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Formulation of the Density Eigenvalue Problem in Neutron Transport for Relevant Engineering Applications

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ABSTRACT

A new formulation of the density eigenvalue problem for the neutron transport equation is presented. This formulation is particularly adequate to study the definition of the material composition in the criticality design process of a multiplying system. The method is then applied for the study of classical problems such as the critical moderation ratio and the poison concentration to control the reactor. Some results are presented in one dimensional configuration using the multi-group spherical harmonics approach. This eigenvalue formulation proves to be a convenient and useful way to attain criticality, also for complex, realistic systems.

KEYWORDS: transport theory, eigenvalue problem, $\mathrm{P_N}$ approximation, density eigenvalue

1. INTRODUCTION

The eigenvalue formulation of the neutron transport balance model is a classic physico-mathematical problem of large interest in the reactor physics field, as the eigenvalue, in its various formulations, is an integral parameter that provides rich physical information on the behavior of a nuclear reactor, with direct applications useful in the reactor engineering field.

The study of the different formulation of the eigenvalue problem for neutron transport has been treated in previous works [1,2], starting from the well-known multiplication eigenvalue k and considering other, physically significant, forms such as the α time-eigenvalue. The analyses have been performed in the context of the transport $\mathrm{P_N}$ model, focusing the attention on aspects related to the convergence of the solution with respect to the angular and spatial variable, also suggesting the application of specific acceleration techniques [3].

All the formulations of the eigenvalue problem can be given a physical interpretation, but all the applicative studies have always been focused on k and α. Instead, the mathematical formulation of the eigenvalue problem can be elaborated in alternative ways, aiming at a form of the problem that is relevant and useful in the engineering design field. This objective requires formulating the eigenvalue problem in a rather unusual form, for instance highlighting aspects related to the control of a multiplying system. All the resulting alternative formulations can be qualified as a novel interpretation of the δ eigenvalue [4], which in the past, in its traditional form, was considered somewhat exotic and not very informative, as it simultaneously modifies all the densities of the nuclides within the system [5].

The approach adopted in this work and its final aim fits, in the Authors' opinion, into the spirit of the legacy that Massimo Salvatores left us, as he was always attentive to the basic physical and mathematical aspects of a reactor physics problem, without losing sight of the application to realistic situations. We therefore hope that this contribution will honour the memory of one of the most important scientists in the world in the field of reactor physics, Massimo Salvatores.

2. THE THEORY OF THE ζ EIGENVALUE

Suppose to study a system defined in a bounded spatial domain $\mathcal{V}$, composed by a mixture of nuclides, each characterized by a local density $N_m(\vec{r})$, for $m = 1, \ldots, M$. As a first step towards an alternative formulation of the density eigenvalue problem, let us suppose to introduce such eigenvalue to act only on the density of a chosen nuclide, identified by index $m^\star$, in a specific zone $\mathcal{Z}$, constituting a sub-domain of $\mathcal{V}$. It is not required that such zone is geometrically simply connected. The general time-dependent source-driven neutron transport equation reads:

$$\begin{aligned}
&\frac{1}{\mathrm{v}}\frac{\partial\phi(\vec{r},E,\vec{\Omega},t)}{\partial t} + \vec{\Omega}\cdot\nabla\phi(\vec{r},E,\vec{\Omega},t) + \sum_{m=1}^{M}\left[N_m(\vec{r})\sigma_{t,m}(E)\right]\phi(\vec{r},E,\vec{\Omega},t) = \\
&\sum_{m=1}^{M}\int dE' \oint d\vec{\Omega}' \left[N_m(\vec{r})\sigma_{s,m}(E')\right] f_{s,m}(\vec{r},E'\to E,\vec{\Omega}'\cdot\vec{\Omega})\phi(\vec{r},E',\vec{\Omega}',t) + \\
&\sum_{m=1}^{M}\int dE' \oint d\vec{\Omega}' \left[N_m(\vec{r})\nu_m(E')\sigma_{f,m}(E')\right]\frac{\chi_m(E)}{4\pi}\phi(\vec{r},E',\vec{\Omega}',t) + S(\vec{r},E,\vec{\Omega},t),
\end{aligned} \tag{1}$$

