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Original Article

Analysis of alpha modes in multigroup diffusion

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ABSTRACT

The alpha eigenvalue problem in multigroup neutron diffusion is studied with particular attention to the theoretical analysis of the model. Contrary to previous literature results, the existence of eigenvalue and eigenflux clustering is investigated here without the simplification of a unique fissile isotope or a single emission spectrum. A discussion about the negative decay constants of the neutron precursors concentrations as potential eigenvalues is provided. An in-hour equation is derived by a perturbation approach recurring to the steady state adjoint and direct eigenvalue problems of the effective multiplication factor and is used to suggest proper detection criteria of flux clustering. In spite of the prior work, the in-hour equation results give a necessary and sufficient condition for the existence of the eigenvalue-eigenvector pair. A simplified asymptotic analysis is used to predict bands of accumulation of eigenvalues close to the negative decay constants of the precursors concentrations. The resolution of the problem in one-dimensional heterogeneous problems shows numerical evidence of the predicted clustering occurrences and also confirms previous theoretical analysis and numerical results.

1. Introduction

The kinetic neutron equation with precursors is an efficient tool for the analysis of the neutron time evolution and, therefore, finds multiple applications in reactor control and the study of accident scenarios. The time-dependent flux depends on the initial conditions for neutrons and precursors, the boundary condition for neutrons, the presence of external sources and the time-dependent changes of the cross-sections, such as those produced by rod motion and changes of Boron concentration or to small stochastic perturbations induced by the coolant flow and, in the long time, by radioactive decay and nuclide depletion and creation from fission.

However, if the cross-sections and boundary conditions remain constant in time and the sources vanish, then the state of the system tends asymptotically in time to an exponential behavior, which is independent of the earlier changes of the system and, specially, of the initial conditions [1].

The exponential behaviors that a given system can adopt are the solutions of an eigenvalue equation and can be used to describe the fast evolution of the system as well as to characterize the reactivity of the system. The solutions of this equation are known as time-dependent modes or, more simply, alpha modes, where "alpha" refers to the most frequently adopted symbol for these eigenvalues.

Alpha modes have been applied to formally derive different forms of the well-known in-hour equation, to obtain solutions of the kinetic equations by expansion techniques [2], to develop numerical solution methods [3] and also as weighting fluxes to homogenize the kinetic equation [4]. These applications, as well as the theoretical interest, of alpha modes have been the object of intense study. However, with the exception of a few scattered mathematical results [5–7], a detailed description of these modes have not yet been given for the diffusion equation. The purpose of this paper is to give a detailed analysis of the alpha modes for a slab geometry using multigroup diffusion theory. We give ample numerical evidence for all the modes predicted from mathematical analysis as well as from physical arguments.

General equations for the alpha eigenvalue problem are discussed in *The alpha eigenvalue equations*, including a perturbation expression in terms of reactivity. In *Summary of results* we summarize our results and observations for the multigroup one-dimensional slab. Some numerical results are illustrated in *Numerical results*, while in *Comparison with Asahi's results* we compare with Asahi's analytical results for the one-group problem [6]. Conclusions follow.

For simplicity we shall use a notation based on a continuous formulation and leave it to the reader to the change to a fully discretized operator which is used in the numerical application.

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2. The alpha eigenvalue equations

Our starting point is the time-dependent kinetic diffusion equations coupled to the precursors equations in a heterogeneous domain $\mathcal{D}$:

$$\begin{cases} \left(\frac{1}{v}\partial_t + \beta_{pr}\right)\psi = \sum_p \chi_p \lambda_p C_p, & \text{(a)} \\ (\partial_t + \lambda_p) C_p = \mathcal{F}_p \psi. & \text{(b)} \end{cases} \tag{1}$$

Here $\psi(x,t)$ is the scalar flux, $x = (\mathbf{r},E)$ stands for the phase space variables, $C_p(\mathbf{r},t)$ is the concentration for precursor p and

$$\beta_{pr} = \mathcal{L} - \mathcal{P}_{pr}$$

is the diffusion kinetic operator with prompt neutron production

$$\mathcal{L} = -\nabla\cdot D\nabla + \Sigma - \mathcal{H}, \tag{2}$$

where $D(x,t)$ is the diffusion coefficient, $\Sigma(x,t)$ is the total macroscopic cross-section, $\mathcal{H}$ stands for the scattering operator and $\mathcal{P}_{pr} = \sum_i \chi_i(1-\beta_i)\mathcal{F}_i$ is the prompt fission operator with the sum in i over the fissile isotopes.

Also in Eqs. (1b) and (2), $\mathcal{F}_p = \sum_i \beta_{i\to p}\mathcal{F}_i$ and $\mathcal{F}_i$ are the production operators for precursor p and neutrons from isotope i, respectively. The latter is defined as $\mathcal{F}_i\psi = \int \nu\Sigma_{f,i}\psi dE$. We note N_p and N_i the number of precursors and fissile isotopes, respectively, and take the prompt and delayed fission spectra, χ_i and χ_p, to be normalized so that $\int \chi dE = 1$.

By introducing the reduced scalar product over the energy E,

$$\langle f,g\rangle = \int \bar{f} g dE, \tag{3}$$

where $\bar{f}$ denotes the complex conjugate of f, the two latter formulas can be written as $\mathcal{F}_i\psi = \langle \nu\Sigma_{f,i},\psi\rangle$ and $\langle 1,\chi\rangle = 1$. Finally, λ_p and $\beta_{i\to p}$ are the decay constants for the precursor p and its fission yield from isotope i, respectively, and $\beta_i = \sum_p \beta_{i\to p}$ is the total precursor yield for isotope i. We shall follow the usual convention of ordering λ_p in increasing values.

The kinetic equations in (1) are supplemented with initial conditions for both ψ and C_p and with boundary conditions for ψ. The cross-sections, external source and boundary conditions may change in time. But at any time $t = t_*$ one might consider a new kinetic problem with the initial and boundary conditions at time t_* and such that for $t > t_*$ the cross-sections and boundary conditions remain constant and the external source vanishes. This defines a kinetic problem with constant cross-sections and boundary conditions and with no external source which will evolve in time according solely to its initial conditions at t_*.

The alpha eigenvalue equations for this t_* -kinetic problem are obtained by introducing an exponential time behavior in (1),

$$\psi(x,t) \sim e^{\alpha t}\psi_\alpha(x), C_p(\mathbf{r},t) \sim e^{\alpha t}C_{p,\alpha}(\mathbf{r}),$$

to obtain:

$$\begin{cases} \left(\frac{\alpha}{v} + \beta_{pr}\right)\psi_\alpha = \sum_p \chi_p\lambda_p C_{p,\alpha}, & \text{(a)} \\ (\alpha + \lambda_p) C_{p,\alpha} = \mathcal{F}_p\psi_\alpha. & \text{(b)} \end{cases} \tag{4}$$

Here $\psi_\alpha(x)$ and $C_{p,\alpha}(\mathbf{r})$ are respectively the scalar flux and the concentration for precursor p of an α-mode, and all other quantities and operators are like those defined for the time-dependent kinetic equation but with the cross-sections evaluated at time t_*.

More generally, by introducing the vector function $\overline{\Psi}_\alpha = \{\psi_\alpha, \overrightarrow{C}_\alpha\}$, where $\overrightarrow{C}_\alpha$ has components $\{C_{p,\alpha}, \alpha = 1, N_p\}$, the set of alpha equations can be written in the form of a classical linear eigenvalue problem:

$$\mathcal{M}\overline{\Psi}_\alpha = \alpha\overline{\Psi}_\alpha, \tag{5}$$

where the structure of the matrix operator $\mathcal{M}$, not stated here, can be inferred from Eq. (4).

