A generalised eigenvalue formulation for core-design applications

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Abstract

The adoption of multiplication eigenvalue is a well established approach for the design of nuclear reactors. However, despite its popularity and nice physico-mathematical properties, this eigenvalue formulation is not able to provide quantitative information about what parameters the designer has to modify. In this paper, a novel generalised eigenvalue formulation is introduced to disclose the full potential of the neutron transport equation for core design applications. To illustrate the advantages of this new design-orient approach with respect to traditional methods, some relevant problems arising in the physics of reactors are solved, such as the determination of the absorber density in the control rods and of the fissile concentration in the molten salt fast reactor.

Keywords — Neutron Transport Equation, Eigenvalue problems, Density eigenvalue problem, Core design

I. INTRODUCTION

The concepts of eigenvalue and eigenfunction of an operator are fundamental in a wide range of applications, from basic physics to statistics to engineering. Since their first appearance in the XIX$^{\text{th}}$ century, they have rapidly become so popular that they are now considered a standard tool of applied mathematics. As reported in [1], there are at least four main reasons behind the success of the eigenvalues and eigenfunctions:

1. the possibility to use them as a basis to solve partial differential equations, when variables can be separated;

2. their use in sensitivity analysis, for example in connection to the physical phenomena of mechanical resonances;

3. their connection to stability and asymptotic analyses, to determine the dominant response of a system to a perturbation;

4. their ability to provide the intimate behaviour, i.e. the *personality*, of an operator by means of its spectrum.

Most of these aspects are particularly relevant in the framework of the physics of fission reactors. The first feature is used to approach analytically the solution of the transport equation [2], while the second one is very useful to estimate the sensitivity of a system with respect to a certain input variation, in order to perform uncertainty quantification or design optimisation [3]. Concerning the third feature, the eigenvalues have been extremely relevant in the development of perturbation methods, which are widely employed in many applications [4]. All these applications implicitly rely on the fourth aspect, which plays a central rôle in fission reactor physics. The fundamental problem of this discipline is to look for the existence of an asymptotic, bounded and non-negative

solution of the Neutron Transport Equation (NTE) for a multiplying medium, which reads

$$
\begin{cases}
\dfrac{1}{\mathrm{v}(E)}\dfrac{\partial\phi(\vec{r},E,\vec{\Omega},t)}{\partial t}+\nabla\cdot(\vec{\Omega}\phi(\vec{r},E,\vec{\Omega}))+\Sigma_t(\vec{r},E)\phi(\vec{r},E,\vec{\Omega},t)= \\
\qquad\displaystyle\int_0^\infty dE'\oint d\vec{\Omega}'\Sigma_s(\vec{r},E')\phi(\vec{r},E',\vec{\Omega}',t)f_s(\vec{r},E'\to E,\vec{\Omega}'\cdot\vec{\Omega})+ \\
\qquad(1-\beta)\dfrac{\chi_p(\vec{r},E)}{4\pi}\displaystyle\int_0^\infty dE'\oint d\vec{\Omega}'\nu\Sigma_f(\vec{r},E')\phi(\vec{r},E',\vec{\Omega}',t)+ \\
\qquad\displaystyle\sum_{r=1}^{\mathrm{R}}\dfrac{\chi_{d,r}(\vec{r},E)}{4\pi}\lambda_r C_r(\vec{r},t) \\
\dfrac{\partial C_r(\vec{r},t)}{\partial t}=\beta_r\displaystyle\int_0^\infty dE'\oint d\vec{\Omega}'\nu\Sigma_f(\vec{r},E')\phi(\vec{r},E',\vec{\Omega}',t)-\lambda_r C_r(\vec{r},t), \\
\qquad r=1,\ldots,R,
\end{cases}
\tag{1}
$$

subject to appropriate initial and boundary conditions. The symbols have the usual meaning:

- $\mathrm{v}(E)$ is the neutron velocity;
- $\phi(\vec{r},E,\vec{\Omega},t)$ is the angular neutron flux as a function of the three-dimensional spatial coordinate $\vec{r}$, the particle energy E, the flying direction $\vec{\Omega}$ and the time instant t;
- $\Sigma_t(\vec{r},E)$ is the total macroscopic cross section: it is useful to recall here that this quantity is given as the sum of total capture, total fission and total scattering interactions, respectively

$$\Sigma_t(\vec{r},E)=\Sigma_c(\vec{r},E)+\Sigma_f(\vec{r},E)+\Sigma_s(\vec{r},E); \tag{2}$$

- $f_s(\vec{r},E'\to E,\vec{\Omega}'\cdot\vec{\Omega})$ is the scattering transfer function, which represents the probability density function that an incident neutron colliding with the medium is transferred from the phase space coordinates (E', $\vec{\Omega}'$) to (E, $\vec{\Omega}$), assuming rotational invariance;
- β is the total neutron delayed fraction, given as

$$\beta=\sum_{r=1}^{\mathrm{R}}\beta_r, \tag{3}$$

  where β_r is the delayed fraction of the r^{th} of the R precursor families;

- $\chi_p(\vec{r}, E)$ is the prompt fission emission spectrum, while $\chi_{d,r}(\vec{r}, E)$ is the delayed fission emission spectrum for the r^{th} family. The emission spectra are assumed to depend on the emission energy only [5].;
- $\nu\Sigma_f(\vec{r}, E)$ is the neutron fission production macroscopic cross section;
- λ_r is the radioactive decay constant for the r^{th} precursor family;
- $C_r(\vec{r}, t)$ is the density of delayed neutron precursor;

The following operators are now introduced in order to express this model in a more compact way:

- the streaming operator,

$$\hat{L} = \nabla \cdot (\vec{\Omega}*); \tag{4}$$

- the removal by collision operator,

$$\hat{R} = \Sigma_t(\vec{r}, E)*; \tag{5}$$

- the scattering operator,

$$\hat{S} = \int_0^\infty dE' \oint d\vec{\Omega}'\, \Sigma_s(\vec{r}, E') f_s(\vec{r}, E' \rightarrow E, \vec{\Omega}' \cdot \vec{\Omega})*; \tag{6}$$

- the prompt fission operator,

$$\hat{F}_p = (1-\beta)\frac{\chi_p(\vec{r}, E)}{4\pi} \int_0^\infty dE' \oint d\vec{\Omega}'\, \nu\Sigma_f(\vec{r}, E')*; \tag{7}$$

- the delayed fission operator for the i^{th} delayed precursor family,

$$\hat{F}_{d,r} = \beta_r \frac{\chi_{d,r}(\vec{r}, E)}{4\pi} \int_0^\infty dE' \oint d\vec{\Omega}'\, \nu\Sigma_f(\vec{r}, E') * . \tag{8}$$

In addition to these definitions, other operators that will be adopted later in the paper are introduced here. The first one is the total fission production operator, which is useful in the steady-state equation, when the neutron population is in equilibrium with the precursors

concentrations,

$$\hat{F} = \hat{F}_p + \sum_{r=1}^{\mathrm{R}} \hat{F}_{d,r}. \tag{9}$$

Recalling eq. (2) the other operators can be defined splitting the removal operator in eq. (5) accordingly to the following three reaction operators,

- total capture operator,

$$\hat{C}_T = \Sigma_c(\vec{r}, E)*; \tag{10}$$

- total fission operator,

$$\hat{F}_T = \Sigma_f(\vec{r}, E)*; \tag{11}$$

- total scattering operator,

$$\hat{S}_T = \Sigma_s(\vec{r}, E) * . \tag{12}$$

These definitions allow casting section I into the more compact form,

$$\begin{cases} \dfrac{1}{\mathrm{v}} \dfrac{\partial \phi}{\partial t} + \hat{L}\phi + (\hat{C}_T + \hat{F}_T + \hat{S}_T)\phi = \hat{S}\phi + \hat{F}_p\phi + \displaystyle\sum_{r=1}^{\mathrm{R}} \lambda_r \epsilon_r \\ \dfrac{\partial \epsilon_r}{\partial t} = \hat{F}_{d,r}\phi - \lambda_r \epsilon_r \quad r = 1, \ldots, R, \end{cases} \tag{13}$$

where the flux and precursors dependencies are omitted, for the sake of conciseness, and we have introduced the delayed emissivity ϵ_r as:

$$\epsilon_r(\vec{r}, E, t) = \frac{\chi_{d,r}(\vec{r}, E)}{4\pi} C_r(\vec{r}, t). \tag{14}$$

When a multiplying, source-free system is able to reach a steady-state condition, it is said to be self-sustaining or *critical*. From a physical perspective, maybe the most intuitive way of approaching criticality is to observe the free evolution of the system under examination, assuming the medium properties to be time-independent, at least on the evolution time scale. Under this hypothesis, it has been observed both experimentally [6] and theoretically [5] that the neutron flux can be factorised into a time exponential behaviour and a distribution in the phase space

$$\phi(\vec{r}, E, \vec{\Omega}, t) = \varphi_\omega(\vec{r}, E, \mu) e^{\omega t}, \tag{15}$$

independently on the initial conditions.

Substituting this physically intuitive factorisation, which is assumed to hold for the precursors concentration C_i as well, into eq. (13) yields the so-called *time* eigenvalue formulation of the transport equation,

$$\begin{cases} \dfrac{\omega}{\mathrm{v}}\varphi_\omega + \hat{L}\varphi_\omega + (\hat{C}_T + \hat{F}_T + \hat{S}_T)\varphi_\omega = \hat{S}\varphi_\omega + \hat{F}_p\varphi_\omega + \displaystyle\sum_{r=1}^{\mathrm{R}} \lambda_r \epsilon_r \\ \omega\epsilon_r = \hat{F}_{d,r}\varphi_\omega - \lambda_r\epsilon_r \quad i = r, \dots, R. \end{cases} \tag{16}$$

The solution of this eigenvalue problem, which could be obtained equivalently also taking the Laplace transform of eq. (13), describes the time frequencies ω characterising the system free evolution. Therefore, the eigenstates associated to this problem are usually identified as the *natural modes* of the neutron transport operator. The Laplace transform is a common approach to tackle time-dependent problems in both physics and engineering, then it is hard to assess who was the first to derive this eigenvalue problem in the reactor physics community. Regardless, Henry [6] was the first to study the time eigenvalue and to highlight its value for different applications.

Since the time eigenvalue, which is also often indicated with the symbol α, can be interpreted as a time frequency, the inverse of the dominant one is related to the system period, say T. When the system reaches a steady state, i.e. it is critical, its time period tends to become infinite, $T \to \infty$. Hence, in practical situations, the criticality condition is achieved when the dominant time eigenvalue, i.e. the one associated to the non-negative, non-trivial eigenstate, tends to zero, $\omega_0 \to 0$.

From another perspective, the criticality is achieved when the net number of neutrons does not change as time goes by, i.e. the loss and the production terms are exactly the same:

$$(\hat{L} + \hat{R} - \hat{S} - \hat{F})\phi = 0. \tag{17}$$

When eq. (17) is satisfied, the neutron population self-sustains and a steady state equilibrium is reached. However, in practice, this condition is never fully achieved: even assuming that the equilibrium is reached at a certain time t, the fissile nuclides would be consumed by fissions at time $t + dt$, changing the material properties of the system and, thus, its ability to sustain fission. From this perspective, operating a real reactor would seem barely impossible. In reality, the constraint expressed by eq. (17) should be interpreted more weakly: in order to achieve and

maintain criticality, it is sufficient that the control actions adopted, i.e. reactivity insertions, are faster than time scale of the reactor stable period, T.

Despite its natural definition and its elegance in connecting an idealised physico-mathematical condition with engineering aspects, the time eigenvalue is not appropriate for the design of a critical system. In this respect, eq. (17) is definitively more useful to formulate design-oriented eigenvalue problems.