where the symbols have their usual meaning in reactor physics, see for instance [2]. Vacuum boundary conditions and an initial condition are needed to complement this equation. To construct the needed eigenvalue problem, the time dependence and the external source are removed. Consequently, an eigenvalue ζ may be introduced to act on the density of nuclide $m^\star$ in zone $\mathcal{Z}$ only. Therefore, the transport equation to be solved for $\vec{r}\in\mathcal{Z}$ takes the following form:

$$\begin{aligned}
&\vec{\Omega}\cdot\nabla\phi(\vec{r},E,\vec{\Omega}) + \sum_{m\neq m^\star}\left[N_m(\vec{r})\sigma_{T,m}(E)\right]\phi(\vec{r},E,\vec{\Omega}) + \frac{1}{\zeta}\left[N_{m^\star}(\vec{r})\sigma_{T,m^\star}(E)\right]\phi(\vec{r},E,\vec{\Omega}) = \\
&\sum_{m\neq m^\star}\int dE' \oint d\vec{\Omega}' \left[N_m(\vec{r})\sigma_{s,m}(E')\right] f_{s,m}(\vec{r},E'\to E,\vec{\Omega}'\cdot\vec{\Omega})\phi(\vec{r},E',\vec{\Omega}') + \\
&\frac{1}{\zeta}\int dE' \oint d\vec{\Omega}' \left[N_{m^\star}(\vec{r})\sigma_{s,m^\star}(E')\right] f_{s,m^\star}(\vec{r},E'\to E,\vec{\Omega}'\cdot\vec{\Omega})\phi(\vec{r},E',\vec{\Omega}') + \\
&\sum_{m\neq m^\star}\int dE' \oint d\vec{\Omega}' \left[N_m(\vec{r})\nu_m(E')\sigma_{f,m}(E')\right]\frac{\chi_m(E)}{4\pi}\phi(\vec{r},E',\vec{\Omega}') + \\
&\frac{1}{\zeta}\int dE' \oint d\vec{\Omega}' \left[N_{m^\star}(\vec{r})\nu_{m^\star}(E')\sigma_{f,m^\star}(E')\right]\frac{\chi_{m^\star}(E)}{4\pi}\phi(\vec{r},E',\vec{\Omega}'),
\end{aligned} \tag{2}$$

while for the $\vec{r}\notin\mathcal{Z}$:

$$\begin{aligned}
&\vec{\Omega}\cdot\nabla\phi(\vec{r},E,\vec{\Omega}) + \sum_{m=1}^{M}\left[N_m(\vec{r})\sigma_{T,m}(E)\right]\phi(\vec{r},E,\vec{\Omega}) = \\
&\sum_{m=1}^{M}\int dE' \oint d\vec{\Omega}' \left[N_m(\vec{r})\sigma_{s,m}(E')\right] f_{s,m}(\vec{r},E'\to E,\vec{\Omega}'\cdot\vec{\Omega})\phi(\vec{r},E',\vec{\Omega}') + \\
&\sum_{m=1}^{M}\int dE' \oint d\vec{\Omega}' \left[N_m(\vec{r})\nu_m(E')\sigma_{f,m}(E')\right]\frac{\chi_m(E)}{4\pi}\phi(\vec{r},E',\vec{\Omega}').
\end{aligned} \tag{3}$$

Of course, the continuity of the angular flux on any internal interface is required.

The choice of the nuclide and region depends on the application envisaged, as this formulation of the problem allows to evaluate the effect on the balance problem of a specific nuclide and on its positioning within the reactor. In general, the eigenvalue ζ could be introduced in a more general way to filter a specific volume in phase space, thus including also the possibility to act on a specific energy range. This generalization is not considered in the present work.