When appropriate we shall use Hilbert spaces for a precise formulation of results. We note that $\mathcal{H}_\mathcal{X}$ the Hilbert space of complex-valued functions defined over phase space $\mathcal{X}$ and satisfying the boundary conditions of problem (4). This space is endowed with the scalar product

$$(f,g) = \int_\mathcal{X} \bar{f}(x)g(x)dx, \tag{6}$$

where $dx{=}d\mathbf{r}dE$ is the volume element in $\mathcal{X}$. We also note $\mathcal{H}_\mathcal{D}$ is the Hilbert space of complex-valued functions defined over the geometrical domain D with scalar product

$$(f,g)_\mathcal{D} = \int_\mathcal{D} \bar{f}(\mathbf{r})g(\mathbf{r})d\mathbf{r}.$$

Thus, we consider problem (5) in the Hilbert space of complex-valued functions $\mathcal{H}_\mathcal{X} \times (\mathcal{H}_\mathcal{D})^{N_p}$ with scalar product

$$\left(\left(\overline{\Psi}, \overline{\Psi}'\right)\right) = (\psi,\psi') + \sum_p \left(C_p, C_p'\right)_\mathcal{D}.$$

A useful form of the alpha-equations can be obtained by solving Eq. (4b) for the precursor concentrations:

$$C_{p,\alpha} = \frac{\mathcal{F}_p\psi_\alpha}{\alpha + \lambda_p}, \quad \alpha\in\mathbb{C}\backslash\Lambda, \tag{7}$$

where $\Lambda = \{-\lambda_p, \ p = 1, N_p\}$. Next, replacing this result in Eq. (4a) yields an expression for the alpha-eigenvalue problem in terms of only the flux:

$$\left(\frac{\alpha}{v} + \overline{\mathcal{B}}\right)\psi_\alpha = -\mathcal{K}_\alpha\psi_\alpha, \quad \alpha\in\mathbb{C}\backslash\Lambda, \tag{8}$$

where $\overline{\mathcal{B}} = \mathcal{L} - \overline{\mathcal{P}}$,

$$\overline{\mathcal{P}} = \sum_i \overline{\chi}_i\mathcal{F}_i \tag{9}$$

is the production operator with the steady-state fission spectrum

$$\overline{\chi}_i = (1-\beta_i)\chi_i + \sum_p \beta_{i\to p}\chi_p \tag{10}$$

and

$$\mathcal{K}_\alpha = \sum_p \frac{\alpha}{\alpha+\lambda_p}\chi_p\mathcal{F}_p \tag{11}$$

comes from the delayed contribution to production. We consider this problem in $\mathcal{H}_\mathcal{X}$.

We note that Eq. (8) is a non linear eigenvalue problem for (α,ψ_α). Moreover, as we will discuss next, except for very pathological cases, Λ is in the resolvent set of the linear operator in Eq. (5) and therefore Eqs. (4) and (8) are equivalent.

Let us analyze in which conditions $\alpha = -\lambda_p$ can be in the spectrum of Eq. (4). If this is true, then one must have from Eq. (4b)

$$\mathcal{F}_p\psi_\alpha = 0. \tag{12}$$

We note that one can write $\mathcal{F}_p = h\pi_p$ where $h(\mathbf{r}) = (\mathcal{F}_p 1)(\mathbf{r})$ and $\pi_p = h^{-1}\mathcal{F}_p$ is a projector $\pi_p : \mathcal{H}_\mathcal{X} \to \mathcal{H}_\mathcal{D}$. Equivalently, constraint (12) can be written as

$$\psi_\alpha \in ker(\pi_p),$$

where $ker(\pi_p)$ is the null space of π_p. For the other precursors one obtains

$$C_{p',\alpha} = \frac{1}{\lambda_{p'} - \lambda_p}\mathcal{F}_{p'}\psi_\alpha, \quad p' \neq p, \tag{13}$$

which yields a source equation for the flux:

$$\widehat{\beta}\psi_\alpha = \chi_p\lambda_p C_{p,\alpha}, \tag{14}$$

where

$$\widehat{\beta} = \overline{\beta} - \frac{\lambda_p}{\nu} - \sum_{p'\neq p}\frac{\lambda_p}{\lambda_{p'} - \lambda_p}\chi_{p'}\mathcal{F}_{p'}.$$

Hence, a solution of Eq. (14) with the constraint in (12) is a pair $(\psi_\alpha,\ C_{p,\alpha} = \widehat{\beta}\psi_\alpha/(\chi_p\lambda_p))$[1] iff[2] (i) $0 \neq \psi_\alpha \in ker(\pi_p)$, (ii) $\widehat{\beta}\psi_\alpha \in \mathcal{E}_p$, where we have defined $\mathcal{E}_p = \{f(x) = \chi_p(E)h(\mathbf{r});\ h(\mathbf{r}) \in \mathcal{H}_\mathcal{D}\}$. In other words $-\lambda_p$ is an alpha-eigenvalue iff $\widehat{\beta}(ker(\pi_p)/\{0\}) \cap \mathcal{E}_p \neq \varnothing$. Although this iff condition does not apparently require operator $\widehat{\beta}$ to have an inverse, an equivalent formulation can be written as $\widehat{\beta}^{-1}\mathcal{E}_p \cap (ker(\pi_p)/\{0\}) \neq \varnothing$. Thus, a solution might exists if operator $\widehat{\beta}$ is degenerated or if it is invertible over $\mathcal{E}_p$; the former condition seems unrealistic but the second looks plausible because ν is large and Σ contains scattering, capture and fission and therefore dominates $\mathcal{H}$. However, in both cases the solution of equation (14) must satisfy the orthogonality condition (12), which most likely will not be feasible. Therefore, with the exception of unrealistic cross-sections, the existence of an alpha eigenvalue equal to minus a precursor decay constant can be excluded.

Clearly the precedent conclusion applies to the case of the one-group diffusion equation. But here we give a counter example for which $-\lambda_p$ is an alpha eigenvalue. Consider the case when the diffusion coefficient does not depend on the energy, $D = D(\mathbf{r})$, and take $\psi_\alpha(x) = f(E)h(\mathbf{r})$ with $\pi_p f = 0$ and $h(r)$ an eigenfunction of the Laplacian equation $-\nabla\cdot D\nabla h = \gamma h$ which satisfies the boundary conditions of the alpha problem. Then $\widehat{\beta}\psi_\alpha = h\widehat{\beta}_\gamma f$, where $\widehat{\beta}_\gamma$ equals $\widehat{\beta}$ with the replacement $-\nabla\cdot D\nabla \to \gamma$. Therefore, by setting $\chi_p = \widehat{\beta}_\gamma f/c$, where $c(\mathbf{r}) = \int \widehat{\beta}_\gamma f dE$, the pair $(\psi_\alpha, C_{p,\alpha} = (c/\lambda_p)h)$ is a solution of the alpha eigenvalue problem for $\alpha = -\lambda_p$. A problem with the definition of χ_p is that it depends on space, but this can be avoided by considering a homogeneous problem. However, even then, one would have to "adjust" the cross-sections, perhaps with nonphysical values, so as to ensure that χ_p remains positive.

2.1. Perturbation formulation

Reactivity is a measure of the disequilibrium of a system and there are several ways to introduce a notion of reactivity in neutron kinetics [8,9], in particular that derived with the help of the adjoint α equation [10]. In this work we define a generalized reactivity as $\rho_\lambda = 1 - 1/\lambda$, where λ is any eigenvalue of the quasi-static eigenvalue equation obtained by setting $\alpha = 0$ in Eq. (8):

$$\overline{\beta}_\lambda\varphi_\lambda = 0, \tag{15}$$

where

$$\overline{\beta}_\lambda = \mathcal{L} - (1/\lambda)\overline{\mathcal{P}}. \tag{16}$$

Here $\lambda \in \sigma_p(\mathcal{L}^{-1}\overline{\mathcal{P}})$, where σ_p denotes the point spectrum of the operator, is an eigenvalue of the quasi-static diffusion operator and $\overline{\mathcal{P}}$ is the steady-state production operator in Eq. (9). The boundary condition for Eq. (15) is that of the parent alpha eigenvalue equations. We note E_λ and N_λ, respectively, the subspace of eigenfunctions of eigenvalue λ and its dimension. We recall that the eigenvalue $\lambda = k$ with maximum absolute value in $\sigma(\mathcal{L}^{-1}\overline{\mathcal{P}})$ is real, non degenerate and has a positive eigenfunction φ_k (a physical flux).

In order to analyze the solutions of the alpha-eigenvalue equation it is advantageous to write Eq. (8) in terms of the quasi-static operator $\overline{\beta}_\lambda$ in (16) and cast the alpha-eigenvalue equation as

$$\overline{\beta}_\lambda\psi_\alpha = \mathcal{K}_{\lambda,\alpha}\psi_\alpha, \tag{17}$$

where $\lambda \in \sigma_p(\mathcal{L}^{-1}\overline{\mathcal{P}})$ and

$$\mathcal{K}_{\lambda,\alpha} = \rho_\lambda\overline{\mathcal{P}} - \left(\frac{\alpha}{\nu} + \mathcal{K}_\alpha\right). \tag{18}$$

The appeal of formulation (17) is that (i) it offers a perturbation expression for the alpha eigenvalue problem in terms of the better known steady-state eigenvalue problem, and (ii) the operator $\overline{\beta}_\lambda$ on the left of the equal sign is singular and therefore the "source" term $\mathcal{K}_{\lambda,\alpha}\psi_\alpha$ must satisfy a solvability condition.