I.A. Design-oriented eigenvalue formulations

Among its peculiarities, eq. (17) is homogeneous. From a mathematical standpoint, this means that non-trivial steady-state distributions exist only as solutions of an eigenvalue problem, namely

$$\hat{A}\vec{\varphi}_{\xi,n} = \xi_n \hat{B}\vec{\varphi}_{\xi,n}, \tag{18}$$

where $\hat{A}$ and $\hat{B}$ are, in principle, any reasonable linear combination of the operators appearing in eq. (17), and $\{\xi_n, \vec{\varphi}_{\xi,n}\}$ is the n^{th} eigenpair, constituted by an eigenvalue ξ_n and an eigenfunction $\vec{\varphi}_{\xi,n}$, respectively. According to the geometric multiplicity of the eigenproblem $g(\xi)$, the number of eigenpairs is $g(\xi)-1$. In the following, the fundamental eigenpair will be indicated as $\{\xi_0, \vec{\varphi}_{\xi,0}\}$. To approach the criticality condition, several eigenvalue formulations have been proposed. Since their common feature is the fact that the various eigenvalues act on one or more terms of the NTE in order to enforce a steady-state neutron distribution, in the following these formulations will be addressed as *design-oriented* eigenvalues, in order to distinguish them from the time eigenvalue problem.

Probably because of the peculiarity of the newly discovered fission phenomenon [7], Fermi [8] firstly introduced an eigenvalue, which he called *reproduction factor* k, in front of the total fission operator:

$$\hat{L}\varphi_{k,n} + (\hat{C}_T + \hat{F}_T + \hat{S}_T)\varphi_{k,n} - \hat{S}\varphi_{k,n} = \frac{1}{k_n}\hat{F}\varphi_{k,n}. \tag{19}$$

In this formalism, the system is critical when no modification of the fission operator is required, i.e. $k = 1$. To the authors' knowledge, the second eigenvalue formulation proposed is due to Davison [9]. He proposed to approach criticality introducing a *collision* eigenvalue to modify all

the interactions leading to a neutron emission, i.e. scattering and fission,

$$\hat{L}\varphi_{\gamma,n} + \hat{R}\varphi_{\gamma,n} = \frac{1}{\gamma_n}\left(\hat{S} + \hat{F}\right)\varphi_{\gamma,n}. \tag{20}$$

The third design-oriented eigenvalue formulation present in the literature is due to Ronen, Shalitin, and Wagschal [10]. In this paper, they cleverly observed that, given a certain medium, it should be possible to attain criticality varying its density, introducing an eigenvalue acting on all the material properties of the system,

$$\hat{L}\varphi_{\delta,n} = \frac{1}{\delta_n}\left(\hat{S} + \hat{F} - \hat{R}\right)\varphi_{\delta,n}\varphi_{\delta,n}. \tag{21}$$

Due to its position in the transport equation, the action of this eigenvalue can be interpreted in different ways. The most intuitive one is probably the modification of the medium density, which introduces a "competition" between positive (fission, scattering) and negative (removal) contributions. Because of this aspect, this eigenvalue is usually known as *density* eigenvalue. However, multiplying the equation by δ, this eigenvalue can be interpreted as well as a *streaming* eigenvalue, which modifies the relationship between the angular current spatial derivative and the angular flux. In this case, the eigenvalue operates a re-scaling of the spatial coordinates, changing the free-flight kernel of the transport process.

In addition to these formulations, it is also possible to introduce an eigenvalue acting on the total capture cross section. To the best of the author's knowledge, this eigenvalue formulation has never been proposed so far. The symbol proposed here to indicate this capture eigenvalue is taken from the ancient Greek word for "capture", "hunting", ϑηράω,

$$\left(\hat{L} + \hat{F}_T + \hat{S}_T - \hat{S} - \hat{F}\right)\varphi_{\vartheta,n} = \frac{1}{\vartheta_n}\hat{C}_T\varphi_{\vartheta,n}. \tag{22}$$

All the eigenvalue problems presented so far can be obtained from a manipulation of eq. (13) [11],

eigenvalue	critical value	ε_k	ε_α	ε_ω	ε_γ	ε_δ	ε_ϑ
k	1	$1/k$	0	0	1	1	0
ω	0	1	ω	ω	1	1	0
γ	1	1	0	0	$1/\gamma$	1	0
δ	1	1	0	0	1	δ	0
ϑ	1	1	0	0	1	1	$1/\vartheta$

TABLE I
The set of ε parameters to be used in eq. (23) to retrieve the different eigenvalue formulations.

$$\begin{aligned}\varepsilon_\delta \hat{L}\phi(\vec{r},\vec{\Omega},E) + \left(\varepsilon_\vartheta \hat{C}_T + \hat{F}_T + \hat{S}_T + \frac{\varepsilon_\alpha}{\mathrm{v}}\right)\phi(\vec{r},\vec{\Omega},E) = \\ \varepsilon_\gamma \left[\hat{S} + \varepsilon_k \left(\hat{F}_p + \sum_{r=1}^{\mathrm{R}} \frac{\lambda_r}{\lambda_r + \varepsilon_\omega}\hat{F}_{d,r}\right)\right]\phi(\vec{r},\vec{\Omega},E),\end{aligned} \tag{23}$$

where the values of the ε parameters are provided in table I. The symbol ϕ is used to indicate the neutron angular flux for an arbitrary eigenvalue formulation. In the following, the symbol φ_{x} will be used to indicate the angular flux associated to a specific eigenvalue formulation x.

Except for the novel capture eigenvalue, all the other formulations have been extensively studied in the literature. For instance, in [12, 13] an assessment of the impact of the various eigenvalue problems on the neutron energy spectra is carried out, in [14, 11] the eigenvalue spectra are analysed in the framework of the $\mathrm{P_N}$ model, while in [15] the time, collision and multiplication eigenmodes are employed in a modal method to analyse some transient scenarios.

Despite the various formulations are very useful to highlight different aspects pertaining to the NTE and have some important practical applications, all of these spectral forms of the NTE share the issue of showing unsatisfactory adherence to the physical constraints that are practically encountered when the design is actually carried out. Hence, their adoption is limited to assess the criticality of a fissile system. However, for industrial design-oriented applications, the k eigenvalue is still the most popular figure of merit used to study the criticality condition.

According to the value of k_{eff}, i.e. the fundamental eigenvalue k_0, the designer can immediately understand how far the system is from criticality. Assuming that a certain system is featured by $k > 1$, the designer guesses that the multiplication properties of the core should decrease, either changing its geometrical features to increase leakage or changing its material properties, e.g. increasing parasitic capture or decreasing fission, but no precise indication on *what* has to

change can be obtained. Most of the times, the other design constraints can guide this selection. For example, the fuel pins should have a minimum surface-to-volume ratio for thermo-hydraulics requirements [16], so the criticality could be attained, in this case, acting only on the material composition. However, the quantitative information provided by k is not sufficient to practically achieve criticality. k can be interpreted as a correction factor for the total fission production, so it can be viewed as a correction either for Σ_f or for ν. In the first case, changing the total fission cross section would imply to change the absorption and the total cross sections as well, while changing ν is not possible unless acting on the mixture of fissile materials, which implies also to change the cross sections of the medium. At this point, it should be clear that the quantitative information delivered by k does not provide a *physically consistent* indication for the design. The same could be argued also for the γ and the ϑ cases.

On the contrary, the other design-oriented formulation, i.e. the density eigenvalue δ, provides a correction factor for the medium density, so it acts simultaneously on all the cross sections. In principle, this information is physically consistent, but it may not be useful from a practical point of view, as it is not always possible to act on the atomic density of a certain material. Moreover, the same correction factor should be applied to each nuclide composing the medium, meaning that this formulation does not allow to handle specific regions, e.g. the fuel pins or the control rods.

This paper presents an innovative formulation of the density eigenvalue, based on a generalised eigenvalue formulation, which overcomes the issues of the traditional δ formulation in order to be applicable for design-oriented applications. In the next section, this new eigenvalue formulation will be derived starting from a generalisation of the NTE eigenvalue problem, while in the rest of the paper some relevant design problems occurring in the physics of fission reactors will be analysed in the light of this new formulation, in order to show its advantages with respect to the legacy calculation approach.

II. THE THEORY OF THE ζ EIGENVALUE

Except for the time eigenvalues, which naturally arise from the Laplace transform of the NTE, all the other design-oriented formulations discussed so far are simply derived introducing an eigenvalue in front of the operator of interest. Recalling eq. (18), it is evident that the eigenvalue ξ_n turns out to be a tuning parameter that is used to force the system to reach the criticality

condition. In this case, this parameter acts on the operator $\hat{B}$ and, consequently, on the phase space where this operator is defined. For example, in case ξ is k, this parameter would act only on those regions of the phase space where $\chi(\vec{r}, E)\nu(\vec{r}, E')\Sigma_f(\vec{r}, E') \neq 0$, i.e. only on the fissile nuclides in the active regions and only on the fission energy range.

As such, it would be still valid, from both a mathematical and a physical point of view, to introduce the eigenvalue to act on a more specific portion of the phase space. Let us assume, for example, that the objective of the design is to determine what is the amount of captures that a cluster of control rods should ensure in order to compensate the excess of reactivity for a fresh fuelled, thermal reactor. In this case, due to the spectrum of the system, we could assume that our control rods are made of a thermal absorber, like cadmium. Since the control rods are localised in a specific position in the core, it is possible to introduce the ϑ eigenvalue as follows,

$$\left(\hat{L} + \hat{F}_0 + \hat{S}_0 - \hat{S} - \hat{F}\right)\varphi_{\theta_n} = \frac{1}{\theta_n(\vec{r}, E)}\hat{C}_T\varphi_{\theta_n}, \tag{24}$$

where the dependence of the eigenvalue with respect to the spatial and energy variable should be interpreted as

$$\theta_n(\vec{r}, E) = \begin{cases} \theta_n & \forall \vec{r} \in \mathcal{V}_{CR}, \forall E \in [E_{min}, E_{max}] \\ 1 & \text{otherwise.} \end{cases} \tag{25}$$

The symbol $\mathcal{V}_{CR}$ indicates the volume of the control rods, while $[E_{min}, E_{max}]$ indicates the thermal range for the capture cross section of cadmium.

With respect to the formulation given in eq. (22), this alternative form of ϑ allows to estimate the capture reaction rate needed to achieve criticality for a specific region, without affecting the other ones. However, from a practical point of view, this form is still unsatisfactory, as it includes also other nuclides in addition to cadmium, e.g., the structural materials composing the rods. Therefore, to achieve the maximum level of flexibility, the eigenvalue formulation should be generalised in order to act only on the nuclides of interest.

In this case, the quantitative information obtained by solving the ϑ eigenvalue problem would be a correction factor $1/\theta_{\text{eff}}$ for the capture cross section of cadmium, $\Sigma_{c,Cd}(E) = N_{Cd}\sigma_{c,Cd}(E)$. Since it is not possible to change $\sigma_{c,Cd}(E)$, which is an intrinsic property of cadmium, the correction factor should be interpreted as a scaling factor for its atomic density N_{Cd}. However, if the cadmium

concentration is re-scaled, also the other cross sections of cadmium, like the scattering one, would change. Hence, in light of this consideration, the only physically meaningful eigenvalue turns out to be the density eigenvalue, which is the only one able to provide scaling factors consistent with the physics. In order to distinguish this generalised eigenvalue from the classic one, hereafter this eigenvalue will be addressed as ζ.