3. APPROXIMATE TRANSPORT MODEL AND DISCUSSION OF PROBLEMS ANALYSED

It is well known that, for a given off-critical system, the criticality condition can be attained adjusting its material composition or its geometrical size and arrangement or both [6]. The search for criticality is usually performed evaluating the effective multiplication factor of the system, $\mathrm{k_{eff}}$. The distance of this parameter with respect to unity suggests what has to be done to approach criticality, e.g. when $\mathrm{k_{eff}} < 1$ the multiplication should be enhanced and/or the particle loss should be reduced. However, no quantitative information is provided on how criticality can be achieved, except that the number of neutrons emitted by fission, ν, should become $\nu/\mathrm{k_{eff}}$. Nevertheless, this variation cannot be practically obtained, since adjusting ν means changing the composition of the fissile material and, thus, Σ_f.

Assuming that the rough system dimensions and arrangement are determined by constraints other than criticality, i.e. thermo-hydraulics and structural requirements, the designer can achieve criticality acting only on the atomic density of one or more nuclides. Therefore, the design process is restricted to the choice of the type of nuclide whose density needs to change, i.e. fissile, absorber or moderator if the system is thermal.

A set of physico-engineering problems relevant in reactor physics will be presented in this section, in order to show the main features of this generalised density eigenvalue formulation. These problems will be all addressed discretising the $\mathrm{P_N}$ multi-group equations in plain geometry with a finite difference scheme and imposing Mark boundary conditions to approximate the vacuum, as done in [2]. The choice of an approximate, one-dimensional numerical transport model instead of an analytical one allows to treat less idealised problems, but also makes the introduction of the ζ eigenvalue easier. All the multi-group constants employed in the calculations are obtained by collapsing a set of starting cross sections, generated with the Serpent 2 Monte Carlo code [7] on the CASMO 70 groups grid. It is worth to mention the fact that the effect induced by the variations in the density of the selected nuclides on the multi-group cross sections self-shielding is neglected at this stage, leaving this aspect as a future development of this approach.

3.1. Approach to criticality for a mixture of fuel and moderator

One of the classical problems of reactor physics is the determination of the critical moderator-to-fuel ratio in a thermal reactor. It is well known that, if the fissile enrichment and the system size are adequate, there can be two critical moderation ratios N_m/N_f [8], as it can be seen in figure 1. When the lowest one is selected, the critical structure is said to be under-moderated, while, when the largest one is employed, the system is said to be over-moderated.

The existence of these two solutions is physically explained by the competition between the neutron slowing down and absorption in the moderator.

Figure 1 shows the $\mathrm{k_{eff}}$ behaviour for a slab filled with a homogeneous mixture of fissile material and light water as a function of the moderation ratio. As usual, the critical moderation ratios, i.e. the red dots in the figure, are determined changing iteratively the moderator density. Therefore, each dot in the Figure corresponds to the solution of a k-eigenvalue problem cast in the two-group $\mathrm{P_1}$ model.

Table I: Critical moderation ratios N_m/N_f to achieve criticality in a two-group homogeneous mixture of fissile material and light water.

ζ calculation		iterative calculation	
N_m/N_f	k_{eff}	N_m/N_f	k_{eff}
379.7	1.00000	384.8	1.00773
21722.5	1.00000	21583.4	0.99674