According to the Riesz-Schauder theory [11], the solvability condition requires the source term to be in the orthogonal complement $E^\perp$ of the eigenspace $E^\dagger_{\overline{\lambda}}$ associated to the eigenvalue $\overline{\lambda} \in \sigma((\overline{\mathcal{P}}\mathcal{L}^{-1})^\dagger)$ of the adjoint operator $\overline{\beta}^\dagger_{\overline{\lambda}}$.[3] More explicitly,

$$\left(\varphi^\dagger, \mathcal{K}_{\lambda,\alpha}\psi_\alpha\right) = 0 \ \forall\varphi^\dagger \in E^\dagger_{\overline{\lambda}}. \tag{19}$$

Thus, the solvability condition results in a system of N_λ one-point-like "kinetic" alpha equations. For each function $\varphi^\dagger \in E^\dagger_{\overline{\lambda}}$ we have an in-hour-type equation:

$$\rho_\lambda = \alpha\left(\Lambda + \sum_p \frac{\Gamma_p}{\alpha + \lambda_p}\right), \tag{20}$$

where

$$\Lambda = \frac{(\varphi^\dagger, \frac{1}{\nu}\psi_\alpha)}{(\varphi^\dagger, \overline{\mathcal{P}}_\alpha)},\ \Gamma_p = \frac{\left(\varphi^\dagger, \chi_p\mathcal{F}_p\psi_\alpha\right)}{(\varphi^\dagger, \overline{\mathcal{P}}\psi_\alpha)}. \tag{21}$$

[1] For simplicity, we assume that χ_p is strictly positive.
[2] if and only if.
[3] It is understood that the adjoint operator is provided with appropriate "adjoint" boundary conditions [12].

As an aside, we note that in Eq. (21) one can write $\Gamma_p = \sum_i \beta_{i\to p}\gamma_{i,p}$ with the effectiveness factors [13] $\gamma_{i,p} = \int \langle \varphi_k^\dagger, \chi_p\rangle \langle \nu\Sigma_{f,i}, \psi_\alpha\rangle d\mathbf{r}/(\varphi_k^\dagger, \overline{\mathcal{P}}\psi_\alpha)$ and $(\varphi_k^\dagger, \overline{\mathcal{P}}\psi_\alpha) = \sum_i \int \langle \varphi_k^\dagger, \overline{\chi}_i\rangle \langle \nu\Sigma_{f,i}, \psi_\alpha\rangle d\mathbf{r}$, recovering thus the formula derived for an infinite homogeneous medium in [14]. Also, because of the projection by $\varphi^\dagger$ the original eigenvalue α is dispersed among the N_p+1 roots of Eq. (20).

Under the solvability constraint (19), the general solution of (17) is an arbitrary multiple of

$$\psi_\alpha = \varphi_\lambda + \psi^\perp, \tag{22}$$

where $\varphi_\lambda = \sum_n a_n\varphi_n$ is written using an arbitrary basis $\{\varphi_n, n = 1, N_\lambda\}$ in E_λ and $\psi^\perp \in E^\perp$. The latter condition entails

$$a_n = \left(\varphi_n^\dagger, \psi_\alpha\right), \tag{23}$$

where the $\{\varphi_n^\dagger, n = 1, N_\lambda\}$ is the dual basis in $E_\lambda^\dagger$, i.e., such that $(\varphi_n^\dagger, \varphi_{n'}) = \delta_{nn'}$.

We end this section with a comment regarding the effect of spatial symmetries on the structure of the in-hour equation. Consider a problem with a spatial involution, that is a symmetry s such that $s^2 = 1$. Then ψ_α obeys the relation $s^2\psi_\alpha = \psi_\alpha$ and, since operator s^2 has eigenvalues 1 and -1, one can write ψ_α as the sum of an even $(+)$ and an odd $(-)$ components $\psi_{\alpha,\pm} = (s\pm 1)\psi_\alpha$ with the property that $\int d\mathbf{r}\psi_{\alpha,+}(\mathbf{r})\psi_{\alpha,-}(\mathbf{r})$ vanishes. Because both the steady-state transport equation and the alpha eigenvalue equation necessarily share the same geometry one concludes that the in-hour equation does not exist when $\varphi^\dagger$ and ψ_α have opposite symmetries.

3. Summary of results

The spectrum of the alpha mode equations is conditioned by the nature of these equations and by the degree of complexity accepted in the delayed neutron term. In the continuous case the eigenmodes, $\overrightarrow{\Psi}_\alpha(x)$, belong to a functional space of infinite dimensions, while in the discretized case they become vectors in a finite-dimensional space. On the other hand, the degree of complexity of the fission delayed contribution depends on the number of fissile isotopes N_i and the number of precursors N_p. The operator in Eq. (11) can be written as a sum of projectors with $\mathbf{r}$-dependent coefficients:

$$\mathcal{K}_\alpha = \sum_p \frac{\alpha}{\alpha+\lambda_p} a_p\pi_p, \tag{24}$$

where $a_p(\mathbf{r}) = \mathcal{F}_p\chi_p$ and $\pi_p = (1/a_p)\chi_p\mathcal{F}_p$ is a projector over the subspace generated by the $\{\chi_p, p = 1, N_p\}$. Therefore, for $\alpha \notin \{0\cup\Lambda\}$, $\mathcal{K}_\alpha$ is a finite linear combination of projectors with finite range equal to the span of the functions $\{\chi_p, p = 1, N_p\}$. Moreover, the null space of $\mathcal{K}_\alpha$ contains the set of all the functions that are orthogonal to the finite set $\{\nu\Sigma_{f,i}, i = 1, N_i\}$.

Simplifications of the fission delayed contributions are typically introduced to facilitate the theoretical analysis of the alpha spectrum. A simplifying assumption can be applied to the delayed fission spectra, to the fission production or to both. The first consists of replacing all the delayed neutron spectra with an averaged one, $\chi_p \sim \chi$, which leads to the simplified form $\mathcal{K}_\alpha = \chi\mathcal{F}_\alpha$, where $\mathcal{F}_\alpha = \sum_p [\alpha/(\alpha+\lambda_p)]\mathcal{F}_p$. In the second one replaces the fission production for all fissile isotopes with a single one, $\nu\Sigma_{f,i} \sim w_i(\mathbf{r})\nu\Sigma_f$, where by convenience we assume $\sum_1 w_i(\mathbf{r}) = 1$. This approximation yield the simplified form $\mathcal{K}_\alpha = \chi_\alpha\mathcal{F}$, where now $\chi_\alpha = \sum_p [\alpha/(\alpha+\lambda_p)\beta_p\chi_p]$ with $\beta_p(\mathbf{r}) = \sum_i w_i(\mathbf{r})\beta_{i\to p}$. Note that these approximations are automatically satisfied if one assumes one single precursor ($\chi = \chi_1$) or one single fissile isotope ($w_1 = 1$ and $\beta_p = \beta_{1\to p}$). Finally, when both approximations are used one has the simplified operator

$$\mathcal{K}_\alpha = f_\alpha(\mathbf{r})\chi\mathcal{F}, \tag{25}$$

where

$$f_\alpha(\mathbf{r}) = \sum_p \frac{\alpha}{\alpha+\lambda_p}\beta_p(\mathbf{r}). \tag{26}$$

Note that for a single fissile isotope $\beta_p(\mathbf{r}) = \beta_p$, while for a homogeneous medium $\beta_p = \sum_i w_i\beta_{i\to p}$. For both cases $f_\alpha(\mathbf{r})$ is independent of $\mathbf{r}$ and is an analytical function of α in $\mathbb{C}\backslash\Lambda$.

