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**Neutron optics: new algorithm based on Green's functions for simulating waveguides with Dirichlet boundary conditions.** (English) [Zbl 1481.78013](#)

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**Summary:** We present a new, efficient and robust method for computing scalar wave propagation for those cases in which Dirichlet boundary conditions play a key role. The algorithm is versatile and it allows to treat reflection, diffraction, waveguiding regime, scattering and free propagation. The analysis is based upon a representation for a slow neutron wavefunction in terms of the incoming wave and integrals, along the boundaries of an unbounded domain, involving a Green's function and certain auxiliary functions (warranting the Dirichlet boundary conditions). The analysis involves Fourier and Hilbert transforms defined only on the boundaries and enables to exploit the detailed advantages of Fast Fourier Transform (FFT) to perform simulations. Our algorithm proves to be highly effective both in terms in running time and memory load, compared to those based on Finite Differences Methods (FDM). Moreover, since the value of the field at each point may be calculated independently, this algorithm allows parallelization in a natural way.

**MSC:**

[78A50](#) Antennas, waveguides in optics and electromagnetic theory

[35Q60](#) PDEs in connection with optics and electromagnetic theory

**Keywords:**

neutron optics; waveguides; Green's functions; Dirichlet boundary conditions; unbounded domain; meshless algorithm

**Software:**

[FFTW](#)

**Full Text:** [DOI](#)

**References:**

- [1] Molina de la Peña, I.; Calvo, M. L.; Álvarez-Estrada, R. F., Neutron waveguides in neutron optics: Green's functions formalism with Dirichlet boundary conditions, *J. Mod. Opt.*, 67, 10, 899-913 (2020)
- [2] Bacon, G. E., *Neutron Diffraction* (2nd Ed.), Monographs on the Physics and Chemistry of Materials (1962), Oxford University Press: Oxford University Press London
- [3] Alvarez-Estrada, R. F.; Calvo, M. L., Chapter 1: Neutron Optics: Fundamentals, (Calvo, M. L.; Alvarez-Estrada, R. F., *Advances in Neutron Optics: Fundamentals and Applications in Materials Science and Biomedicine* (2019), CRC Press: CRC Press Boca Raton (FL), 3-78
- [4] De Wames, R. E.; Sinha, S. K., Possibility of guided-neutron-wave propagation in thin films, *Phys. Rev. B.*, 7, 3, 917-921 (1973)
- [5] Alvarez-Estrada, R. F.; Calvo, M. L., Neutron fibres: a possible application of neutron optics, *J. Phys. D: Appl. Phys.*, 17, 3, 475-502 (1984)
- [6] Calvo, M. L.; Alvarez-Estrada, R. F., Neutron fibres (II): some improving alternatives and analysis of bending losses, *J. Phys. D: Appl. Phys.*, 19, 6, 957-973 (1986)
- [7] Feng, Y. P.; Majkrzak, C. F.; Sinha, S. K., Direct observation of neutron-guided waves in a thin-film waveguide, *Phys. Rev. B.*, 49, 15, 10814-10817 (1994)
- [8] Pogossian, S. P.; Menelle, A. Le; Gall, H., Experimental observation of guided polarized neutrons in magnetic-thin-film waveguides, *Phys. Rev. B.*, 53, 21, 14359-14363 (1996)
- [9] Menelle, A.; Pogossian, S. P.; Le Gall, H., Observation of magnetic films neutron waveguides, *Phys. B.*, 234, 510-512 (1997)
- [10] Pogossian, S. P.; Menelle, A. Le; Gall, H., Observation of neutron guided waves from the open end of a thin film waveguide and a waveguide interferometry, *J. Appl. Phys.*, 83, 3, 1159-1162 (1997)
- [11] Pogossian, S. P., Enhanced neutron concentration in uranium thin film waveguides, *J. Appl. Phys.*, 102, 10, Article 104501 pp. (2007)