Considering a system defined in a limited spatial domain $\mathcal{V}$, filled by a mixture of M nuclides, each characterised by a local atomic density $N_m(\vec{r}), m = 1, \ldots, \mathrm{M}$, the generalised eigenvalue problem ζ for a specific isotope, identified as $m^\star$ and located in a region $\mathcal{V}_{m^\star}$, would yield

$$\begin{aligned}
&\vec{\Omega}\cdot\nabla\phi(\vec{r},E,\vec{\Omega}) + \sum_{\substack{m=1\\m\neq m^\star}}^{\mathrm{M}} [N_m(\vec{r})\sigma_{t,m}(E)]\phi(\vec{r},E,\vec{\Omega}) + \frac{1}{\zeta}[N_{m^\star}(\vec{r})\sigma_{t,m^\star}(E)]\phi(\vec{r},E,\vec{\Omega}) = \\
&\sum_{\substack{m=1\\m\neq m^\star}}^{\mathrm{M}} \int dE' \oint d\vec{\Omega}' \, [N_m(\vec{r})\sigma_{s,m}(E')] f_{s,m}(\vec{r},E'\to E,\vec{\Omega}'\cdot\vec{\Omega})\phi(\vec{r},E',\vec{\Omega}') + \\
&\frac{1}{\zeta}\int dE' \oint d\vec{\Omega}' \, [N_{m^\star}(\vec{r})\sigma_{s,m^\star}(E')] f_{s,m^\star}(\vec{r},E'\to E,\vec{\Omega}'\cdot\vec{\Omega})\phi(\vec{r},E',\vec{\Omega}') + \\
&\sum_{\substack{m=1\\m\neq m^\star}}^{\mathrm{M}} \int dE' \oint d\vec{\Omega}' \, [N_m(\vec{r})\nu_m(E')\sigma_{f,m}(E')]\frac{\chi_m(E)}{4\pi}\phi(\vec{r},E',\vec{\Omega}') + \\
&\frac{1}{\zeta}\int dE' \oint d\vec{\Omega}' \, [N_{m^\star}(\vec{r})\nu_{m^\star}(E')\sigma_{f,m^\star}(E')]\frac{\chi_{m^\star}(E)}{4\pi}\phi(\vec{r},E',\vec{\Omega}'),
\end{aligned} \tag{26}$$

for $\vec{r}\in\mathcal{V}_{m*}$, while, for $\vec{r}\notin\mathcal{V}_{m*}$,

$$\begin{aligned}
&\vec{\Omega}\cdot\nabla\phi(\vec{r},E,\vec{\Omega}) + \sum_{m=1}^{\mathrm{M}} [N_m(\vec{r})\sigma_{T,m}(E)]\phi(\vec{r},E,\vec{\Omega}) = \\
&\sum_{m=1}^{\mathrm{M}} \int dE' \oint d\vec{\Omega}' \, [N_m(\vec{r})\sigma_{s,m}(E')] f_{s,m}(\vec{r},E'\to E,\vec{\Omega}'\cdot\vec{\Omega})\phi(\vec{r},E',\vec{\Omega}') + \\
&\sum_{m=1}^{\mathrm{M}} \int dE' \oint d\vec{\Omega}' \, [N_m(\vec{r})\nu_m(E')\sigma_{f,m}(E')]\frac{\chi_m(E)}{4\pi}\phi(\vec{r},E',\vec{\Omega}'),
\end{aligned} \tag{27}$$

imposing the continuity of the angular flux on any internal interface. It should be noticed that it is not required that the zone $\mathcal{V}_{m*}$ is physically connected, meaning that the same eigenvalue can be applied also to disjoint zones in the reactor at the same time.

Equations (26) and (27) constitute a general eigenvalue problem that allows to estimate the effect of a specific nuclide and its positioning within the reactor on the total neutron balance in a completely self-consistent way. In general, the eigenvalue ζ could be defined to filter a more specific

volume in phase space, as for the example of cadmium, thus including the possibility to select a specific energy window and a specific reaction channel. In this sense, each eigenvalue formulation discussed so far can be interpreted as a particular case of the ζ model:

- k is restricted to the phase space region featured by $\Sigma_f(\vec{r}, E) \neq 0$;
- γ is applied to each phase space region and nuclide featured by a particle emission;
- ϑ filters the specific capture reaction, extending to the whole phase space and to each nuclide;
- δ is defined over the whole phase space and applies to each nuclide.

Due to its generality, it is extremely difficult to provide a formal proof concerning the existence and uniqueness of an eigenfunction with uniform sign over the phase space. If ζ is cast into a k form, it would be always possible to assess the existence and uniqueness of a fundamental eigenpair. However, if ζ is cast as ϑ, the existence of a positive eigenvalue would not be guaranteed. Despite this lack of formal evidences could seem a bit disappointing, it is not an issue from a practical standpoint. In the framework of the core design, the designer is aware that, in the design process, different possibilities may arise: the lack of a fundamental solution would simply mean that it is not possible to obtain a steady state system acting on that particular isotope and region of the phase space, while, if one or more fundamental eigenpair exist, this would mean that the problem can be solved.

The following sections present a set of relevant applications of this new eigenvalue problem, showing in more detail these different possibilities.

II.A. Implementation in the TEST code

The numerical results presented and discussed in the following have been produced with an *in-house* Python package, denoted in the following as TEST (Transport Equation Solver at Turin). This code, which has been extensively benchmarked for the eigenvalue analysis in [14, 11], allows first to assemble the spatially discretised operators of the multi-group NTE, and then to construct the desired eigenvalue formulation. The eigenproblem is then solved using the SLEPc/PETSc (Scalable Library for Eigenvalue Problem Computations and Portable, Extensible Toolkit for Scientific Computation) libraries [17, 18], which implement very efficient methods for the determination of the higher-order eigenmodes [19, 20].

Exploiting the built-in classes already implemented in TEST to handle the various eigenvalue formulations presented in section I, an *ad hoc* sub-class was defined to properly handle the ζ formulation and its action on specific nuclides and/or portions of the phase space. Aiming at maximising the code flexibility, the full set of matrix operators appearing in eq. (23) are first assembled for the initially off-critical system. Then, the formulation is built acting on the different operators, according to a user-defined object that represents the volume of the phase space and the nuclides on which ζ should operate. If the nuclide of interest does not exist in the starting off-critical system, e.g., the boron to be diluted in water, its few-group cross sections are read and the set of the matrix operators are defined accordingly in order to yield eq. (26). Because of the additional implementation complexities that may arise, TEST does not currently support matrix-free, iterative solution of eq. (26), like the transport-sweep algorithm.

III. DETERMINATION OF THE MODERATION RATIO FOR A HOMOGENEOUS 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. Due to the competition between the neutron slowing down and the parasitic captures that both occur in the moderator, it is usually possible to find two critical moderation ratios N_m/N_f, where N_m and N_f are the atomic density of the moderator and of the fuel material, respectively [21]. A typical example of the behaviour of the effective multiplication constant for a thermal system moderated by light water can be found in fig. 1, which has been constructed iteratively changing N_m, for a fixed value of N_f. In case the lowest value of N_m is selected, the critical structure is said to be *under-moderated*, while, in case the largest one is employed, the system is said to be *over-moderated*. The existence of a maximum in this curve induces the designer to choose the under-moderated configuration, because of its better behaviour in presence of instabilities. There are at least two physical justifications for this choice. From a purely neutronic point of view, this configuration is more spatially coupled, so it is less sensitive to localised perturbations. Consequently, the under-moderated arrangement is featured by a larger eigenvalue separation (ES), which is a well established figure of merit to assess the spatial stability of a reactor [22, 23]. From a thermo-hydraulics point of view, an increase of the average temperature of the system would cause a larger variation in the density of the moderator, meaning that the

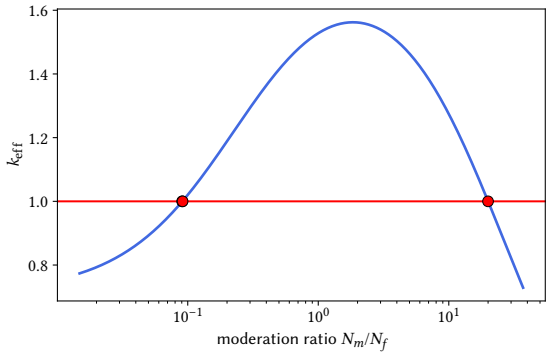


Fig. 1. *Effective multiplication factor as a function of the moderation ratio for a two-group, P_1 homogeneous system 140 cm thick and filled with a mixture of uranium oxide enriched at 3% and light water.*

moderation ratio of the system would decrease and that, consequently, the multiplication factor of the system would increase, destabilising the system.

TABLE II
Critical moderation ratios N_m/N_f for a slab thick 170 cm filled with a mixture of fissile material and light water.

ζ formulation		iterative approach	
N_m/N_f	k_{eff}	N_m/N_f	k_{eff}
0.09096	1.00000	[0.09060, 0.09132]	[0.99918, 1.00082]
20.01752	1.00000	[19.98347, 20.14059]	[1.00074, 0.99734]

Figure 1 shows the k_{eff} behaviour for a slab, thick 140 cm and filled with a homogeneous mixture of fissile material and light water, as a function of the moderation ratio. Following the common practice, the critical moderation ratios, i.e. the red dots in the figure, are determined increasing iteratively the moderator density, using 1000 uniformly-spaced values. Therefore, each dot in the figure corresponds to the solution of a k-eigenvalue problem cast in the two-group P_1 model.

Both solutions can be obtained "exactly", without iterations, introducing the ζ eigenvalue in front of the moderator density. Table II provides the density correction factors needed to attain criticality computed with the two methods. For the iterative approach, the range including the critical values is reported. The presence of two critical configurations is reflected by the existence of two fundamental eigenfunctions, both featured by a uniform sign across the domain. These modes are showed in fig. 2 with the first and second order harmonics. By inspection, it is easy

to notice that the solution associated to the larger value of ζ, i.e. the one requiring the largest moderator density reduction, is associated with a harder spectrum, featured by a global spectral index roughly equal to 0.6, with respect to the second arrangement, featured by a global spectral index about 71. Figure 3 represents the full ζ eigenvalue spectrum. Thanks to the detail on the right of the figure, it is possible to appreciate the existence of two batches of eigenvalues around the star symbols, which represent the fundamental eigenvalues. The largest value represents the under-moderated configuration, while the other star represents the over-moderated one. These figures are very informative. First, it is extremely interesting to notice that the eigenvalue separation ES in the first batch is much larger than the second one, where the eigenvalue are very close to each other. Moreover, it is possible to notice that the over-moderated fundamental is the lowest values in its batches, meaning that the corresponding ES is negative.

This fact, which can be appreciated also looking at the eigenvalues reported in the legend of fig. 2, is consistent with the known relationship between ES and the core spatial decoupling degree, and would have an important implication: the designer could look only for the dominant eigenpair, avoiding the determination of the full spectrum. However, this peculiarity depends on the system initial configuration. When the starting off-critical configuration is featured by a larger moderation ratio, closer to the critical over-moderated configuration, the situation is reversed, i.e. the largest ζ corresponds to the over-moderated solution. Since the ζ spectrum behaviour is case-dependent, computing only the dominant eigenvalue could be risky. This observation seems to suggest that, in order to find all the physically meaningful solutions and to choose the best one, the complete spectrum should be estimated. In case this would not be affordable, a smart computational strategy for the reduction of the computational burden could be to use a low-order transport model (e.g. with fewer energy groups and less angular detail) to look for the approximated fundamental eigenvalues, which then could be used in the well known shift-and-invert procedure to enhance the eigenvalue solver convergence towards more precise estimates of the eigenvalues [24]. Alternatively, if some basic knowledge of the various possible critical arrangements was available, the calculation could be made more efficient starting from a configuration close to the desired one.