There is a sizable number of theoretical studies of the alpha spectrum in transport theory but, to our knowledge, there are only three communications pertaining to diffusion theory. Porsching [5] used algebraic techniques to analyze the spectrum of the alpha mode discretized diffusion equations in a homogeneous medium with a single fissile isotope. However his equations were based on a synthetic expression for the time-dependent flux and, regarding the present standard alpha eigenvalue problem, Porsching's results apply only to the one-group diffusion equation. A generalization to the multigroup diffusion equation was carried out by Devooght [7] for the fully discretized diffusion equation in a heterogeneous medium with no upscattering and with a single fissile isotope. To simplify the delayed fission term, Devooght assumes that all the fissile neutron spectra are identical, i.e., not only that $\chi_p \sim \chi$ but also $\overline{\chi}_1 \sim \chi$, which lead him to lump prompt and delayed fission in a single term and work with the function $f(\alpha) = 1 - f_\alpha$, which is also analytical in $\mathbb{C}\backslash\Lambda$. This function was used in the general study of the spectrum. The analysis of the fast spectrum, based on a perturbation result for the case of degenerated operators discussed in Kato [15], was carried out for the case with no precursors, while a technique early introduced by Wings [1] was applied to the investigation of the degeneracy of the delayed spectrum. The result of the analysis is that the spectrum consists of $N_g + N_p$ clusters of N_r eigenvalues each, where N_g and N_r are the number of groups and the number of spatial components, respectively. The delayed spectrum has N_p clusters of real eigenvalues with the p-th cluster confined to the open interval[4]

$$I_p = \left(-\lambda_p, -\lambda_{p-1}\right) \tag{27}$$

with the convention that $-\lambda_0 = \infty$. The only theoretical result for the one-group continuous diffusion equation in the one-dimensional heterogeneous slab geometry was given by Asahi [6] a few years earlier than Devooght's paper but seemingly unknown to the latter. Asahi demonstrated that for an arbitrary geometry, the eigenvalues were real and bounded and that the $-\lambda_p$ values were not in the spectrum. He also gave a more detailed analysis for the case of the one-dimensional slab, classifying the

[4] In reality, the result obtained by Devooght is that the $-\lambda_p$ also belongs to the p-th clusters and that, therefore, the precursor clusters contain N_r+1 eigenvalues each. However, he recognized that this pathological result occurred because he had artificially replaced the precursor concentrations $C_p(\mathbf{r})$ with the energy dependent functions $C_p^\clubsuit(\mathbf{r}, E) = \chi_p(E)C_p(\mathbf{r})$ resulting in the associated eigenvalue problem having $N_rN_p(N_g-1)$ more eigenvalues than the original one.

eigenfunctions by the number of nodes and showing that there are a countable infinite number of eigenvalues in each interval I_p which accumulate at $-\lambda_p$ as well as in the open interval

$$I^L_{N_p} = \left(-\infty, -\lambda_{N_p}\right). \tag{28}$$

The rightmost eigenvalue in each interval has an eigenfunction with positive flux (zero nodes) and the number of nodes of the eigenfunction fluxes increases monotonously by one for the other eigenvalues in the interval. Finally, as shown in Appendix A, an analytical solution can be obtained for the one-group homogeneous case which confirms the structure of the prompt and delayed spectrum as well as the emergence of flux clustering. This result leads to a new derivation of Asahi's results for the one-group homogeneous finite slab (see Appendix B).

In the second part of this section, we give general observations in the nature of the spectrum of the alpha eigenvalue problem derived from robust arguments and from numerical exploration of multigroup diffusion in a slab geometry. Our results match the known theoretical predictions in their restricted domain of validity [5–7]. Our discretization was done for the one-dimensional piecewise heterogeneous slab geometry by writing the linear alpha eigenvalue equations (5) in their multi-group form and by introducing a numerical discretization for the spatial dependence of both ψ and $\vec{C}$. We observe that the number of degrees of freedom (DOF) of the discretized system of equations is

$$N_{DOF} = N_r\left(N_g + N_p\right). \tag{29}$$

A natural ordering is built in the kinetic equations. This ordering stems from the observation that most of the neutrons resulting from fission are prompt and that, therefore, the contribution of delayed neutrons to the overall neutron production in the kinetic equations can be considered as small. In addition, the frequencies of emission of delayed neutrons are also much smaller than the neutron collision frequency. These two conditions can be expressed as

$$\beta_p \ll 1 \quad \text{and} \quad \lambda_p \ll \nu\Sigma.$$

In the following we shall assume that all cross-sections are $O(1)$ and we shall define $\varepsilon_\beta = O(\beta)$ and $\varepsilon_\nu = O(1/\nu)$. Physical data tells us that ε_β~10^{-3}–10^{-4} and ε_ν~10^{-5}–10^{-9}.

This ordering has direct implications on the distribution of the alpha spectrum, which can be sorted out into two subsets: delayed and prompt eigenvalues.

3.1. Delayed spectrum

These modes appear in the range $|\alpha| \sim O(\lambda_p)$, in N_p clusters of N_r eigenvalues each, for a total of N_rN_p eigenvalues (see Fig. 1). The eigenvalues in the p-th cluster gather on the right of $-\lambda_p$:

$$-\lambda_p < \alpha_{p,N_r} < \ldots < \alpha_{p,2} < \alpha_p < -\lambda_{p-1},$$

where $\alpha_{p,i}$ is the i-th eigenvalue of the cluster in the interval I_p. Also, we have written $\alpha_{p,1}$ simply as α_p to indicate the special

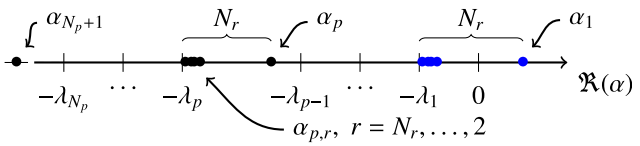

Fig. 1. Clusterings of eigenvalues approaching the negative values of the precursor's decay constants.

nature of the dominant mode in the cluster. While the other eigenvalues in the cluster are very close to $-\lambda_p$ and their values do not change much with the reactivity, the value of the dominant eigenvalue α_p increases with the reactivity towards $-\lambda_{p-1}$. The delayed eigenvalues are simple and real negative with the exception of α_1 which becomes positive for positive reactivity. This latter eigenvalue admits a positive eigenvector (both fluxes and concentrations are positive). The remaining dominant eigenvalues (α_p,$p > 1$) have positive fluxes but the concentrations change sign.

The p-th cluster can be analyzed using the expression

$$\alpha + \lambda_p = \varepsilon_p \tag{30}$$

and considering the eigenvalue problem for $|\varepsilon_p| \to 0$. The analysis shows that there is a leading concentration for each of the N_p clusters which, because of the special variation degenerates into N_r independent distributions. Hence, this part of the spectrum can also be named "precursor" spectrum. We have also made the conjecture that the eigenmodes concentrations in each cluster are linearly independent and this has been supported by all our calculations.

In order to analyze the clustering results we resort to an approach different from the ones adopted in the literature. We recognize that the behavior of the delayed spectrum is directly related to the changes undergone by the precursors concentrations and, therefore, replace Eq. (8) with an "equivalent" equation for the concentrations. We use Eq. (7) to write the delayed contribution in Eq. (8) in terms of the concentrations and by making the ψ_α in the resulting equation explicit we write

$$\psi_\alpha = -\left(\alpha/\nu + \overline{\beta}\right)^{-1} \alpha \sum_p \chi_p C_{p,\alpha},\ \alpha \notin \sigma\left(-\nu\overline{\beta}\right). \tag{31}$$

Next operating on this equation with $(\alpha + \lambda_p)^{-1}\mathcal{F}_p$ yields a finite system of equations for the concentrations, which we choose to write as:

$$\left(\alpha + \lambda_p\right) C_{p,\alpha}(\mathbf{r}) = -\alpha \sum_{p'} \left(\mathcal{T}_{pp',\alpha} C_{p',\alpha}\right)(\mathbf{r}),\ \alpha \notin \sigma\left(-\nu\overline{\beta}\right), \tag{32}$$

where $\mathcal{T}_{pp',\alpha}$ is an integral operator over E and $\mathbf{r}$ with kernel

$$t_{pp',\alpha}(\mathbf{r}' \to \mathbf{r}) = \int dE \nu\Sigma_{f,p}(x) \int dE' \chi_{p'}(E') g_\alpha(x' \to x), \tag{33}$$

where $\nu\Sigma_{f,p} = \sum_i \beta_{i\to p}$ is the fission production term for precursor C_p, $x = (E, \mathbf{r})$ and $g_\alpha(x' \to x)$ is the Green's function of operator $(\alpha/\nu + \overline{\beta})^{-1}$. We note that Eq. (32) is not equivalent to Eq. (8) for the simple reason that the energy variable does not appear in the former equation. This can be stated more precisely for the discretized case where the number of DOF for Eq. (32) is N_rN_p whereas Eq. (8) has $N_rN_gN_p$ DOF. This shows that, except for the one-group case, the two equations are not equivalent. However, if α is an eigenvalue of Eq. (32) with eigenvector $\vec{C}_\alpha(\mathbf{r})$ and $\alpha \notin \sigma(-\nu\overline{\beta})$, then α is also an eigenvalue of the full alpha problem in Eq. (8) with the eigenvector given by Eq. (31).