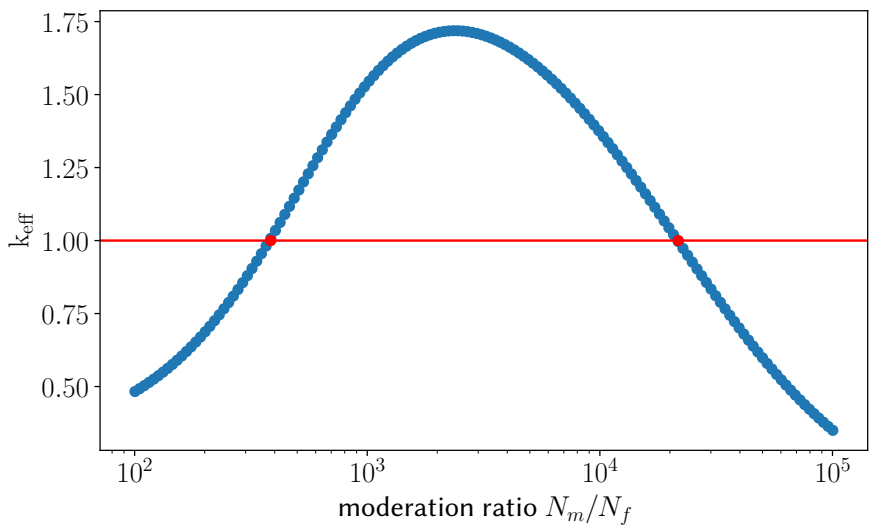

Figure 1: Effective multiplication factor as a function of the moderation ratio for a two-group homogeneous system.

The same solutions can be obtained introducing the ζ eigenvalue in front of the moderator density. In Table I it is possible to observe that the ζ approach allows to determine the "exact" values of the moderation ratio, while the iterative method yields only approximate values.

Figures 2 and 3 show the first four higher-order ζ harmonics and the full eigenvalue spectrum for this problem. These figures are very informative. First, it is remarkable to notice that, due to the existence of two possible critical moderation ratios, there are two positive eigenfunctions, associated to the fundamental eigenvalues, which are represented as blue stars in the graph. By inspection it is possible to see that the fundamental ζ yielding the over-moderated system corresponds to the dominant eigenvalue, i.e. the largest one, while the under-moderated solution, which is usually preferred for stability requirements, falls around zero and it is very close to the other eigenvalues.

This behaviour seems to suggest that, in order to find all the physically meaningful solutions, the complete spectrum should be found. In case this was not computationally affordable, a simpler transport model could be employed to look for the approximated spectrum and, thus, fundamental eigenvalues, which then could be used as eigenvalue shifts to enhance the eigenvalue solver convergence [9].

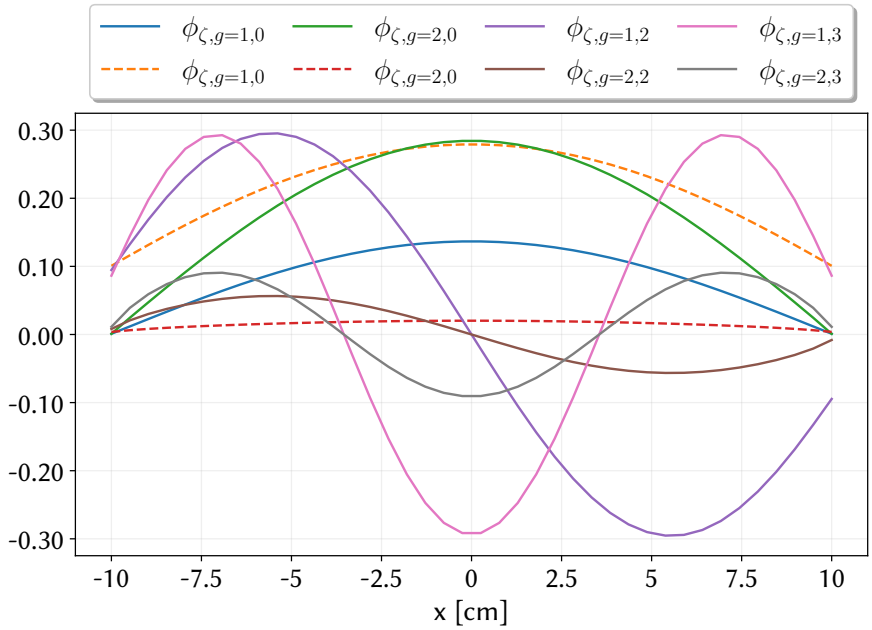

Figure 2: Higher-order, two-group ζ modes for a homogeneous mixture of light water and fissile material. Each harmonic is normalised to yield a unitary integral of the total flux corresponding to the same spatial harmonic.