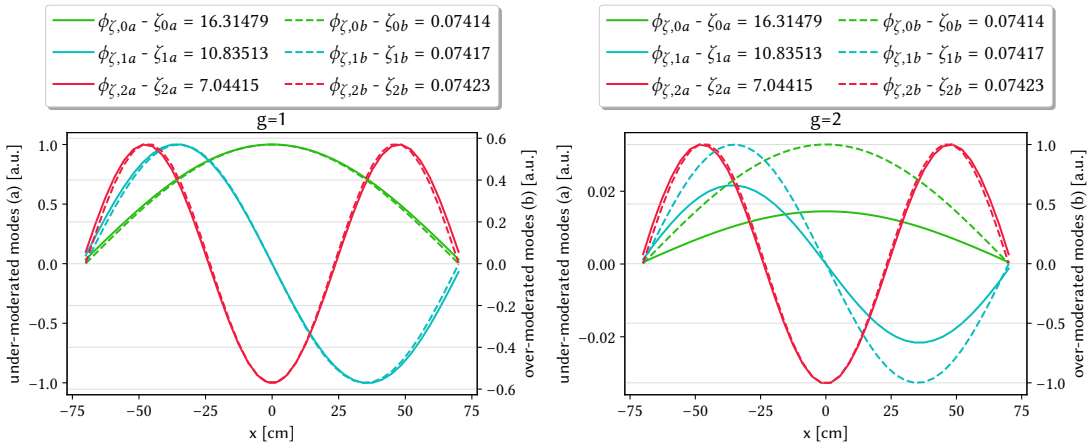
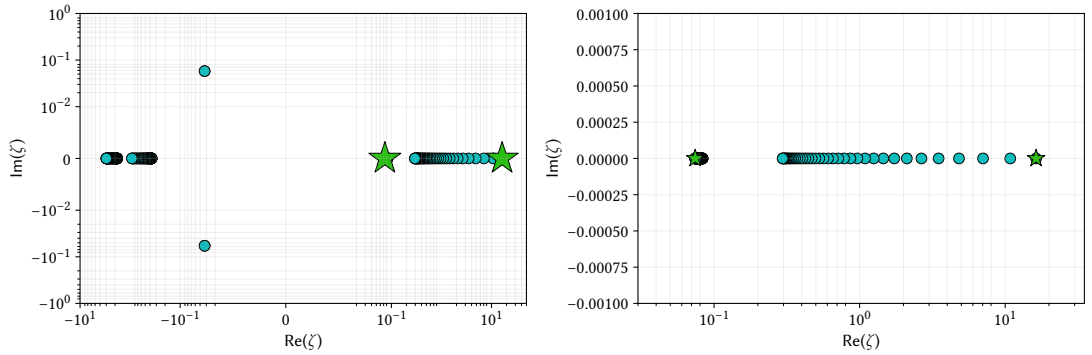


Fig. 2. *Higher-order, two-group total flux ζ modes for a homogeneous mixture of light water and fissile material. The spectral index ϕ_1/ϕ_2 of the systems is equal to 70.3 and 0.6 for the under- and over-moderated cases, respectively.*



(a) (b)

Fig. 3. *ζ eigenvalue full spectrum (a) and zoom on the real part of the spectrum (b) for a homogeneous mixture of light water and fissile material. The stars are the eigenvalues associated to positive modes.*

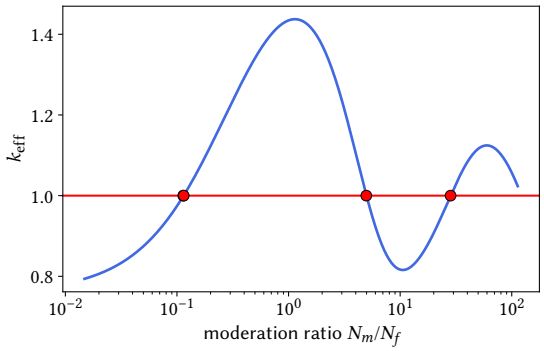


Fig. 4. *Effective multiplication factor as a function of the moderation ratio for a two-group heterogeneous system composed of alternating layers of fuel and moderator.*

IV. DETERMINATION OF THE MODERATION RATIO FOR A REGULAR LATTICE

Due to its great flexibility, ζ can be used to deal with more complex problems, for example the determination of the moderation ratio for a heterogeneous arrangement of fuel and moderator layers, surrounded by a reflector. In this case, the iterative search of the critical moderation ratio is more expensive, due to the larger number of spatial nodes needed to resolve the spatial gradients. Of course, the design is usually carried out using effective, non-linear root-finding algorithms, like the Newton-Raphson method [25], to minimise the number of static calculations required. However, the presence of more solutions, like in this case, can have a detrimental effect on such techniques, limiting their effectiveness. This aspect is even more important when the design calculation includes other parameters, like the thermo-hydraulics quantities [26]. As visible from fig. 4, which has been again obtained iterating the calculations, three critical configurations could be devised for a lattice composed by 17 sheets, 3 cm thick and composed of uranium oxide enriched at 3%, and 16 layers of water 3 cm thick, surrounded at both sides by 20 cm of water used as a reflector. It is important to remark here that, despite the curve seems to approach a fourth zero around $N_m/N_f = 10^2$, it was not possible to found a solution to the static, k problem around these values of N_m, due to the ill conditioning of the moderator cross sections, which assume very large, unphysical values.

In this case it is possible to determine three possible critical eigenstate, casting the ζ eigen-

value problem as follows,

$$\begin{cases} \mu\dfrac{\partial\phi(x,E,\vec{\Omega})}{\partial x}+\dfrac{1}{\zeta}N_m\sigma_{t,m}(E)\phi(x,E,\mu)= \\ \dfrac{1}{\zeta}\displaystyle\int_0^\infty dE'\int_{-1}^1 d\mu' N_m\sigma_{s,m}(E')f_{s,m}(E'\to E,\mu')\phi(x,E',\mu') \qquad x\in\mathcal{X}_m, \\ \\ \mu\dfrac{\partial\phi(x,E,\mu)}{\partial x}+\Sigma_t(x,E)\phi(x,E,\mu)= \\ \displaystyle\int_0^\infty dE'\int_{-1}^1 d\mu'\Sigma_s(x,E')f_s(x,E'\to E,\mu')\phi(x,E',\mu')+ \qquad x\notin\mathcal{X}_m, \\ \displaystyle\int_0^\infty dE'\int_{-1}^1 d\mu'\nu_m(x,E')\Sigma_{f,m}(x,E')\frac{\chi(x,E)}{2}\phi(x,E',\mu') \end{cases} \tag{28}$$

where $\mathcal{X}_m$ is defined as $\{[x_1,x_2],\cup[\ldots]\cup[x_i,x_{i+1}]\}$. In the first equation, the eigenvalue acts only on the nuclide density N_m featuring the homogeneous water sheets, while in the second one the cross sections are expressed as space-dependent functions since they refer to the reflector and to the fuel regions.

Equation (28) makes possible, also in this case, to determine the three scaling factors $1/\zeta$ for the moderator density identified by the iterative procedure used to draw the curve in fig. 4. In order to distinguish the eigenvalues belonging to the fundamental set, i.e. the eigenvalues associated to eigenfunctions with uniform sign over the phase space, they will be indicated in the following as $\zeta_{0}*$, where $*$ is replaced by a letter. In this specific case, the largest eigenvalue in the fundamental set will be indicated as ζ_{0a}, while the smallest fundamental eigenvalue will be indicated as ζ_{0c}.

The thermal and fast fluxes associated to these configurations are represented on top of the lattice geometry in fig. 5. These eigenfunctions correspond to the critical neutron distribution in the phase space, provided that the moderator density was modified by a factor $1/\zeta_{0^*}$. The black curve, associated to the largest fundamental eigenvalue, i.e. to the under-moderated solution, presents smaller spatial gradients in the core, consistently with the larger degree of spatial coupling, while the red curve, associated to the over-moderated solution ζ_{0b}, shows significant oscillations in both the fast and the thermal fluxes. These local oscillations in the fluxes are due to the stronger interplay between slowing down and fission for larger moderator densities: the moderation is a sink for the fast population and a source for the thermal one, while the fission produces fast neutrons and removes thermal ones. This mechanism is exacerbated when the moderator density

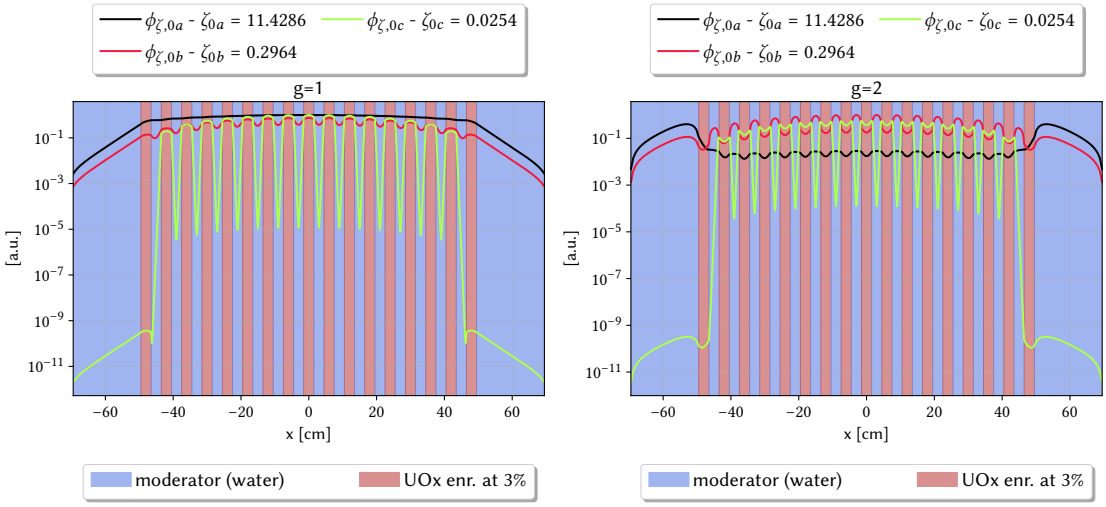


Fig. 5. *Fundamental two-group ζ modes for the heterogeneous arrangement of light water and fissile material.*

is further increased adopting the scaling factor $1/\zeta_{0c}$. Similar considerations hold also for the spatial behaviour of the first harmonic, represented in fig. 6. In this case, only the a and the b modes are showed in order to make the figure readable.

As for the homogeneous case, the eigenvalue spectrum for ζ, in fig. 7, presents batches of eigenvalues near the fundamental ones. The first batch is well separated, while the other two batches, related to the over-moderated configurations, are less and less separated, as visible in the right part of the figure (b).

The fact that the largest fundamental eigenvalue, ζ_{0a}, is featured by the largest dominance ratio ζ_{0a}/ζ_{1a} is a very nice feature of the ζ formulation. From a numerical point of view, the convergence speed of the numerical algorithms for the solution of the eigenvalue problems is always somehow proportional to the dominance ratio, especially for the legacy power method. Thus, if the system is closer to the desired configuration, the convergence should be enhanced, avoiding the risk of finding one of the other possible critical arrangements.

As pointed out in this paper, one of the advantages of ζ is that the consistency of the cross sections of the system is guaranteed by acting only on the atomic density of one or more nuclides. Notwithstanding this inherent advantage, it is not always possible to practically act on the atomic density. According to the medium considered, the atomic density could be interpreted macroscopically as a chemical concentration or as a physical density. In the first case, the range

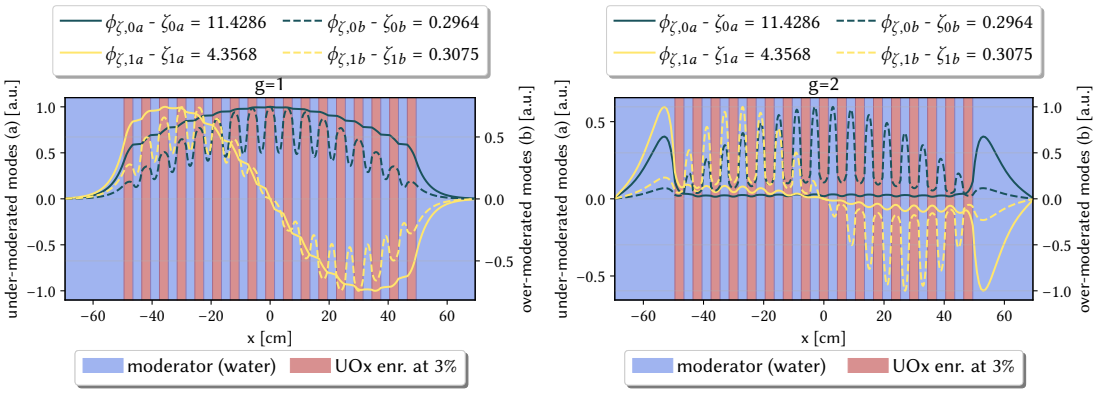


Fig. 6. *Fundamental two-group ζ modes for the heterogeneous arrangement of light water and fissile material.*

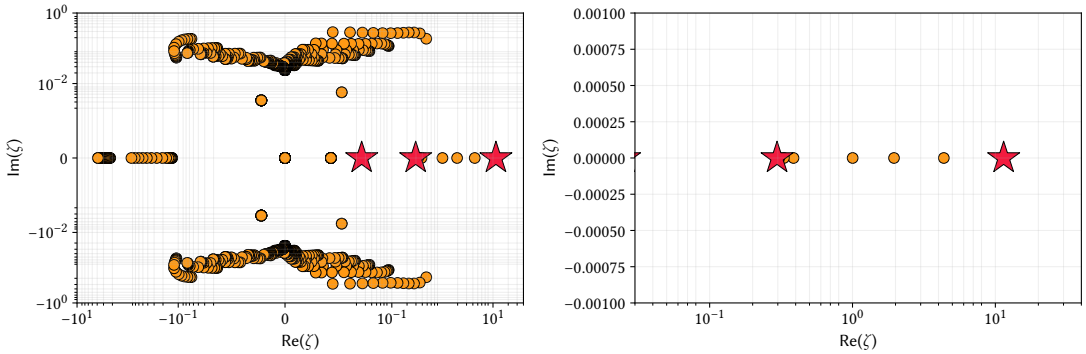


Fig. 7. *ζ eigenvalue spectrum for the heterogeneous arrangement of light water and fissile material. The stars are the eigenvalues associated to positive modes.*

of variation for the isotope atomic density is determined by the solubility of the solute into the solvent. This situation is often encountered in nuclear engineering, for example when the boric acid H_3BO_3 is dissolved in water to control the reactivity in PWRs or when some fissile nuclides like ^{233}U or ^{239}Pu are added to a molten salt reactor. In these cases, the solubility range is usually wide enough to allow a fine regulation of the atomic concentration that is useful in most situations [27]. Hence, the scaling factor $1/\zeta$ could be effectively achieved.