Thus, we can safely use Eq. (32) to analyze the delayed alpha spectrum. We introduce the assumption in Eq. (30) and use asymptotic analysis to study the behavior of the spectrum near $-\lambda_p$. A full analysis would consist of expanding the concentrations and the eigenvalue as a sum of increasing powers of ε_p, but here we use a rough approximation and keep only the leading terms in the equation. However, the discussion is awkward when working with

Eq. (32) and we shall instead take a step back and work with Eqs. (7) and (8). We notice first that, consistently with Eq. (7), we have $C_{p,\alpha} = \mathcal{F}_p\psi_\alpha/\varepsilon_p \sim \varepsilon_p^{-1}$ and, for $p' \neq p$, $C_{p',\alpha} = \mathcal{F}_{p'}\psi_\alpha/(\lambda_{p'} - \lambda_p + \varepsilon_p) \sim O(1)$.

Hence, we can neglect the contribution from the $p' \neq p$ precursors in the sum in the right-hand-side of Eq. (8). Following the derivation of Eq. (32), this implies that the system of equations in (32) uncouples and, in particular, yields a single equation for $C_{p,\alpha}$. To simplify our notation we write this equation as follows

$$\varepsilon_p C_{p,\alpha}(\mathbf{r}) = \lambda_p\left(\mathcal{T}_\alpha C_{p,\alpha}\right)(\mathbf{r}), \alpha \notin \sigma\left(-\nu\overline{\beta}\right) \tag{34}$$

with ε_p now playing the role of the eigenvalue. Still, this last equation is difficult to analyze and we should simplify the operator by keeping only the leading contributions. Going back to Eq. (8), we observe that because $\mathcal{F}_p \sim \varepsilon_\beta$, the order of the right-hand term in this equation is $\varepsilon^{-1} = \varepsilon_\beta/\varepsilon_p$ instead of ε_p^{-1}. So, in order to have $\varepsilon \ll 1$, we have to assume $\varepsilon_p \ll \varepsilon_\beta$. Having made sure that the right-hand-side of Eq. (8) is $\sim\varepsilon^{-1}$, we observe that on the left-hand-side $(\alpha/\nu + \Sigma - \mathcal{H} - \overline{\beta})\psi \sim O(1)$ so we have $\alpha/\nu + \overline{\beta} \sim -\nabla\cdot D(E,\mathbf{r})\nabla$. The spectrum of this operator consists of a countable infinite number of real positive eigenvalues growing towards $+\infty$; these eigenvalues have finite multiplicity and the corresponding eigenfunctions form a complete basis in L_2 [16]. It follows that the inverse of this operator is compact and definite positive and its Green's function is of the form $g_\alpha(E,\mathbf{r}' \to \mathbf{r})$, where E appears only as a parameter. This implies that the operator $\mathcal{T}$ is also compact, and therefore it has real eigenvalues, but it is not necessarily definite positive. However, it is easily verified that for a homogeneous medium, as well as in the one-group case, $\mathcal{T}$ is definite positive and therefore its eigenvalues are positive and accumulate at zero. This proves that the eigenvalues α which converge towards $-\lambda_p$ do this from the right $(\alpha > -\lambda_p)$.

3.2. Prompt spectrum

The remaining part of the spectrum lies on the complex plane $\Re(\alpha) < -\lambda_{N_p}$ and consists of simple eigenvalues that are real or complex conjugated in the range $|\alpha| \sim O(\nu\Sigma)$; the exception is the first dominant eigenvalue α_{Np+1} which is real and, with increasing reactivity tends to $-\lambda_{Np}$. The eigenvectors have negligible concentration values and they are dominated by energy modes.

To analyze these eigenvalues we use again an asymptotic approach by assuming that $\alpha \sim O(\nu)$. Hence, one can neglect the contribution of the delayed neutrons and write the alpha eigenvalue equation by keeping only the leading terms as

$$\left(\frac{\alpha}{\nu} + \beta_{pr}\right)\psi_\alpha \sim 0. \tag{35}$$

This shows that the prompt spectrum is closely related to the spectrum of the diffusion equation with prompt fission, $\alpha \in \sigma(-\nu\mathscr{B}_{pr})$.

3.3. Flux clustering

We use the expression *flux clustering* to refer to a set of distinct eigenvalues which have very close fluxes. Flux clustering for the alpha eigenvalue transport problem was discussed earlier by Gozani [17] and by Henry [10]. Gozani applied his analysis also to diffusion theory, but the most interesting result was Henri's analysis of the two-group P1 transport equation, which is closely related to diffusion; by using the analytical solutions of this problem, Henri was able to give a satisfactory argument, albeit non rigorous, in support of flux clustering.

The flux components of the N_{p+1} dominant alpha modes can be shown to cluster about the dominant mode of the quasi-static equation φ_k. This includes the dominant modes in the delayed spectrum (α_p,$p = 1$,N_p) plus the dominant mode of the prompt spectrum (α_{Np+1}). It can also be expected that non-dominant delayed modes can exhibit some form of flux clustering, like sharing the same number of spatial fluctuations in the slab case, and that this type of flux clustering might even apply to prompt modes. However, in our numerical calculations we have not observed yet any such clustering, except for the fact that for each energy group one might be able to identify N_r modes that are associated, in the sense that they have a similar spatial behavior.

Our analysis of flux clustering is based on the perturbation approach discussed in *Perturbation formulation*, whose main results are the in-hour equation and the flux perturbation formula, Eqs. (20) and (22), respectively. For simplicity, hereafter we shall only consider the case when λ is the dominant eigenvalue of the quasi-static diffusion operator, which we denote by k. This eigenvalue is simple, real positive and its eigenvector φ_k is the so-called fundamental flux. Hence, the system of in-hour equations in (20) simplifies to a single equation which we write as

$$\rho_k = \omega\left(\Lambda_\alpha + \sum_p \frac{\Gamma_{p,\alpha}}{\omega + \lambda_p}\right), \tag{36}$$

where, to stress the fact that the equation has N_p+1 roots of which only one is the original alpha eigenvalue, we have replaced α with ω and we have used the lower index α to indicate that the coefficients Λ and Γ_p depend on the eigenvector ψ_α.

The in-hour equation can have complex roots and we refrain here from considering this case. But, as shown in Appendix C, if the coefficients Λ_α and the $\Gamma_{p,\alpha}$ in the in-hour equation have the same sign, which we take to be positive, then all the N_p+1 roots are real. Therefore, since the associated steady-state adjoint flux $\varphi_k^\dagger$ is positive, we shall consider only the case when the alpha eigenvector ψ is also positive. Note that this implies that the eigenvalue α is real. This is in fact the more clear-cut and best understood example of flux clustering.

A substantial argument in support of flux clustering can be made by looking for alpha modes with fluxes close to the fundamental static flux φ_k. We proceed by writing the flux perturbation formula, Eq. (22), in the form

$$\psi_\alpha = (1 + \varepsilon)\varphi_k + \psi^\perp, \tag{37}$$

where $|\varepsilon| \ll 1$ and where we have adopted the normalizations $||\varphi_k|| = ||\psi_\alpha||$. Next, we use this expression to compute the coefficients in the in-hour equation Eq. (36) and observe that in the leading term in ε, the coefficients depend only on the static flux φ_k. The reason is that $\left\|\psi^\perp\right\| \sim \sqrt{\varepsilon}$. As an aside, we point out that another reason for neglecting $\psi^\perp$ is that the coefficients depend on integrals of a product of a positive function times ψ_α and that the impact of $\psi^\perp$ in the value of the integrals is further reduced because, as opposed to φ_k, $\psi^\perp$ must necessarily change sign.