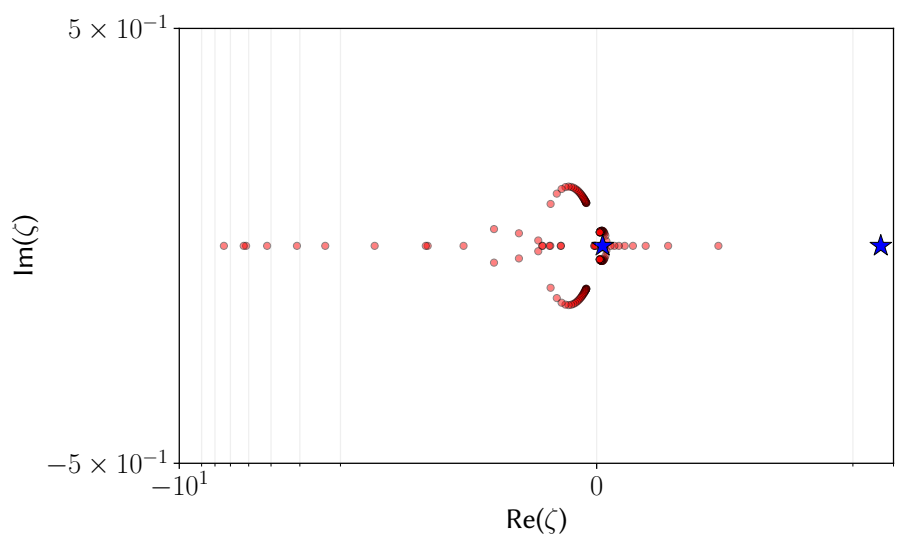

Figure 3: ζ eigenvalue spectrum on the complex plane for a homogeneous mixture of light water and fissile material. The blue stars are the eigenvalues associated to positive modes.

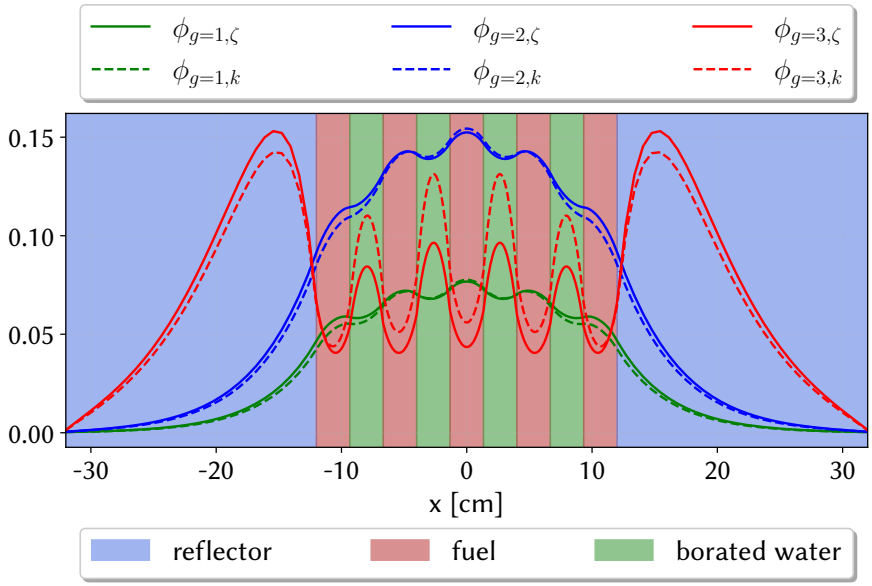

Figure 4: Three-group fundamental k and ζ modes for a heterogeneous arrangement of fuel and borated water layers, surrounded by a light water reflector. The k modes represent the initial off-critical flux distribution, while the ζ modes represent the critical flux when the boron density is adjusted with a 1/ζ factor. The fluxes are normalised to have a unitary total flux integral.