On the contrary, when the atomic density corresponds to the physical density, as in the case of the moderator choice, the designer is not free to change N, which is a physical property of the medium that depends on its thermodynamic conditions. From this perspective, ζ seems to provide a quantitative information that is not practically achievable, as for the other eigenvalue formulations. However, under some rather mild assumptions, it is possible to prove that $1/\zeta$ can be interpreted as a scaling factor for the geometrical volumes containing the isotope under investigation, in analogy to what occurs with the δ formulation, for which ζ is a generalisation.

In [10] it is proved that scaling the system geometry by a factor β, $\vec{\mathcal{R}} = \beta\vec{r}$, scales the density eigenvalue δ by the same factor. Due to their similarities, the same feature can be proved for (28) as well in the specific case of a one-dimensional cartesian system, provided that the scaling is applied only to the geometrical volume where ζ is actually operating. In particular, by choosing $\beta = 1/\zeta_{\text{eff}}$, i.e. $\mathtt{x} = 1/\zeta_{\text{eff}}x$ and $\mathcal{Z}_m = 1/\zeta_{\text{eff}}\mathcal{X}_m$, it is possible to obtain a critical system,

$$\begin{cases} \mu\dfrac{\partial\phi(\mathtt{x},E,\mu)}{\zeta_{\text{eff}}\partial\mathtt{x}} + \dfrac{1}{\zeta_{\text{eff}}}N_m\sigma_{t,m}(E)\phi(\mathtt{x},E,\mu) = \\ \dfrac{1}{\zeta_{\text{eff}}}\displaystyle\int_0^\infty dE'\int_{-1}^1 d\mu' N_m\sigma_{s,m}(E')f_{s,m}(E'\to E,\mu')\phi(\mathtt{x},E',\mu') \qquad \mathtt{x}\in\mathcal{Z}_m, \\ \\ \mu\dfrac{\partial\phi(x,E,\mu)}{\partial x} + \Sigma_t(x,E)\phi(x,E,\mu) = \\ \displaystyle\int_0^\infty dE'\int_{-1}^1 d\mu'\Sigma_s(x,E')f_s(x,E'\to E,\mu')\phi(x,E',\mu') + \qquad x\notin\mathcal{Z}_m. \\ \displaystyle\int_0^\infty dE'\int_{-1}^1 d\mu'\nu_m(x,E')\Sigma_{f,m}(x,E')\frac{\chi(x,E)}{2}\phi(x,E',\mu') \end{cases} \tag{29}$$

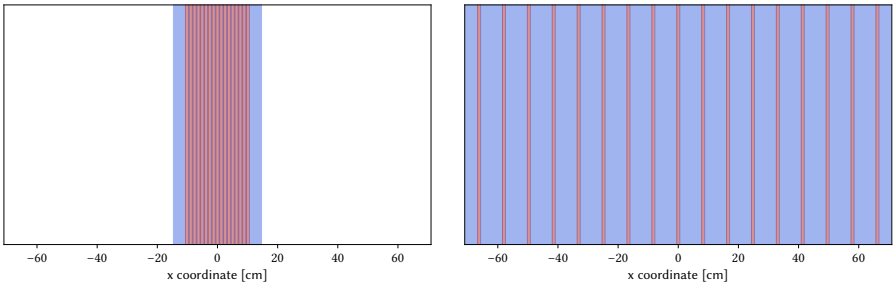
as the $1/\zeta_{\text{eff}}$ terms cancel out. As for the δ eigenvalue, the physical consistency of this local volume scaling can be justified intuitively referring to the fact that the microscopic cross sections are not altered by this procedure, which only affects the streaming term.

This relationship cannot be extended in a straightforward manner also to more complex 2D and 3D systems, due to the fact that scaling a certain region would imply a modification also to the surface-to-volume ratio of the surrounding regions. Due to these intricacies, it is likely that this property holds only for some very specific cases, for example when ζ is formulated in a δ fashion, i.e. it acts on all the regions of the system. Hence, further analyses are left for a future development of this work.

In addition to these assumptions, ζ should act on all the isotopes contained in the phase space volume $\mathcal{V}_{m*}$. It is easy to prove that, in case ζ is introduced in front of a specific isotope m^* inside the selected phase space volume $\mathcal{V}_{m^*}$, scaling the geometrical volume would not be equivalent changing the density of that specific nuclide, since the factor $1/\zeta_{\text{eff}}$ would operate on the volume containing also the other nuclides $m \neq m^*$. Therefore, ζ_{eff} can be interpreted either as a density scaling factor with constant geometry (always) or as a geometrical volume scaling factor for constant density and cross sections (under some assumptions). Despite the volume is scaled only in some non-simply connected zones of the system, the consistency of the system of equations is ensured by enforcing the continuity of the angular flux at the interfaces.

In the following, an example involving the estimation of the geometrical scaling is provided for a sub-critical (k_{eff}=0.92070) lattice composed by 17 fuel sheets, each 1 cm thick and made of 3% enriched uranium oxide, and 16 water layers, each 0.2 cm thick, surrounded by a 4 cm thick water reflector on both sides. Solving the ζ eigenvalue problem for the moderator provides two correction factors, namely $1/\zeta_{0a} = 1.54392$ and $1/\zeta_{0b} = 37.76805$. Figure 8 provides a graphical sketch of the critical configurations obtained adjusting the moderator volume inside the lattice according to the two values of ζ, while fig. 9 shows the off-critical system and the under-moderated configuration on the same scale. As expected, the under-moderated design, obtained with a slight increase of the moderator thickness between each couple of fuel sheets, is more compact than the other one, proving once again its better spatial stability. The spatial distribution of the thermal and fast critical fluxes for the two cases, visible in fig. 10, further confirms this observation: the under-moderated case, on the left, is featured by a rather smooth profile, similar to what occurs in a homogeneous system, while the over-moderated case presents local spikes in both groups.

As mentioned previously, the decoupling degree of a system can be inferred in a more rigorous way from the eigenvalue separation (ES) or from the dominance ratio (DR) of the system under



(a) (b)

Fig. 8. *Under-moderated critical lattice (a) and over-moderated critical lattice (b) designed using the ζ eigenvalue.*

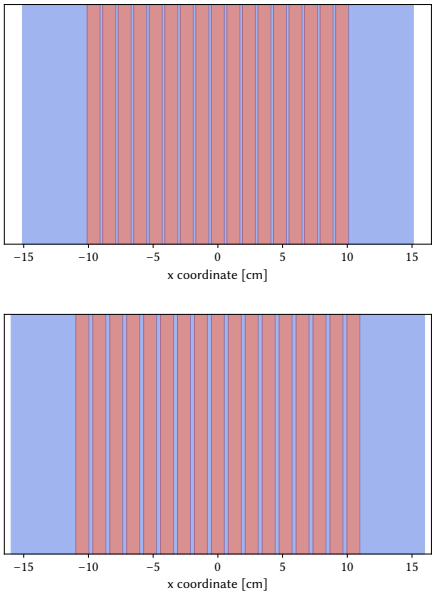
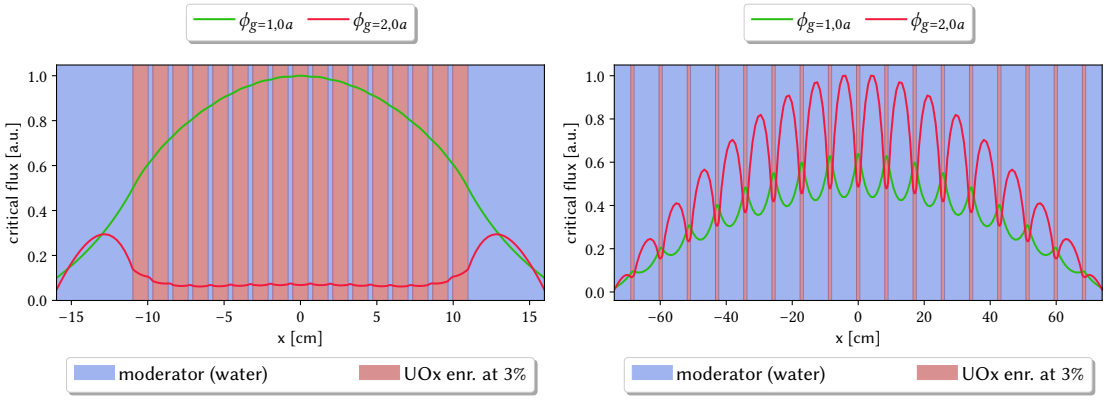


Fig. 9. *Initial off-critical lattice (top) and under-moderated critical lattice.*



(a) (b)

Fig. 10. *Fast and thermal fluxes for the under- (a) and over-moderated (b) design solutions.*

design. An intuitive relationship between of the ES and the system stability can be found in the framework of the Generalised Perturbation Theory, which was mainly developed during the '80s in [28, 29].

The ES may not be a very informative figure of merit *per se*, but it becomes a powerful indicator when it is computed for different system configurations. In this respect, the ES is a valuable criterion to guide the neutronic design of a reactor [30]. In this specific case, it is interesting to compare the values of the ES computed with different eigenvalue formulations for the possible design solutions determined by the ζ problem. To this aim, these figures of merit and the related dominance ratios, defined as the ratio between the eigenvalue featuring the first-order harmonics and the fundamental eigenvalue, are reported in table III.

TABLE III
Critical moderation ratios N_m/N_f for a slab thick 170 cm filled with a mixture of fissile material and light water.

	$\zeta_{0a} = 0.74697$		$\zeta_{0b} = 0.02748$	
eig.	ES	DR	ES	DR
ω	$-2.09226 \times 10^{7}\,\mathrm{s}^{-1}$	-3.24026×10^{-12}	$-2.78505 \times 10^{6}\,\mathrm{s}^{-1}$	-8.80089×10^{-10}
γ	1.43712×10^{-2}	1.01437	3.77510×10^{-4}	1.00038
δ	1.41445	2.41445	-2.32373×10^{-1}	7.67627×10^{-1}
k	8.59768×10^{-1}	1.85977	3.83623×10^{-2}	1.03836
ϑ	-9.60989	-8.60989	-6.01560×10^{-2}	9.39844×10^{-1}

As it could be expected, the critical solution featured by the largest value of ζ presents the largest eigenvalue separation for the different eigenvalue formulations, despite some significant

variations. The prompt time eigenvalue yields the largest eigenvalue separation, while the collision eigenvalue γ yields the smallest one. The other formulations falls between these two. The capture eigenvalue ϑ yields a negative ES, since the fundamental eigenvalue is smaller than the one associated to the first harmonic. It is interesting to notice that δ presents two fundamental harmonics in addition to the critical one, as a consequence of the competition between scattering and absorption triggered by the density modification. This aspect makes ambiguous to evaluate the ES, thus, in this case, the distance between the fundamental critical eigenvalue ($\delta = 1$) and the first harmonic is evaluated.

