ON PERTURBATION THEORY AND REACTOR KINETICS: FROM WIGNER'S PILE PERIOD TO ACCELERATOR DRIVEN SYSTEMS

D.G. CACUCI
Forschungszentrum Karlsruhe (FZK)
Institute for Reactor Safety (IRS)
76021 Karlsruhe, Germany
cacuci@irs.fzk.de

ABSTRACT

This Eugene P. Wigner Keynote Lecture at the PHYSOR 2002 International Meeting in Seoul, Korea, addresses the fundamental basis for formulating the equations that model the time and space-dependent behavior of an Accelerator Driven Sub-Critical Core System (ADS), and highlights the limited applicability to ADS of the traditional Wigner-type perturbation theory formulation of neutron kinetics. In particular, a paradigm ADS neutron-kinetics model is presented, and its exact solution is compared with the incomplete results produced by the traditional approaches originally developed for critical reactors. It is shown that the exact ADS-model is basically non-perturbative; consequently, the exact model cannot be obtained by using the traditional perturbation theory-based approaches as developed originally for critical reactors. In particular, the point-kinetics equations obtained in previous works by using traditional perturbation theory methods are shown to be inadequate for describing the space- and time-behavior of the neutron distribution in the target and the dynamic phenomena at the interface between the ADS target and the ADS sub-critical core regions. In retrospect, this conclusion is not surprising, since the problem for a critical reactor is that of maintaining and controlling a self-sustained reaction (much like treating small perturbations around equilibrium in a self-sustaining harmonic oscillator), whereas the problem for an ADS should be that of optimal control (however complicated) of an externally driven system (much like an externally driven oscillator). Not only physically, but also mathematically, the two problems are fundamentally distinct: mathematically, the critical reactor is described by a homogeneous eigenvalue problem for the non-zero (self-sustaining) flux solution, whereas the ADS is described by an inhomogeneous problem where the corresponding homogeneous problem should by design admit only the identically zero flux solution. This is the basic reason why, for example, it is quite difficult to find a practically useful "fictitious ADS steady-state", which is required by the traditional perturbation-theory-based methods to work.

In this Wigner Keynote Lecture, a new conceptual framework is proposed for treating an ADS, by adopting an optimal control theory point of view rather than the traditional perturbation theory point of view. This new conceptual framework encompasses not only the time- and space behavior of the coupled neutron kinetics but also the ADS thermal-hydraulic balance equations, and is based on optimization and optimal control of ADS operational objectives, which would include minimization of local flux disturbances, load and source following, etc. In particular, this new conceptual framework makes no use of a "fictitious ADS steady-state", as required by the traditional approaches, and, also in contradistinction to the traditional approaches, delivers the correct and complete (i.e., including sources) adjoint equations, without leaving any room for ambiguities. Thus, this new conceptual framework provides a natural basis for developing new computational methods,

specifically tailored for the control and operation of ADS. It also follows that traditional experiments will have limited relevance to the actual operation and control of full-size ADS systems; this is because traditional experiments are also based on traditional methods, which were designed for critical reactors rather than ADS. Hence, the need for complementary, appropriately focused experiments and new computational methods, relevant for the operation and control of ADS, also becomes apparent within the optimal-control-based conceptual framework proposed here for treating ADS.

1. INTRODUCTION

I am very pleased and honored to have the opportunity of presenting the Eugene P. Wigner Keynote Lecture on the occasion of the PHYSOR 2002 International Meeting in Seoul, Korea. As is well known, reactor physics was not the only topic of interest to Wigner, but it was certainly a topic in which he left an everlasting mark. Given the high level of current interest for describing the time-dependent behavior of Accelerator Driven Sub-Critical Systems (ADS), it seems particularly appropriate to revisit Wigner's seminal introduction into reactor physics of perturbation theory and adjoint operators for the space- and time-dependent neutron balance equations for a critical reactor. Wigner did this in his originally classified Manhattan Project document CP-G 3048, dated June 13, 1945, and entitled "Effect of Small Perturbations on Pile Period" (see also Wigner, 1992). Noteworthy is also the fact that Wigner was the first to interpret physically the adjoint functions as "importance functions", in this same article. Referring to the critical reactor (in the jargon of those days) as the "pile", Wigner's stated purpose was "to find a method for calculating the effect of small perturbations on composite piles and to separate the effects on fast, resonance and slow neutrons". He showed that the effects of small changes in a critical reactor can be calculated to first-order changes in the flux most easily by solving the "adjoint of the pile equation". Wigner thus introduced the definition of an "adjoint neutron density", depending on the position and the energy of the neutron, and showed that "the weight factor for a perturbation is the product of the ordinary neutron density and the adjoint density". Wigner focused his perturbation theory procedure on calculating the changes in the "pile period" caused by the introduction of small amounts of extraneous materials into the pile, such as impurities, additional fissionable material, etc. For benchmark purposes, Wigner explicitly developed the adjoint equation both for the one- and two- group "pile theory", and solved them for a "simple pile without reflector".