Hence, to leading order in ε, we might conclude that Eq. (36) is independent of ψ_α and also of small variations in ε. Since this equation has N_p+1 real roots we can safely assume that each one of these roots corresponds, to order ε, to an alpha eigenvalue. However, there are two conundrums regarding the precedent conclusion. The first one is that if the in-hour equation were to depend only on φ_k, then this flux will be a solution of the equation, but the only case in which this might happen is for $k = 1$ which entails, of

course, $\alpha = 0$. The second problem arises from the fact that the inhour equation is only a necessary condition for (α,ψ_α) to be an eigenpair of the alpha eigenvalue problem. Hence, the problem has to be resolved with a simultaneous consideration of both the inhour equation and the original alpha eigenvalue equation. For the present approach this involves showing that solutions of the form in Eq. (37) are truly solutions of the alpha eigenvalue problem. This is what, in a limited way, Henry did for the two-group P1 equation. A more general approach may consist perhaps of using a direct perturbation analysis between the alpha eigenvalue equation and the equation satisfied by φ_k.

Finally, we observe that the leading eigenvalue α_1 dominates the alpha spectrum and consequently it has a positive flux. It remains to show, however, that the fluxes of the other N_p dominant eigenvalues α_p,$p = 2$,N_p are also positive, a fact that is confirmed by previous speculations and by all our calculations. In view of formula (37), this could perhaps be demonstrated by a dominance argument.

4. Numerical results

We have used finite differences to discretize the multigroup diffusion alpha eigenvalue equation in a 1D slab geometry as well as the eigenvalue equations for the quasi-static equation and its adjoint, and implemented three different criteria, all based on the L_2 norm $\left\|\psi_{ref}-\psi_\alpha\right\|_2 = \sqrt{\sum_{g,r}(\psi_{ref}-\psi_\alpha)^2_{g,r}} < \varepsilon_{clus}$, to explore flux clustering about alpha modes ($\psi_{ref} = \psi_{\alpha'},\ \forall\alpha'$), about the modes of the quasi-static equation ($\psi_{ref} = \varphi_\lambda,\ \forall\lambda$) and by using perturbation analysis $\|\psi_\perp\|_2, |1-a| < \varepsilon_{clus}$, where the latter formula has been obtained from Eqs. (22) and (23) for the case of a non degenerated eigenvalue ($N_\lambda = 1$). Calculations are performed in double precision by a Python module (v.2.7), using the numerical numpy library (v.1.11.0). Our program solves the multigroup diffusion, rod geometry and discrete ordinates transport equations in a 1D heterogeneous slab for the α and λ eigenvalue problems with reflection, periodic and void boundary conditions; the full set of eigenpairs is computed from the linear set of equations in (5).

We have analyzed a large number of problems for the infinite homogeneous case as well as for some finite cases with 1, 8 and 281 energy groups and for increasing values of N_r. Flux weighting was used to homogenize and collapse the cross-sections for a PWR fuel assembly at different conditions (see Table 1). Thus, the corresponding α-sets are close. The calculations where done with 8 groups of precursors and 6 fissile isotopes ($N_p = 8$ and $N_i = 6$). We present here a sample of the results.

For all cases in Table 1, the neutron flux components of the ψ_α corresponding to the dominant eigenvalues α_p clustered within $\varepsilon_{clus} = 10^{-2}$. The dominant eigenvalues for cases 3 and 4 are reported in Tables 2 and 3, respectively.

Table 1
Physical conditions of the cross-section preparation in the PWR fuel assembly.

Case nb.	Tfuel (°C)	Tmod (°C)	Boron concentration (ppm)	ρ(pcm)
1	286	286	0	+6880.6
2	286	286	400	+3405.6
3	286	286	600	+1690.3
4	286	286	800	−9.3
5	650	306	0	+4915.5
6	650	306	400	+1624.2
7	650	306	600	+0.1
8	650	306	800	−1611.3
9	1100	306	600	−1302.5
10	1800	306	600	−3037.1

Table 2
Comparisons of the fundamental and delayed reactor periods with 1, 8 and 281 energy groups for case 3 ($k_\infty = +1.017200$).

α's	Relative difference (%)	
281G	8G	1G
+5.8029093620e + 02	−25.514	+0.214
−1.2552000351e − 02	−0.033	+0.002
−2.9640277111e − 02	−0.235	−0.074
−4.3562900973e − 02	−0.139	−0.005
−1.4048345489e − 01	−0.282	−0.030
−3.2792305224e − 01	−0.680	−0.118
−7.0546045788e − 01	−0.379	−0.054
−1.7081304062e + 00	−0.301	−0.041
−3.6271274472e + 00	−0.139	−0.027

Table 3
Comparisons of the fundamental and delayed reactor periods with 1, 8 and 281 energy groups for case 4 ($k_\infty = +0.999910$).

α's	Relative difference (%)	
281G	8G	1G
−1.4397459518e − 03	+4.003	+2.054
−1.4020587820e − 02	+0.056	+0.171
−3.7787664954e − 02	−0.011	−0.133
−8.2605497512e − 02	+0.023	−0.063
−2.0561160002e − 01	−0.016	+0.056
−5.9302199351e − 01	−0.019	−0.016
−1.4945472270e + 00	−0.034	−0.011
−3.4222886970e + 00	−0.017	+0.014
−2.6351110679e + 02	−35.019	−0.972

Table 4
Eigenvalue clustering in the delayed spectrum for increasing number of spatial cells, one energy group, case 4 (α eigenvalues as x.xx+y are to be read as x.xxe+y).

$N_r = 1$	$N_r = 2$	$N_r = 4$
−1.3821081 − 3	−1.3821081 − 3	−1.3821081 − 3
	−1.2466691 − 2	−1.2466692 − 2
		−1.2466698 − 2
		−1.2466699 − 2
−1.4012729 − 2	−1.4012729 − 2	−1.4012729 − 2
	−2.8291558 − 2	−2.8291579 − 2
		−2.8291665 − 2
		−2.8291679 − 2
−3.7791806 − 2	−3.7791806 − 2	−3.7791806 − 2
	−4.2524306 − 2	−4.2524320 − 2
		−4.2524377 − 2
		−4.2524386 − 2
−8.2586186 − 2	−8.2586186 − 2	−8.2586186 − 2
	−1.3304127 − 1	−1.3304138 − 1
		−1.3304182 − 1
		−1.3304189 − 1
−2.0564488 − 1	−2.0564488 − 1	−2.0564488 − 1
	−2.9246435 − 1	−2.9246477 − 1
		−2.9246649 − 1
		−2.9246678 − 1
−5.9313437 − 1	−5.9313437 − 1	−5.9313437 − 1
	−6.6648497 − 1	−6.6648537 − 1
		−6.6648702 − 1
		−6.6648730 − 1
−1.4950512 + 0	−1.4950512 + 0	−1.4950512 + 0
	−1.6347760 + 0	−1.6347767 + 0
		−1.6347797 + 0
		−1.6347803 + 0
−3.4228559+0	−3.4228559 + 0	−3.4228559 + 0
	−3.5545951 + 0	−3.5545958 + 0
		−3.5545988 + 0
		−3.5545993 + 0
−3.5578919 + 2	−3.5578919 + 2	−3.5578919 + 2
	−1.1008588 + 7	−1.2897302 + 7
		−4.4033287 + 7
		−7.5169271 + 7

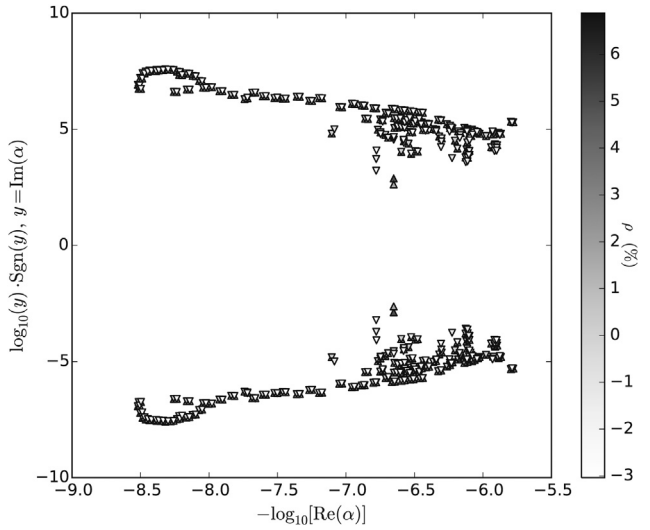

Fig. 2. Distribution on the complex plane of the prompt eigenvalues with 281 groups for the cases in Table 1.

By increasing the number of regions, the delayed eigenvalues cluster very close to the negative decay constants and are only clearly visible for the one-group calculation, as shown in Table 4. The table also shows that the dominant eigenvalue of the clustering, α_p, does not change with the number of regions.