When the design solution is over-moderated, all the eigenvalues exhibit a reduction of their distance from the first harmonic, meaning that the system is more spatially decoupled, i.e. it is more sensitive to the localised perturbation than to the neutron leakages. The eigenvalue formulations featuring the largest variation from one case to the other are the capture eigenvalue, the collision eigenvalue and the density eigenvalue, suggesting that it is worth investigating their capability of delivering information about the system stability in alternative to the ES computed referring to k.

V. DETERMINATION OF THE BORON CONCENTRATION FOR REACTIVITY CONTROL

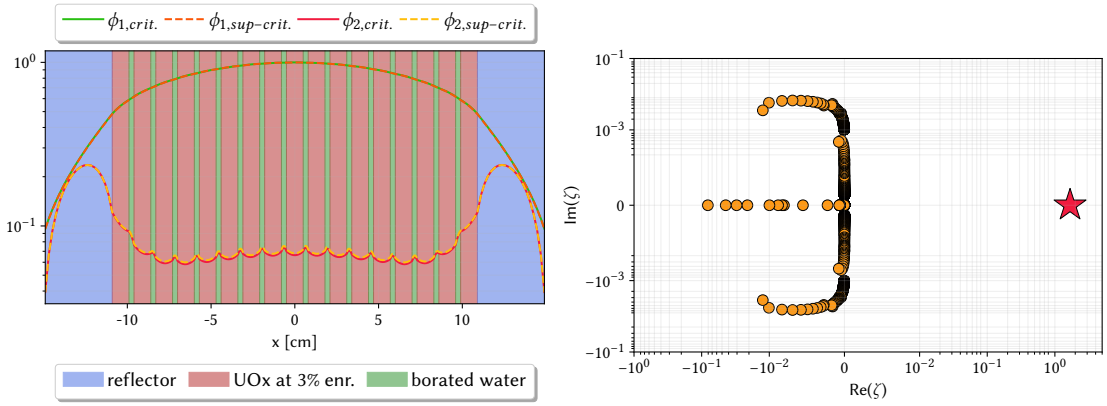
Another fundamental problem in the operation of PWRs is the search for the critical boron concentration to be diluted in the water to control the reactivity during normal conditions. Even in this case, the common approach to determine this parameter is resorting to iterations. Exploiting the generalised density eigenvalue, it is possible to avoid iterations, by looking for the fundamental ζ eigenvalue. Assuming that the moderator surrounding the fuel sheets can be modelled as a homogeneous material, the ζ eigenvalue problem can be cast as follows,

$$
\begin{cases}
\mu\dfrac{\partial\phi(x,E,\mu)}{\partial x}+\dfrac{1}{\zeta}N_a\sigma_{t,a}(E)\phi(x,E,\mu)+N_m\sigma_{t,m}(E)\phi(x,E,\mu)= \\
\displaystyle\int_0^\infty dE'\int_{-1}^1 d\mu' N_m\sigma_{s,m}(E')f_{s,m}(E'\to E,\mu')\phi(x,E',\mu')+ \\
\dfrac{1}{\zeta}\displaystyle\int_0^\infty dE'\int_{-1}^1 d\mu' N_a\sigma_{s,a}(E')f_{s,a}(E'\to E,\mu')\phi(x,E',\mu') \qquad x\in\mathcal{X}_a, \\
\\
\mu\dfrac{\partial\phi(x,E,\mu)}{\partial x}+\Sigma_t(x,E)\phi(x,E,\mu)= \\
\displaystyle\int_0^\infty dE'\int_{-1}^1 d\mu'\Sigma_s(x,E')f_s(x,E'\to E,\mu')\phi(x,E',\mu')+ \qquad x\notin\mathcal{X}_a, \\
\displaystyle\int_0^\infty dE'\int_{-1}^1 d\mu'\nu_m(x,E')\Sigma_{f,m}(x,E')\frac{\chi(x,E)}{2}\phi(x,E',\mu')
\end{cases}
\tag{30}
$$

where N_a indicates the absorber atomic density, N_m indicates the moderator absorber atomic density and $\mathcal{X}_m$ is defined as $\{[x_1,x_2],\cup[\ldots]\cup[x_i,x_{i+1}]\}$. This equation is then cast in a two-group, P_1 model assuming linearly anisotropic scattering, using the group constants computed with Serpent 2 [31].

Figure 11 (left) shows the two-group, off-critical flux ($k_{\text{eff}} = 1.02420$), computed with the k eigenvalue problem, for a super-critical system with no boron in water and the two-group eigenfunction that corresponds to the critical flux in case some boron with density multiplied by $1/\zeta$ is added to the water inside the coolant layers. The geometrical representation refers to the critical case. As expected on a physical ground, the addition of a thermal absorber to the coolant has an impact on the energy spectrum of the system, which shows a slight spectrum hardening.

Figure 11 (a) presents the full ζ spectrum. Since the phase space where the eigenvalue is defined comprises only a neutron poison, there is only one possible critical configuration, associated to the fundamental eigenvalue, while most of the spectrum degenerates around zero. This behaviour can be justified on a physical ground. When the moderator density is changed, it is possible to identify more critical solutions, due to the competition between absorption and scattering of the moderator. On the contrary, the absorber influences the reactivity of the system monotonically, thus only one configuration can be devised.



(a) (b)

Fig. 11. *Two-group fundamental off-critical (k) and critical (ζ) modes for a heterogeneous arrangement of fuel and borated water sheets, surrounded by a light water reflector (a) and eigenvalue spectrum (b).*

VI. FISSILE CONCENTRATION FOR REACTIVITY CONTROL IN THE MOLTEN SALT FAST REACTOR

Similarly to the case concerning the determination of the critical boron concentration, the ζ spectrum appears to have a unique solution when the objective of the analysis is the determination of the critical concentration for a fissile material. Solving this problem efficiently is very important in several situations. For example, one could be interested in estimating which is the minimum fissile enrichment needed to sustain criticality for a given fuel composition, e.g., mixed oxides (MOX) of uranium and plutonium coming from reprocessed spent fuel. Alternatively, the same problem would be relevant for the evaluation of the fissile inventory needed to operate a fluid core system, like the Molten Salt Fast Reactor (MSFR) design, conceived through the European Union funded projects EVOL, SAMOFAR and SAMOSAFER. One of the advantages of using a fluid core would be the possibility to continuously adjust criticality acting on its composition, through the injection of fresh fuel and the extraction and reprocessing of the fuel containing the fission products. From this perspective, the ζ formulation could be extremely valuable, as it could be employed to estimate the fissile concentration needed in different operating configurations of the system.

Having this application in mind, in the following the generalised eigenvalue formulation will be applied to determine the critical concentration of ^{233}U to be diluted in the core of the MSFR

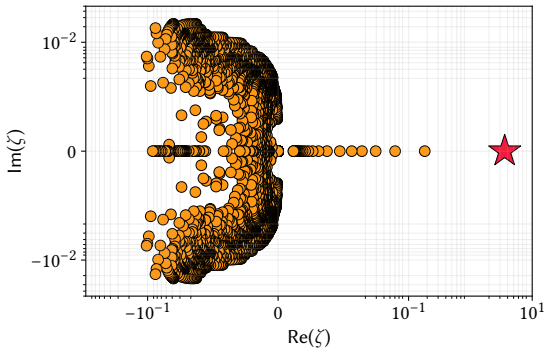


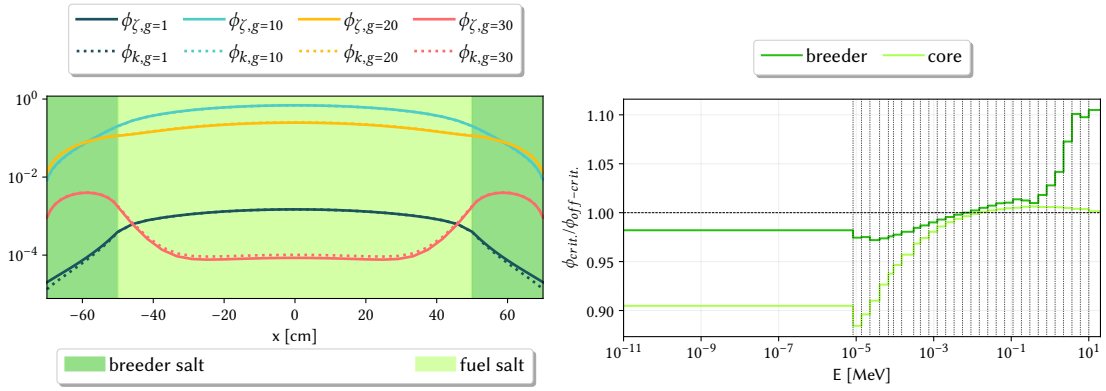
Fig. 12. *Eigenvalue spectrum computed for the MSFR case.*

[32], starting from an initial sub-critical configuration ($k_{\text{eff}} = 0.98072$),

$$
\begin{cases}
\mu\dfrac{\partial\phi(x,E,\mu)}{\partial x} + \dfrac{1}{\zeta}N_f\sigma_{t,f}(E)\phi(x,E,\mu) + N_s\sigma_{t,s}(E)\phi(x,E,\mu) = \\
\displaystyle\int_0^\infty dE' \int_{-1}^{1} d\mu' N_s\sigma_{s,s}(E') f_{s,m}(E'\to E,\mu')\phi(x,E',\mu') + \\
\dfrac{1}{\zeta}\displaystyle\int_0^\infty dE' \int_{-1}^{1} d\mu' N_f\sigma_{s,f}(E') f_{s,f}(E'\to E,\mu')\phi(x,E',\mu') + \\
\displaystyle\int_0^\infty dE' \int_{-1}^{1} d\mu' \nu_s(x,E')\Sigma_{f,s}(x,E')\frac{\chi(x,E)}{2}\phi(x,E',\mu') + \\
\displaystyle\int_0^\infty dE' \frac{1}{\zeta}\int_{-1}^{1} d\mu' \nu_f(x,E')\Sigma_{f,f}(x,E')\frac{\chi(x,E)}{2}\phi(x,E',\mu') \qquad x \in \mathcal{X}_f, \\
\\
\mu\dfrac{\partial\phi(x,E,\mu)}{\partial x} + \Sigma_t(x,E)\phi(x,E,\mu) = \\
\displaystyle\int_0^\infty dE' \int_{-1}^{1} d\mu' \Sigma_s(x,E') f_s(x,E'\to E,\mu')\phi(x,E',\mu') + \qquad x \notin \mathcal{X}_f, \\
\displaystyle\int_0^\infty dE' \int_{-1}^{1} d\mu' \nu_n(x,E')\Sigma_{f,n}(x,E')\frac{\chi(x,E)}{2}\phi(x,E',\mu')
\end{cases}
\tag{31}
$$

where N_f indicates the fissile atomic density, N_s indicates the atomic density of the FLiTh salt, N_n indicates the nuclides constituting the liquid breeding blanket and $\mathcal{X}_f$ is defined as $[-H, H]$, where H is the half-thickness of the core region. This equation is then cast in a 30-group structure matching the ECCO-33 grid except for the last three thermal groups, which are collapsed to avoid statistical issues in the effective group constant generation performed in Serpent 2.

The eigenvalue spectrum for this case, shown in fig. 12, supports the hypotheses made for the boron case: in the absence of competing phenomena, only one configuration can yield a critical system, like in the presence of a fissile isotope, which is directly proportional to the reactivity.



(a) (b)

Fig. 13. *Critical (ζ) modes obtained diluting N_f/ζ moles of ^{233}U in the molten salt fast reactor (a) and the off-to-critical ratio for the energy spectrum (b).*

In contrast with the boron case, here it is possible to observe more than one real and positive eigenvalue, associated to higher-order spatial harmonics.

Figure 13 provides, on the right (b), the spatial behaviour of the group-wise, critical fluxes, while, on the left (a), the ratio between the critical energy spectrum, obtained adjusting the ^{233}U concentration by $1/\zeta_{\text{eff}}$, and the off-critical one is shown for both the regions composing the core. This last graph helps to appreciate the fact that, for a given set of multi-group constants, the ζ formulation takes automatically into account the spectral effects induced by the change in the system composition or volume. In this case, the intermediate group structure allows to get a deeper insight the spectral variations occurring after the fissile concentration adjustment. The addition of 10.79 mg cm^{-3} of ^{233}U to the FLiTh salt has a relatively small impact on the overall energy spectrum. By inspection of this graph, it is possible to appreciate a reduction in the low-energy spectrum, consistently with the fact that the fission cross section of ^{233}U is maximum in the thermal region, and, conversely, a slight increase in the fast spectrum, caused by the additional fast neutrons emitted by fissions. The other large spectral variation involves the blanket: since it is composed only by FLiTh, which can produce fissions only at high energy (see fig. 14), the flux spectrum increases as a consequence of the larger fraction of fast neutrons diffusing from the core to the blanket.