3.2. Boron concentration in a water reactor

Another fundamental problem in the physics and engineering of pressurised water reactors is the search for the boron concentration to be diluted in the coolant to ensure criticality. Even in this case, the common approach to solve this problem is resorting to iterations. However, thanks to the generalised density eigenvalue, it is possible to solve this problem directly, by solving for the fundamental ζ eigenvalue. Figure 4 shows the three-group k flux for a super-critical system with no boron in water and the three-group ζ eigenfunction. This last eigenfunctions corresponds, by definition, to the critical flux of the system when some boron with density multiplied by 1/ζ is mixed with water inside the coolant layers. This fact has also been assessed numerically: after the addition of boron with a 1/ζ density correction, the system yields a unitary k and the same flux distribution obtained in the ζ calculation. As one could expect, the addition of the poison to the coolant layers composition has an important impact on the energy spectrum of the system, featured by a strong spectrum hardening.

Figure 5 shows the full ζ spectrum for a heterogeneous arrangement of fuel and coolant layers, surrounded by a water reflector. In this case, there is only one fundamental eigenvalue, which is strictly positive, as most of the spectrum degenerates around zero.

As a consequence of this spectrum degeneracy, the typical oscillating higher-order harmonics are missing, and only numerically noisy solutions are found. In order to explain this behaviour, it should be remarked here that, contrarily to the k fundamental eigenvalue, which is always strictly positive if some fissile material is present, the existence and uniqueness of a positive ζ eigenvalue is not guaranteed. At a first glance, this fact may sound as an unpleasant feature of this eigenvalue formulation with respect to the k eigenproblem: however, from a practical standpoint, the ζ problem is, to the authors' opinion, the most natural way to approach criticality consistently.

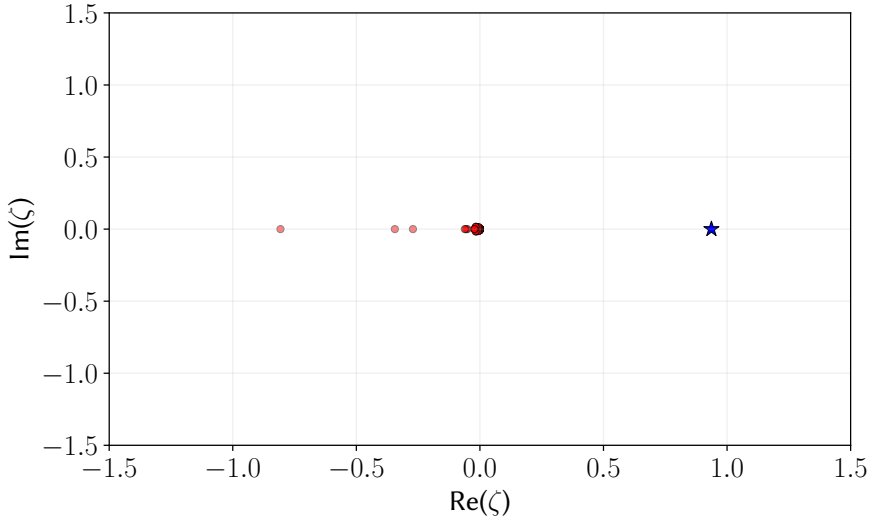

Figure 5: ζ eigenvalue spectrum on the complex plane for a homogeneous mixture of light water and fissile material. The blue stars are the eigenvalues associated to positive modes.

3.3. Approach to criticality via control rod positioning

The last application presented in the paper is the calculation of the absorber density in a control rod device needed to achieve criticality. Also in this case, the ζ eigenvalue allows to determine directly the absorber concentration needed to achieve criticality for an initially super-critical system featured by alternate layers of fuel and coolant. Figure 6 reports both the three-group super-critical k flux and the ζ flux which corresponds to the critical flux when the two layers in green are replaced by the absorber material, i.e. the control devices are inserted. With respect to the boron dilution in water, this reactivity control system introduces a larger distortion in the energy spectrum, as clearly visible in Figure 6.

Figure 7 shows the eigenvalue spectrum for this study case. With respect to the boron dilution case, see Figure 5, there are two eigenvalues larger than one. However, only one of them is associated to a positive eigenfunction, being thus the only physical solution. The other positive eigenvalue is associated with an oscillating eigenfunction. The two first thermal eigenfunctions are depicted in Figure 8.