- [12] Kozhevnikov, S. V.; Khaydukov, Y. N.; Keller, T., Polarized neutron channeling as a tool for the investigations of weakly magnetic thin films, *JETP Lett*, 103, 1, 36-40 (2016)
- [13] Kumakhov, M. A.; Sharov, V. A., A neutron lens, *Nat.*, 357, 6377, 390-391 (1992)
- [14] Chen, H.; Downing, G.; Mildner, D. F.R., Guiding and focusing neutron beams using capillary optics, *Nat.*, 357, 6377, 391-393 (1992)
- [15] Kearney, P.; Klein, A.; Opat, G., Imaging and focusing of neutrons by a zone plate, *Nat.*, 287, 5780, 313-314 (1980)
- [16] Yee, K. S., Numerical solution of initial boundary value problems involving Maxwell's equations in isotropic media, *IEEE Trans. Antennas Propagat.*, A14, 3, 302-307 (1966) · [Zbl 1155.78304](#)
- [17] Nagel, J. R., A review and application of the finite-difference time-domain algorithm applied to the schrödinger equation, *Aces J*, 24, 1, 1-8 (2009)
- [18] Alvarez-Estrada, R. F.; Molina de la Peña, I.; Calvo, M. L., Focalizing slow neutron beams at and below micron scales: discussion on BNCT. Phosphorus, Sulfur Silicon Relat Elems., 193, 2, 64-73 (2018)
- [19] Shojaei, A.; Galvanetto; Rabczuk, T. U.; Jenabi, A., F.; Zaccariotto, M., A generalized finite difference method based on the peridynamic differential operator for the solution of problems in bounded and unbounded domains, *Comput. Methods. Appl. Mech. Engrg.*, 343, 100-126 (2018) · [Zbl 1440.65157](#)
- [20] Shojaei, A.; Mossaiby, F.; Zaccariotto, M.; Galvanetto, U., A local collocation method to construct Dirichlet-type absorbing boundary conditions for transient scalar wave propagation problems, *Comput. Methods. Appl. Mech. Engrg.*, 356, 629-651 (2019) · [Zbl 1441.65080](#)
- [21] Balian, R.; Bloch, C., Distribution of eigenfrequencies for the wave equation in a finite domain: I. Three-dimensional problem with smooth boundary surface, *Ann. Phys. (N.Y.)*, 60, 2, 401-447 (1970) · [Zbl 0207.40202](#)
- [22] Nieto-Vesperinas, M., Propagación de luz y otras ondas electromagnéticas: difracción y esparcimiento [Light and electromagnetic waves propagation: scattering and diffraction], (Calvo, M. L., *Óptica Avanzada [Advanced Optics]* (2002), Ariel Ciencias: Ariel Ciencias Barcelona, Spanish), 41-82
- [23] Nieto-Vesperinas, M., *Scattering and Diffraction in Physical Optics* (1991), Wiley-Interscience: Wiley-Interscience New York (NY) · [Zbl 1110.78001](#)
- [24] Mandel, L.; Wolf, E., *Optical Coherence and Quantum Optics* (1995), Cambridge University Press: Cambridge University Press Cambridge
- [25] Kellogg, O. D., *Foundations of Potential Theory*, 175-211 (1967), Springer-Verlag: Springer-Verlag Berlin-Heidelberg-New York · [Zbl 0152.31301](#)
- [26] Cooley, J. W.; Turkey, J. W., An algorithm for the machine calculation of complex Fourier series, *Math. Comp.*, 19, 90, 297-301 (1965) · [Zbl 0127.09002](#)
- [27] Frigo, M.; Johnson, S. G., The design and Implementation of FFTW3, *Proc. IEEE*, 93, 2, 216-231 (2005)
- [28] Schwinger, J.; Deraad Jr, L.; Milton, K.; Tsai, W. Y., *Classical Electrodynamics* (1998), CRC Press: CRC Press Boca Raton
- [29] Calvo, M. L., Linear behaviour in the aperture pupil of single photoreceptors: consequences related to the degree of inhomogeneity, *Biol. Cybern.*, 54, 3, 201-210 (1986)
- [30] Ojeda-Castaneda, J.; Gomez-Reino, C., *Selected Papers on Zone Plates* (1996), SPIE Press: SPIE Press Washington
- [31] Carnal, O.; Sigel, M.; Sleator, T.; Takuma, H.; Mlynek, J., Imaging and focusing of atoms by a Fresnel zone plate, *Phys. Rev. Lett.*, 67, 23, 3231-3234 (1991)
- [32] Reisinger, T.; Holst, B., Neutral atom and molecule focusing using a Fresnel zone plate, *J. Vac. Sci. Technol. B*, 26, 6, 2374-2379 (2008)
- [33] Arndt, M.; Nairz, O.; Vos-Andreae, J.; Keller, C.; van der Zouw, G.; Zeilinger, A., Wave-particle duality of C-60 molecules, *Nat.*, 401, 6754, 680-682 (1999)
- [34] Alvarez-Estrada, R. F., Quantum diffractive reflection for a periodic non-penetrable surface: a multiple scattering approach, *Ann. Phys.*, 204, 1, 124-154 (1990)

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