As we show next, this follows from the fact that an infinite homogeneous medium sustains a uniform flux solution, regardless of the spatial discretization. The equation describing the energy spectrum of the uniform solution results from setting the spatial derivatives in Eq. (8) to zero:

$$\left(\frac{\alpha}{\nu}+\Sigma-\mathcal{H}-\overline{\mathcal{P}}\right)\psi_\alpha=-\mathcal{K}_\alpha\psi_\alpha,\quad \alpha\in\mathbb{C}\backslash\Lambda,$$

This equation is independent of the spatial discretization, be it continuous or not, and therefore its solutions are present for any value of N_r. Moreover, according with the analysis in the Flux clustering section, these uniform solutions appear in a cluster which contains all the N_p+1 leading modes.

Contrary to the few group cases, complex eigenvalues appear with 281 groups in the infinite homogeneous problem (i.e. one spatial cell and zero current at the boundary), and for different reactivities, see Fig. 2. The distribution of the prompt eigenvalues is in general weakly influenced by the reactivity.

Table 5
Eigenvalues with the relative difference (%) to Asahi's results: delayed spectrum (left), prompt spectrum (right).

$\alpha_{1,(\cdot)}$	Relative difference (%)	$\alpha_{2,(\cdot)}$	Relative difference (%)
−0.000009	—	-6.593×10^{1}	+0.046
−0.095135	$-3.307e-04$	-1.340×10^{3}	+0.027
−0.098363	$-2.959e-04$	-3.957×10^{3}	−0.084
−0.099205	$-4.805e-04$	-8.107×10^{3}	−0.040
−0.099536	$-2.496e-04$	-1.382×10^{4}	+0.153
−0.099697	$+3.656e-04$	-2.098×10^{4}	−0.076
−0.099788	$-3.637e-04$	-2.790×10^{4}	+14.352
−0.099843	$-2.955e-05$	-2.961×10^{4}	+0.033
−0.099879	$+2.620e-04$	-3.205×10^{4}	−0.160
−0.099904	$+3.194e-04$	-4.114×10^{4}	+15.417
−0.099922	$+3.322e-04$	-5.168×10^{4}	−0.037
−0.099936	$-2.921e-04$	-5.736×10^{4}	−0.071
−0.099946	$-9.027e-05$	-6.038×10^{4}	+0.962
−0.099954	$-1.342e-04$	-6.950×10^{4}	−5.892
−0.099960	$+1.894e-04$	-8.366×10^{4}	−0.044
		-9.781×10^{4}	+0.006

5. Comparison with Asahi's results

Asahi applied a continuous space description to the one-group, one precursor problem and computed results for a symmetric reflected critical slab reactor with a central core of half width $a=10$ cm surrounded by two reflectors of width $b=10$ cm [6]. He computed the first 15 eigenvalues in the delayed spectrum and the first 16 in the prompt spectrum by progressively increasing the number of zeros of the associated fluxes. Asahi presented his results with 6 and 3 digits, respectively, for the delayed and prompt eigenvalues.

We have used our numerical approach to recalculate Asahi's reactor by subdividing each cm into M equal regions, for a total of $N_r=40\times M$ spatial DOF, and by gradually increasing M until convergence. For $M=32$ the corresponding delayed and prompt eigenvalues (15+16), out of a total of $N_{DOF}=2560$ eigenvalues, converged to 6 digits and their associated fluxes exhibit the same number of zeros as those from Asahi's. Table 5 shows our 31 eigenvalues and the relative difference in % to the Asahi's values. Note that there are large differences in the prompt eigenvalues. We think that some of Asahi's values lacked precision. Our results prove that, as the number of DOF increases, our numerical technique approaches the more and more closely the full spectrum of the operator.

6. Conclusions

We have presented theoretical arguments about the alpha eigenvalue problem in multigroup neutron diffusion, in support of the general behavior observed in our calculations including the distribution of the prompt and delayed spectrum as well as flux clustering. Our analysis and numerical results confirm the few theoretical and numerical results found in the literature regarding the diffusion problem.

We have used a perturbation formulation, based on the steady state eigenvalue problem of the effective multiplication factor, to derive a generalized form of the in-hour equation. As opposed to previous derivations of the in-hour equation, which have been derived by projection of the original alpha equation, in our formulation this equation arises as a necessary and sufficient condition for the existence of the alpha eigenvalue-eigenvector pair.

We have also conducted many numerical simulations for one-dimensional homogeneous and heterogeneous configurations in multigroup diffusion theory. In all cases, our numerical results support the theoretical predictions.

The characterization of the alpha modes in multigroup neutron transport is deferred to a future study.

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Appendix A. Analysis of the one-group, homogeneous case

The analysis for the one-group case is made especially simple because $\chi_i=\chi=1$ and one can add all fissile isotopes into a single one with $\nu\Sigma_f=\sum_i \nu\Sigma_{f,i}$. Moreover, for a homogeneous medium we can also define $\beta_p=\sum_i \beta_{i\to p}\nu\Sigma_{f,i}/\nu\Sigma_f$ and cast Eq. (8) into the simplified form

$$f(\alpha)\psi = -\overline{\beta}\psi, \tag{38}$$

where

$$f(\alpha) = \frac{\alpha}{v} + \sum_p \beta_p \frac{\alpha}{\alpha + \lambda_p} \nu\Sigma_f, \tag{39}$$

and $\overline{\beta}$ is the diffusion operator with steady-state neutron fission spectrum (unity in the present case). Finally, using the boundary conditions one can construct the eigenfunctions of problem $\overline{\beta}\psi_\zeta = \zeta\psi_\zeta$ and then any (α, ψ_ζ), where α is a root of

$$f(\alpha) = \zeta \tag{40}$$

is an alpha eigenpair.

Consider a homogeneous slab of thickness a. For the case with zero flux boundary conditions, one has the eigenfunctions $\psi(z) \sim \sin(B_n z)$ and the eigenvalues

$$\zeta_n = \nu\Sigma_f - \Sigma_a - DB_n^2,$$

where $B_n = (n+1)\pi/a$. Note also that

$$\zeta_n = -\rho_n \nu\Sigma_f,$$

where $\rho_n = 1 - 1/\lambda_n$ is the generalized reactivity associated to the classical reactor eigenvalues λ_n.

There are $N_p + 1$ roots of (40) and they split into $N_p + 1$ different groups; new roots are added progressively to each group as n increases. We show next that the higher N_p groups cluster on the right of each $-\lambda_p$, but for the group at the left of $-\lambda_{Np}$, the eigenvalues decrease without bounds towards $-\infty$.

We examine first the behavior of the α's that are close to $-\lambda_p$ so that $\alpha + \lambda_p = \varepsilon$ with $|\varepsilon| \ll 1$ (this assumption will be proved by the following analysis). For these α's the critical condition (40) can be written to leading order in ε as $-\beta_p \lambda_p \nu\Sigma_f \varepsilon^{-1} = \zeta_n$, where now ε plays the role of the eigenvalue α. The solution is

$$\varepsilon_n = -\frac{\beta_p \lambda_p \nu\Sigma_f}{\zeta_n} \rightarrow \alpha_n = -\lambda_p \left(1 - \frac{\beta_p \nu\Sigma_f}{\zeta_n}\right).$$

For increasing n, ζ_n becomes negative and increases as $(n+1)^2$ so that the factor between parentheses remains positive but diminishes very fast towards 1. Remember that we have assumed ε_n to be small, which implies $|\zeta_n| \gg \beta_p \lambda_p \nu\Sigma_f$. Clearly, this can only happen if $\zeta_n < 0$.

Consider, finally, the case with $\alpha \ll -\lambda_{N_p}$. Here we can neglect precursor contributions and write $\alpha = v\zeta$, which implies that ζ is negative. Note that in this case the first ζ of this group is the smallest root of (40) for $n = 0$, which we know is $\ll -\lambda_{N_p}$. Here we have

$$\alpha_n - \alpha_{n-1} = vD\left(\frac{\pi}{a}\right)^2 (2n+1).$$

This implies that the distance between two successive eigenvalues in this group increases with n and that $\lim_{n\to\infty} \alpha_n = -\infty$. It follows that the eigenvalues in this group do not cluster.

Appendix B. Asahi problem revisited

The simple technique in Appendix A can be extended to a general analysis of a piecewise homogeneous slab geometry. The basic idea is to use the Laplacian eigenfunctions in each homogeneous piece and impose interface and boundary conditions in order to obtain a general solution for the problem which is then replaced in Eq. (38). Unfortunately, as we show next, this leads to a complicated system of trigonometric equations for the determination of the alpha spectrum.