It should be noticed that, if the system is sub-critical, all the non-zero ζ eigenvalues would be negative. Despite a negative density lacks of physical meaning, a negative eigenvalue suggests that it is not possible to attain criticality with the nuclide whose concentration is considered to be a free parameter unless its cross sections change sign, i.e. the absorption becomes a production.

4. CONCLUSIONS

In this paper, a novel formulation to the neutron transport eigenvalue problem has been proposed, generalising the density eigenvalue. This new eigenvalue, named ζ, can be introduced freely in the transport model, acting on a selected portion of the phase space. Despite its broader applications and its connection with the nature of the transport operator, the ζ eigenvalue has been presented here mainly as a design-oriented technique for the efficient evaluation of the critical concentration for a specific nuclide (or mixture of nuclides).

The application of this approach to realistic problems in reactor physics provided remarkable results. First, the ζ eigenvalue yields equivalent results to the iterative method commonly applied in such framework, but

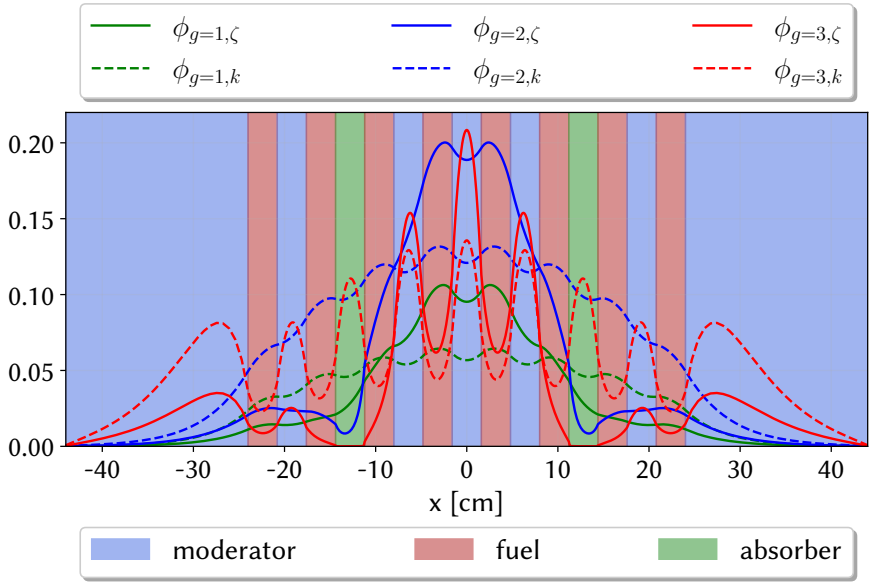

Figure 6: Three-group fundamental k and ζ modes for a heterogeneous arrangement of fuel, coolant and absorber layers, surrounded by a light water reflector. The k modes represent the initial off-critical flux distribution, while the ζ modes represent the critical flux when the boron density is adjusted with a 1/ζ factor. The fluxes are normalised to have a unitary total flux integral.

