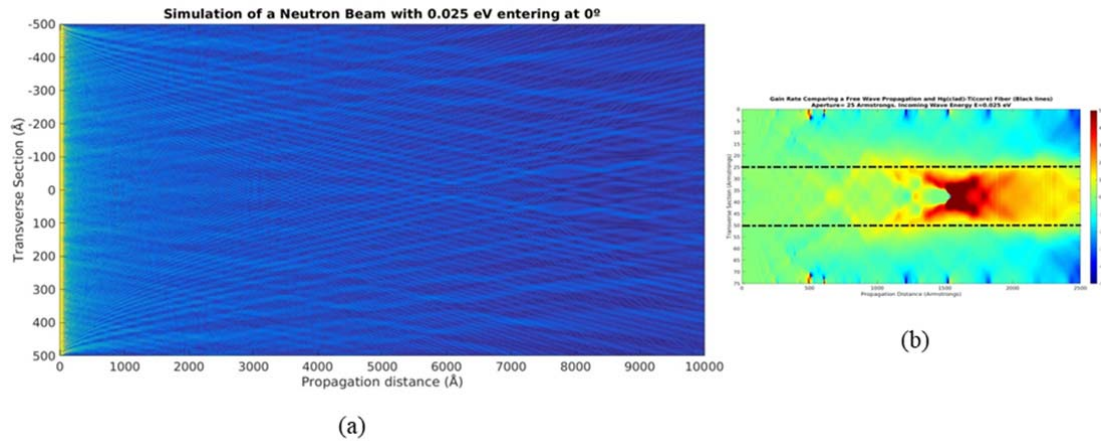

Figure 3. Numerical simulations of the neutron beam confined in the waveguide. (a) Results obtained with the algorithm implemented based upon the Green's function formalism with Dirichlet boundary conditions. Aperture dimension: 1000 Å. (b) Results obtained by the FDTD method. Aperture dimensions 50 Å. Notice that comparative real scale between (a) and (b) is not displayed for convenience. Larger computational time is required for case (b), (80 hours), compared with case (a), (20 minutes).

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