As an example of this analytical approach we consider the Asahi problem discussed in *Comparison with Asahi's results*. This problem contains a central core of width $2a$ and a bilateral reflector of width b. The domain is symmetric with respect to the middle plane. We shall treat only the right half of the domain for $z \in [0, a+b]$, with vacuum boundary conditions on the right at $z = a+b$ and either the current or the flux vanishing on the left at $z = 0$. The latter conditions are necessary because the initial problem is symmetric and therefore accepts even and odd solutions. Given the boundary conditions, the solutions are $\psi_c(z) \sim f_c(B_c z)$ for $z \in [0, a]$ and $\psi_r(z) \sim f_r(B_r(a+b-z))$ for $z \in [a, a+b]$. The core function f_c can be either a cosine or a sine, depending on whether the alpha eigenfunction is symmetric or antisymmetric, while f_r is a sine. We impose continuity of the flux and current at the core-reflector interface $z = a$:

$$A_c f_c(B_c a) = A_r f_r(B_r b),$$
$$A_c D_c B_c f_c'(B_c a) = -A_r D_r B_r f_r'(B_r b),$$

where the A's are two constants and f' is the derivative of f. Dividing the second equation by the first we get the dispersion relation:

$$D_c B_c \widehat{f}_c(B_c a) = B_r D_r \widehat{f}_r(B_r b). \tag{41}$$

Here $\widehat{f}_r$ is the cotangent function while $\widehat{f}_c$ is the tangent function for the symmetric solution or minus the cotangent for the antisymmetric one.

We have now a solution that satisfies boundary and interface conditions with B_c and B_r constrained by Eq. (41). Next, we replace our solution in the alpha eigenvalue Eq. (38) to obtain

$$\begin{cases} f(\alpha) = \nu\Sigma_f - \Sigma_{a,c} - D_c B_c^2, & \text{(a)} \\ \dfrac{\alpha}{v} = -\Sigma_{a,r} - D_r B_r^2, & \text{(b)} \end{cases} \tag{42}$$

where $f(\alpha)$ has been defined in (39).

Equation (41) and the two latter equations form a system of nonlinear equations for the triplet (α, B_c, B_r). We now proceed to eliminate B_c and B_r and obtain a final equation for α. From the two equations in (42) we obtain:

$$B_r^2 = -\frac{\alpha + \nu\Sigma_{a,r}}{\nu D_r},$$
$$B_c^2 = -\frac{f(\alpha) + \nu\left(\Sigma_{a,c} - \nu\Sigma_f\right)}{\nu D_c}, \tag{43}$$

and use of these expressions in the dispersion relation results in a nonlinear equation $F(\alpha) = 0$ for α. In practice one might proceed with a zero search for this nonlinear equation, where given a value of $\alpha \in \mathbb{R}$, one evaluates B_r and B_c via relations (43) and, then calculates $F(\alpha)$ as the difference between the left minus the right hand sides of Eq. (41).

Clearly, $B_r = 0$ is a singular point at which the solution vanishes in the reflector and in the core. Note that B_r^2 is negative for $\alpha > -\nu\Sigma_{a,r}$, in which case the cotangent $\widehat{f}_r$ becomes a hyperbolic cotangent and the reflector flux, which can be taken as positive, decreases from the interface to vanish at the boundary. This case, for which the dispersion relation is easy to solve, at least graphically, corresponds to the delayed spectrum calculated by Asahi, whose eigenfunctions have no zeros in the reflector. In the opposite

case, with $B > 0$ or, equivalently, with $\alpha < -\nu\Sigma_{a,r}$, the flux in the reflector can change sign. This is the case of Asahi's prompt spectrum. The numerical analysis of Asahi's problem is further simplified because of the simple form of $f(\alpha)$ for the case of a single precursor, but we do not pursue this development further here.

Appendix C. Roots of the generalized Nordheim equation

Equation (20) is the condition for the existence of the eigenpair (α,ψ_α). We write this equation in the form $\rho = \rho(\omega)$:

$$\rho = \omega\left(\Lambda + \sum_p \frac{\Gamma_p}{\omega + \lambda_p}\right),$$

where the $\Lambda(\psi_\alpha)$ and $\Gamma_p(\psi_\alpha)$ are defined in Eq. (23). The above equation can be written as a polynomial in ω of order $N_p + 1$ and therefore has as many roots but not all necessarily real. We assume that Λ and the Γ_p 's are bounded and that $\Gamma_p \neq \Gamma_{p'}$ for $p \neq p'$. To simplify the analysis, we shall assume that these coefficients are real and positive. Under these assumption we show that for any $\rho \in \mathbb{R}$ the equation has exactly $N_p + 1$ real distinct roots. As an aside, we recall that for $\rho = \rho_\lambda$ one of the roots must be $\omega = \alpha$.

Let $\mathbb{R}_0 = \mathbb{R}\backslash\Lambda$ be the real line excluding the N_p points $\Lambda = \{-\lambda_p, p = 1, N_p\}$. We note that $\rho(\omega)$ is C_∞ over $\mathbb{R}_0$. It is clear that every one of these points is a vertical asymptote. Let $\varepsilon > 0$, then for $\varepsilon \to 0$ we find that $\rho(-\lambda_p \pm \varepsilon) \to \mp\lambda_p\Gamma_p/\varepsilon$. Therefore, $\rho(\omega)$ goes to $-\infty$ at the right of the asymptote and to ∞ at its left. Moreover, the derivative

$$\partial_\omega\rho = \Lambda + \sum_p \frac{\lambda_p\Gamma_p}{(\omega + \lambda_p)^2}$$

shows that, $\rho(\omega)$ is a monotonously increasing function in $\mathbb{R}_0$. The roots of $\rho(\omega) = 0$ give the locations at which the function changes sign. Note that there is a single root in each interval $(-\lambda_{p+1}, -\lambda_p)$ for $p = 1, N_p - 1$. Clearly $\omega = 0$ is another root and, since the function monotonously increases, there are no roots for strictly positive ω. Next, we check the behavior as $\omega \to \pm\infty$ to find that, for large ω, $\rho(\omega) \to \omega\Lambda$. Therefore there is a last root at some value smaller than $-\lambda_{N_p}$. The general aspect of the graph is depicted in Fig. 3.

Let us discuss what happens when not all of the coefficients are positive. Assume that only one, say Λ, is negative. This changes the behavior for $\omega \to \pm\infty$ and now we find that $\rho(\omega) \to \mp\infty$ for $\omega \to \pm\infty$. This agrees with the fact that presently the derivative has two zeros. Hence, $\rho(\omega)$ has a positive minimum $\rho_{min} > 0$ for $\omega < -\lambda_{N_p}$ and a positive maximum $\rho_{max} < \rho_{min}$ for $\omega > -\lambda_1$. The number of roots is $N_p + 1$ except for $\rho \in (\rho_{max}, \rho_{min})$ where it is $N_p - 1$. Note that for $\rho = \rho_{max}$ or $\rho = \rho_{min}$ there is a double real root.

Finally, we consider the case when the coefficient Γ_p is negative for one intermediary p value, while all other coefficients remain positive. Here a positive minimum $\rho_{min} > 0$ appears in the interval $(-\lambda_{p+1}, -\lambda_p)$ while a positive maximum $\rho_{max} < \rho_{min}$ appears in the interval $(-\lambda_p, -\lambda_{p-1})$. The discussion is similar to the previous case. We left the analysis of more complicated cases, where more than one coefficient is negative, to the interested reader.

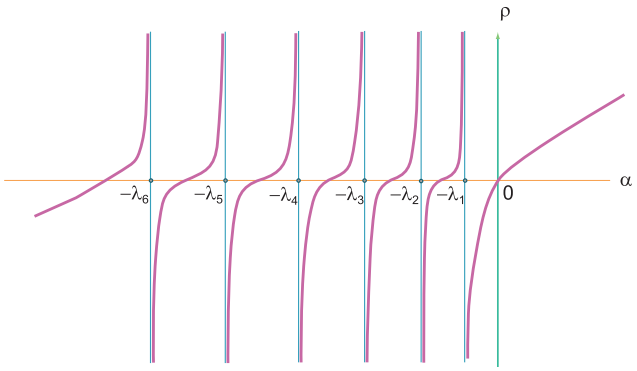

Fig. 3. Sketch of generalized Nordheim in-hour equation for $N_p = 6$.

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