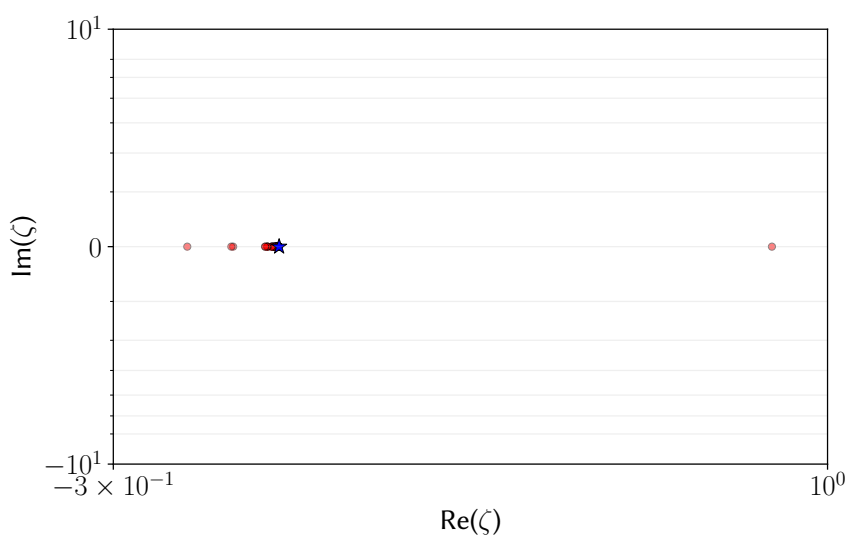

Figure 7: ζ eigenvalue spectrum on the complex plane for a heterogeneous arrangement of coolant, absorbers and fissile material. The blue star is the eigenvalue associated to the positive mode.

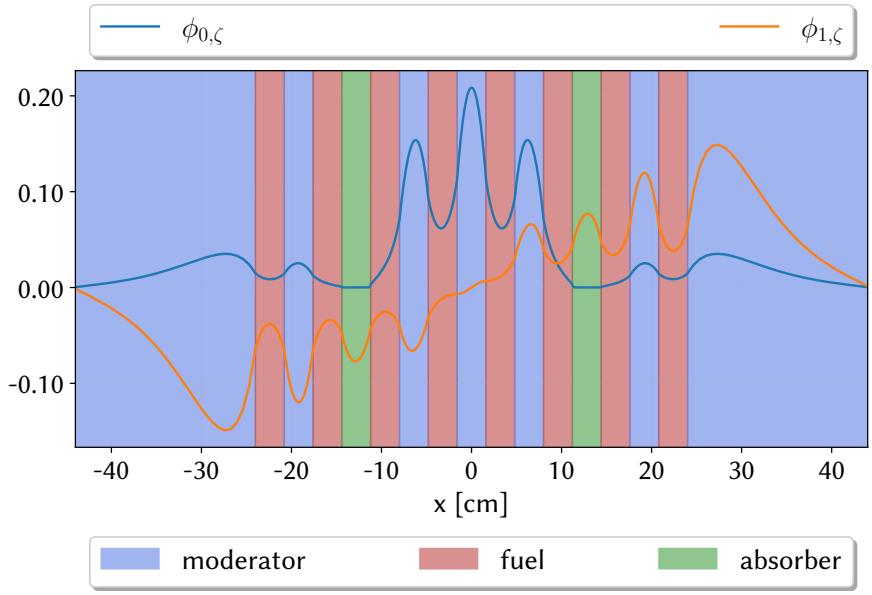

Figure 8: Thermal higher-order ζ modes for a heterogeneous arrangement of fuel, coolant and absorber layers, surrounded by a light water reflector. Each spatial harmonic is normalised to yield a unitary integral of the total flux corresponding to the same harmonic order.

with a strong reduction of the computational effort. More importantly, the existence of one or more design solutions seems related to the presence, in the ζ spectrum, of one or more real and positive eigenvalues associated to positive eigenfunctions. This is a remarkable feature, which should facilitate to rigorously assess whether criticality can be attained or not acting on the selected nuclides, even in case of complex systems. Finally, this study of the ζ eigenvalue spectrum suggests that, in some situations, like the study of control systems, the eigenvalue separation is large enough to ensure an efficient numerical convergence on the dominant one.

Due to its novelty, there are many open questions that should be addressed in future works. First of all, the ζ spectrum should be studied thoroughly, taking into account the impact of the different spatial, angular and energy approximations of the neutron transport equation. In particular, the issue of multiplicity of eigenvalues associated to physically meaningful eigenfunctions should be investigated, especially for non-thermal systems. Moreover, the physical meaning of the higher-order ζ harmonics should be investigated more deeply. Then, also the action of the eigenvalue on more specific portions of the phase space should be studied, involving for example only some reaction channel, e.g. the capture, and a reduced energy range, e.g. the thermal region.

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