The graphs in fig. 13 leads to the conclusion that the ζ formulation allows to naturally take into account the spectral and spatial effects occurring as a consequence of the density (or

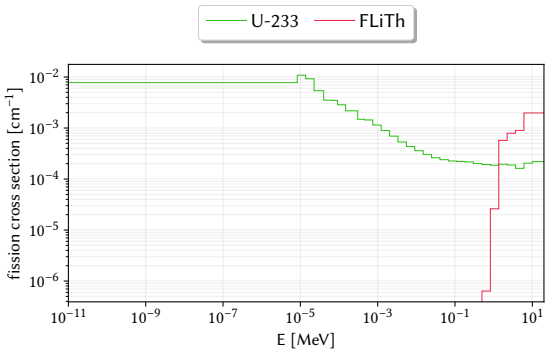


Fig. 14. *Fission cross section collapsed on the 30-group grid based on the ECCO-33 structure.*

volume) adjustments. Henceforth, in addition to the modelling and numerical errors, the only physical approximations induced by the adoption of the ζ approach are due to the fact that the self-shielding of the input multi-group cross sections are computed *a priori*, without taking into account the additional self-shielding effects induced by the $1/\zeta$ correction in the density or in the volume of the selected region. The most natural way to tackle this issue would be to perform a ζ calculation for a configuration close to the studied one during the multi-group cross section calculation stage, similarly to what is usually done for standard k calculations. In this way, most of the spatial and the energy self-shielding effects on the flux would be automatically accounted for, thus ensuring that the small spectral adjustments induced by the solution of the ζ problem for the coveted configuration do not affect significantly the accuracy of the self-shielded cross sections. Since both the cases involving the search for the critical boron concentration and the search for the critical fissile concentration are loosely off-critical, they do not induce sharp variations in the flux spectrum, suggesting that this approach should be adequate. Nonetheless, since this is the first application of the ζ eigenvalue problem and since TEST does not currently support too fine group calculations, this aspect will not be addressed in more detail in the following.

VII. DETERMINATION OF THE COOLANT VOLUME IN A LEAD FAST REACTOR

Similarly to the discussion in section IV, this section presents the solution of the ζ eigenvalue problem for the case of a lattice composed by fuel sheets made of MOX of minor actinides (MAs) and cooled by liquid lead. As for the MSFR, also this system is featured by a fast spectrum. Due

TABLE IV
Six-group energy grid adopted to perform the macroscopic cross sections energy collapsing [33].

Energy [MeV]	$2.000 \cdot 10^{1}$	$1.353 \cdot 10^{0}$	$1.832 \cdot 10^{-1}$	$6.738 \cdot 10^{-2}$	$9.119 \cdot 10^{-3}$	$2 \cdot 10^{-5}$	10^{-11}

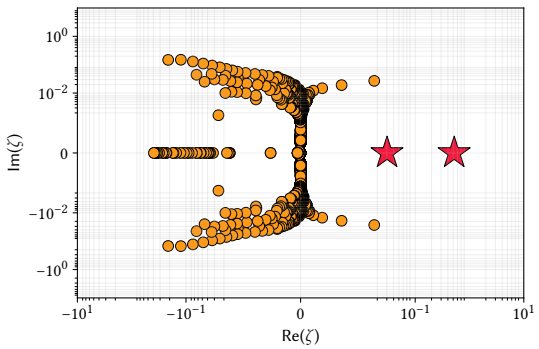
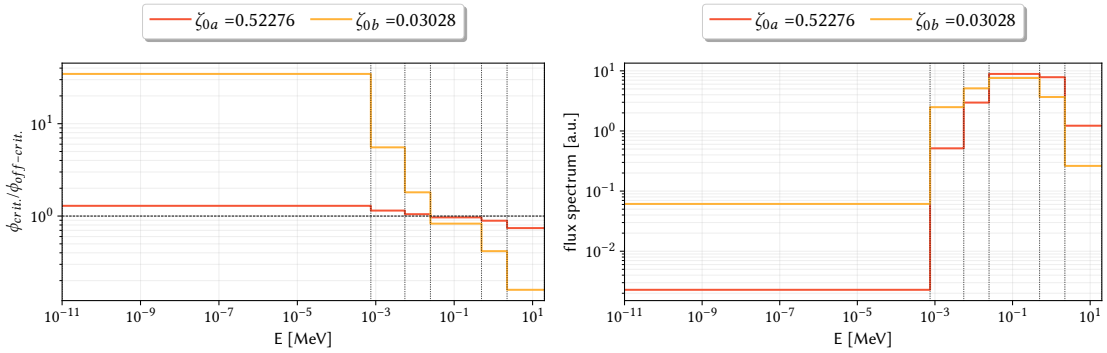


Fig. 15. *Eigenvalue spectrum for the MOX-lead lattice.*

to the absence of a moderator, the MOX fuel is usually highly enriched in the fissile component ($\approx 20\%$), thus allowing to achieve higher power densities and more compact core arrangements with respect to light water reactors. ^{208}Pb, which constitutes roughly half of the natural lead, has an average capture cross section that is very small and, thus, adequate for the neutron economy of the system. Moreover, due to its relatively heavy nucleus, neutrons are not significantly slowed down by scattering interactions, thus making lead one of the best coolant options for MOX-fuelled, fast-spectrum reactors. The fact that there is not a dominant phenomenon between capture and slowing down allows the existence of more than one possible critical configurations.

Given a sub-critical ($k_{\text{eff}} = 0.96298$) lattice constituted by 14 MOX sheets, each 1.5 cm thick, surrounded by sheets of lead, each 1 cm thick, the ζ approach allows to identify two different configurations. This system has been analysed employing a P_1 model, collapsing the cross sections on the six-group structure used in [33, 34], reported in table IV and casting the eigenproblem as in eq. (28), *mutatis mutandis*. Similarly to what occurs for a light water lattice, one solution is featured by a slight adjustment in the coolant volume, while the other is featured by a substantially larger volume fraction. The dominant mode, associated to the largest ζ, allows to realise a critical arrangement with ES= 1.01922, while the other solution yields a more decoupled critical structure, characterised by ES= 0.12770. Interestingly, fig. 15 shows *ictu oculi* that there are no other positive, real eigenvalues except the fundamental ones, implying that there are no real higher-order flux harmonics.



(a) (b)

Fig. 16. *Ratio between the critical and the sub-critical energy spectra for the two possible critical configurations (a) and the critical energy spectra (b) for a lattice of MOX and liquid lead.*

Figure 16 provides the six-group spectrum of the two critical configurations (a) and the ratio between each of the two critical spectra and the starting, sub-critical one (b). The first configuration slightly perturbs the spectrum, because of the smaller increase in volume of lead ($V'_{\mathrm{Pb}} = 1/\zeta_{0a}V = 1.913V$), while the other ($V'_{\mathrm{Pb}} = 1/\zeta_{0b}V = 33.02V$) shows a strongly softer spectrum, increasing the thermal population roughly by a factor 30. Of course, the preferable solution among the two is the first one since, in addition to its better neutronic stability, it allows to minimise the volume of lead, reducing both the weight of the reactor and its size. Nevertheless, being aware that criticality could be reached also for a larger coolant-to-fuel volume ratio is certainly very important for the safety assessment of the reactor.

The flux spatial distribution in the lattice is shown in fig. 17 for some selected groups. The solution for the configuration that requires the minimum lead volume is characterised by a spatial trend that is very close to the one typical of a homogeneous system, while the solution associated to the more decoupled configuration exhibits strong variations passing from the fuel to the coolant sheets, similarly to what occurs for a moderated system.

VIII. DETERMINATION OF NEUTRON ABSORBERS FOR REACTIVITY CONTROL

The last application presented in this section concerns another classical problem in reactor physics, namely the evaluation of the absorber density required for a control rod device in order to achieve criticality. Assuming that the control rods are located in some specific volumes, $\mathcal{X}_{CR} =$

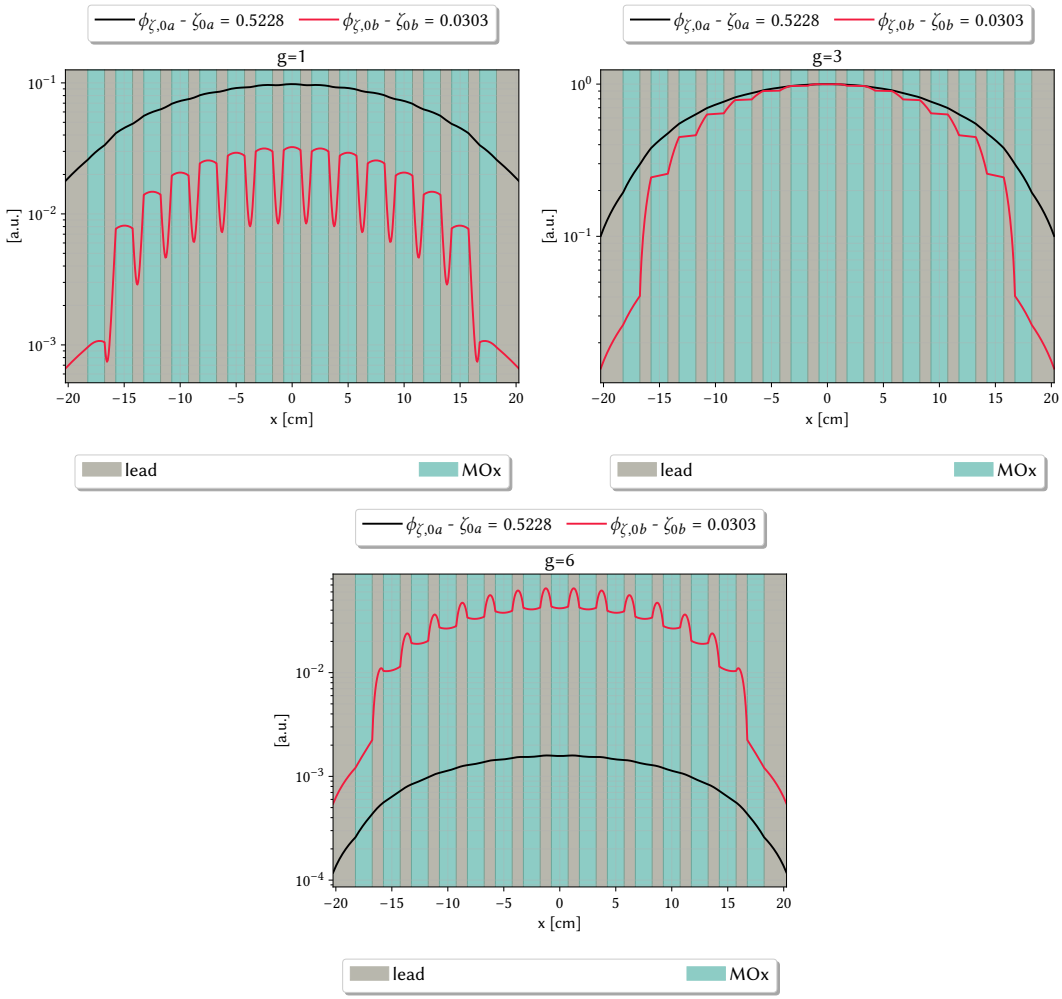


Fig. 17. *Group-wise fluxes for the two critical configurations for the MOX-lead lattice.*

$[x_i, x_{i+1}], \ldots, [x_j, x_{j+1}]$, the eigenproblem can be cast as follows,

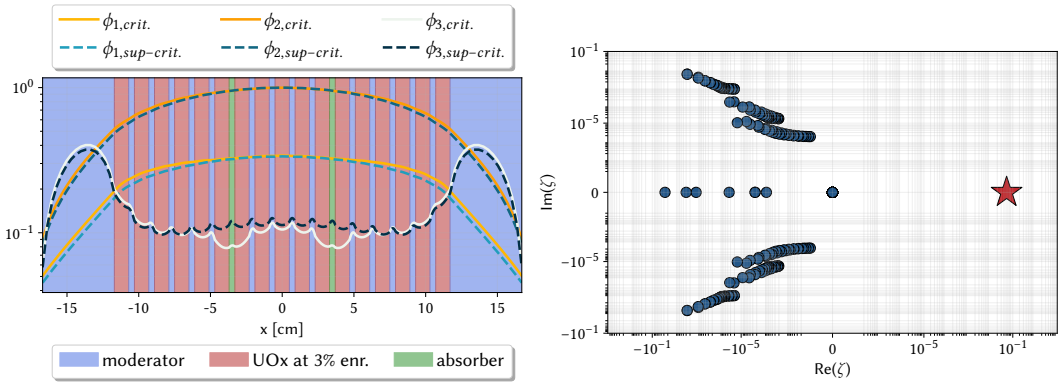
$$\begin{cases} \mu \dfrac{\partial \phi(x,E,\mu)}{\partial x} + \dfrac{1}{\zeta} N_{CR}\sigma_{t,CR}(E)\phi(x,E,\mu) = \\ \dfrac{1}{\zeta}\displaystyle\int_0^\infty dE' \int_{-1}^1 d\mu' N_{CR}\sigma_{s,CR}(E') f_{s,CR}(E' \to E, \mu')\phi(x,E',\mu') \qquad x \in \mathcal{X}_{CR}, \\ \\ \mu \dfrac{\partial \phi(x,E,\mu)}{\partial x} + \Sigma_t(x,E)\phi(x,E,\mu) = \\ \displaystyle\int_0^\infty dE' \int_{-1}^1 d\mu' \Sigma_s(x,E') f_s(x,E' \to E, \mu')\phi(x,E',\mu') + \qquad x \notin \mathcal{X}_{CR}, \\ \displaystyle\int_0^\infty dE' \int_{-1}^1 d\mu' \nu_m(x,E')\Sigma_{f,m}(x,E')\frac{\chi(x,E)}{2}\phi(x,E',\mu') \end{cases} \tag{32}$$

where N_{CR} indicates the atomic density of the control rod.

In the following, the critical absorber density (or volume) is searched for different control rod arrangements and initial off-criticality levels, dealing with a thermal system similar to the one discussed in section IV. Since the characteristics of the control rods are usually determined when most of the core parameters as the moderation ratio and the fuel enrichment have been selected, the initial configuration will be assumed to be super-critical. This is the only reasonable situation that could be considered, as, in the case of sub-criticality, it may not be possible to achieve a steady state configuration in general, unless considering unphysical, negative density corrections.

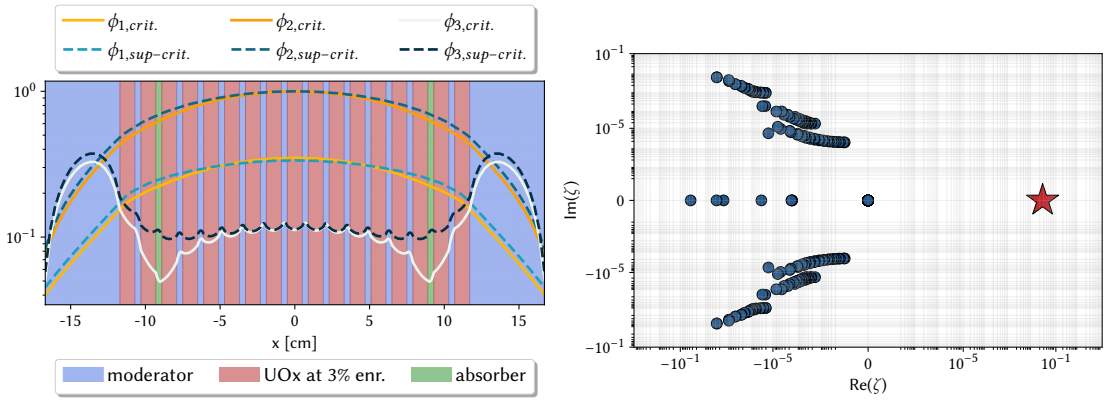
All the problems treated in the following have been solved using the P_1 model and collapsing the group constants on the CASMO-3 grid [35]. The determination of the whole ζ eigenvalue spectrum reveals that only one density allows to achieve criticality for an initially super-critical system, provided that the reactivity excess is not too large. Figure 18 reports the three-group fundamental k mode for the super-critical configuration ($k_{\text{eff}} = 1.11155$) and the fundamental ζ mode which corresponds to the critical flux when the two sheets of absorber are localised near the centre of the core. With respect to the boron dilution in water, this reactivity control system introduces a larger distortion in the energy spectrum, especially in the thermal group. The ES associated to this critical configuration amounts to 0.8, while $1/\zeta_{\text{eff}} = 18.93716$.

When the control devices are placed in the periphery of the core, see fig. 19, the spatial decoupling of the system is reduced, ES=1.12759. However, due to the proximity with the boundaries, also the effectiveness of the control devices is reduced, i.e. their worth reduces when they



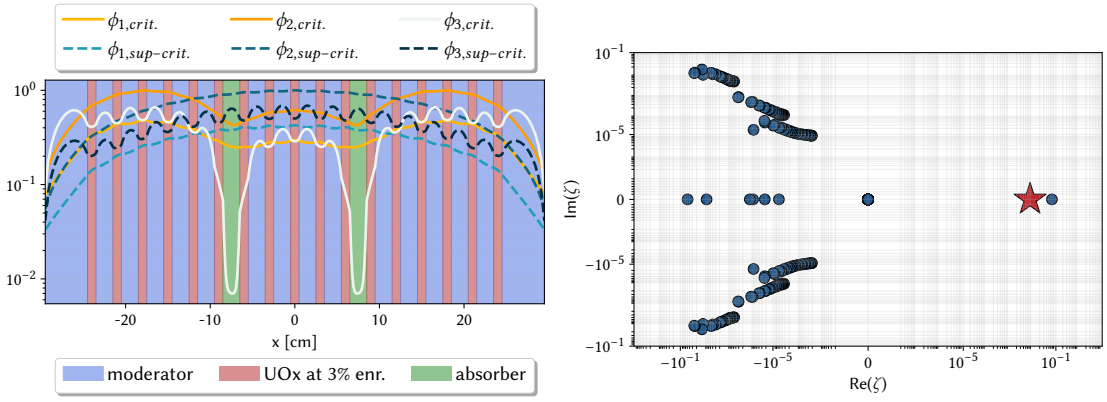
(a) (b)

Fig. 18. *Three-group critical and off-critical fluxes (a) and eigenvalue spectrum (b) for the case considering the control rods near the center of the lattice.*



(a) (b)

Fig. 19. *Three-group critical and off-critical fluxes (a) and eigenvalue spectrum (b) for the case considering the control rods near the reflector.*



(a) (b)

Fig. 20. *Three-group critical and off-critical fluxes (a) and eigenvalue spectrum (b) for the case considering the control rods near the center of the lattice.*

are located far from the centre of the core, where fluxes and importances of neutrons are higher. Hence, the same static reactivity ($\rho = 10035$ pcm) should be compensated with a larger absorber concentration, $1/\zeta_{\text{eff}} = 37.18518$. Also in this case, there is only one solution to the design problem, i.e. only one real and positive value of ζ can be found.

Figures 20 and 21 refer to a different initial configuration, characterised by a larger moderation ratio with respect to the previous case and, thus, by a larger departure from criticality ($k_{\text{eff}} = 1.39879$, $\rho = 28509$ pcm). When the control rods are positioned at the core centre, the ζ spectrum (see right of fig. 20) exhibits two real and positive eigenvalues, associated to the fundamental and to the first-order harmonic. As for some cases discussed previously, the fundamental eigenvalue is smaller than the first-order one. The appearance of a higher-order real and positive eigenvalue is related to the larger departure from criticality with respect to the previous case. Following this intuition, the same problem is addressed placing the control rods in a peripheral position. In this case, there is no solution to the problem, i.e. it is not possible to determine a correction factor for the control devices such that they are able to remove the excess of reactivity. As visible in fig. 21, no fundamental eigenvalue, represented with a star marker throughout the paper, appears in the spectrum. Therefore, the appearance of higher-order eigenvalues could be related to the offset to criticality, although a deeper investigation would be required.

Concerning the spatial profile displayed in fig. 20, it is easy to notice the strong flux depression in correspondence of the control sheets, which is caused by the spatial self-shielding effects induced

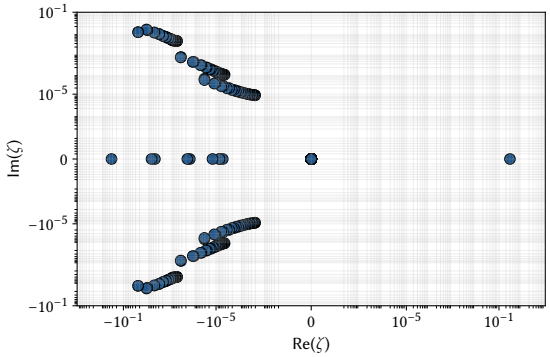


Fig. 21. *Eigenvalue spectrum for the case considering the control rods near the reflector.*

by the adjusted absorber density. The overall effect of these flux spikes is an increase of the core spatial decoupling, ES=0.04787. The significant self-shielding effect raises again the issue of the few-group constant generation: in practical applications, the ζ method should be applied during the group constants generation process, to avoid the under-/over-estimation of the self-shielding effects.

It is interesting to notice how, focusing only on the neutronic aspects of the core design, the location of the control rods should require a compromise between the core stability and their worth. An analogous discussion applies also to the number of control rods in relation to the core decoupling and to the offset from criticality, although this aspect has not been taken into account in this section. In light of these considerations and of the results of this section, the proposed eigenvalue formulation seems to well suit the needs of the design process, providing an efficient computational framework. As a matter of fact, the existence of only one physical solution, due to the absence of competing phenomena, would allow to compute only a few dominant eigenpairs instead of the full spectrum, which could be a considerable reduction of the computational time in practical applications.

IX. CONCLUSIONS

In this paper, it has been shown how the eigenvalue formulations for the neutron transport equation could be traced back to a generalised eigenvalue formulation, called ζ. This eigenvalue can be introduced in order to filter specific regions of the phase space. In particular, bearing in mind the possible practical constraints arising during the core-design process, the ζ eigenproblem

has been cast into a form that extends the applicability of the density eigenvalue δ to specific nuclides and regions of the phase space.

This novel approach has been applied to a wide range of different classical yet realistic problems in reactor physics, considering the main types of materials encountered in the design of a reactor core, e.g., the fuel, the coolant, the moderator and the localised absorbers. These applications provided remarkable results. First, the ζ eigenvalue yields equivalent results to the iterative method commonly applied in such framework, but with a strong reduction of the computational effort. More importantly, the existence of one or more design solutions is related to the presence, of one or more real and positive eigenvalues associated to positive eigenfunctions in the ζ spectrum. 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. Moreover, the knowledge of all the possible criticality arrangements of a system is of the utmost importance for the safety studies involving the re-criticality phenomena. This study of the ζ eigenvalue spectrum suggests that, in some situations, in particular in the absence of competing interaction phenomena, there can exist only one positive solution, associated to an eigenvalue separation which 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 activities. First of all, the ζ spectrum should be studied more thoroughly, starting from a more rigorous physico-mathematical framework and taking into account the impact of the different spatial, angular and energy approximations of the neutron transport equation. Moreover, the physico-mathematical meaning of the higher-order ζ harmonics should be investigated as well. A better comprehension of the ζ higher modes could disclose the possibility to apply perturbation methods, like the Generalised Perturbation Theory, which would be very useful for design-purpose calculations. Furthermore, 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 radiative capture, and a reduced energy range, e.g. the thermal region. At last, some research efforts should be devoted to incorporate the ζ calculation in the cross sections collapsing and homogenisation process, in order to directly account for the self-shielding effects.

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