This Wigner Keynote Lecture is organized as follows: In Sec. 2, Wigner's seminal ideas on the use of perturbation theory and adjoint operators to calculate reactivity coefficients, which were originally called "danger coefficients", will be revisited in order to highlight the profoundness of his insightful analysis of a critical reactor. In the jargon of that time, Wigner generally observed that the effect of small perturbations (localized impurities, etc.) on the pile is important not only because of the theory of danger coefficient measurements but also because the effect of certain influences cannot be taken into account easily by any other than the perturbation method. Wigner's remarkable original report "endeavors to go beyond Fermi's simple theory which applies only to a uniform bare pile and recognizes only one kind of neutrons (thermal)".
Section 3 presents Wigner's eigenfunction expansion method using the adjoint eigenfunctions of a critical reactor which, together with his use of perturbation theory, provided the basis for designing both experiments and the world's first reactors. In particular, Wigner conceived the "pile oscillator" and the "multiplication-rate" techniques, which, along with the "exponential experiment" conceived by Fermi, still remain the classic experiments performed all over the world today.

Section 4 presents a paradigm ADS neutron kinetics model, which (for the first time) considers the ADS target and sub-critical core regions separately, in order to examine properly the time- and space-dependent dynamic effects of the spallation neutron source on the sub-critical core. The time- and space-dependent neutron balance equations, including the production of delayed neutrons in the sub-critical ADS core, are solved exactly, in order to highlight the fundamental properties of this exact solution. In particular, the exact solution highlights the importance of treating correctly the spallation source neutrons in the target region, and the coupling between the ADS target and sub-critical core regions. In Section 5, the exact solution is compared to results produced by the methods, based on the traditional perturbation theory-type approaches, which have recently been proposed for simulating the time-dependent behavior of an ADS. This comparison clearly highlights the limited applicability of traditional analysis methods and experiments (e.g., source importance, reactor oscillator techniques, source multiplication) to the operation and control of a full-power ADS. Thus, Section 6 presents a new conceptual framework for the development of computational methods specifically designed for ADS design, operation and control. This new conceptual framework uses optimization theory/optimal control in order to establish the proper mathematical equations for modeling the operation and control of an ADS. In particular, this new framework clearly shows that the form of the proper adjoint equations, including adjoint source terms, are derived unambiguously from the design objective, without the need to consider a “fictitious ADS steady-state”; all this is in contradistinction to the currently proposed methods based on traditional perturbation-theory as applied to critical reactors. Finally, the concluding remarks underscore the need for appropriately focused experiments and the development of new methods, specifically designed for the operation and control of an ADS.

2. WIGNER’S “GENERAL PERTURBATION THEORY”

Wigner’s remarkable insight is certainly worth citing in the original wording: “It was customary so far to express the effect of small perturbations as a change in the multiplication constant. However, this is a possible procedure only in the case of a uniform, bare pile. A composite pile, or even a simple pile with a reflector, has no single multiplication constant and it was thought best to express the effect of perturbations in terms of the change in reciprocal pile period”

Wigner considers homogeneous “pile equations” (i.e., equations for critical reactors) of the form

$$\frac{\partial n}{\partial t} = Mn \tag{1}$$

where the neutron density n is a function of the position, energy, and direction of the neutron velocity. Obviously, Eq. (1) applies to critical reactors. Wigner then solves Eq. (1) by considering solutions which depend on time exponentially and satisfy “characteristic value” (i.e., “eigenvalue”) equations of the form

$$Mn = \lambda n \tag{1a}$$

where λ is a constant. Noting that the reciprocal of λ is the “period of the pile”, Wigner demonstrates that λ is not unique, but that the steady solution of the critical pile satisfies the equation $Mn = 0$ corresponding to $\lambda = 0$, and underscores that one is interested in the largest λ, which for a critical reactor “is in the neighborhood of zero, all other λ of the pile being negative”.

Wigner then proposes to calculate the change in λ due to a change V in the pile equation, which "may be caused by the introduction of some additional absorber into the pile, or of a fissionable element or something similar”, and which would cause the perturbed, *yet still critical*, pile equation to become

$$(M+V)n' = \lambda' n' , \tag{2}$$

since the change V causes "a change in both the neutron distribution n, which will become n', and also in the period, which changes from λ to λ'".

At this point, Wigner makes the crucial observation that, "the above problem is very much the same as the one occurring in quantum mechanics where it is solved by the Rayleigh-Schrödinger perturbation theory", but with the difference "that M is not i times a self adjoint (Hermitian) operator". For this reason, Wigner considers, in addition to Eq. (1a), the adjoint equation

$$M^{+}N = \lambda N \tag{3}$$

where the operator M^{+} is defined by the equation

$$(\varphi, M\psi) = (M^{+}\varphi, \psi) \tag{4}$$

and where, in Wigner's original wording: "φ and ψ are two arbitrary functions satisfying the boundary conditions of the problem and M^{+} is defined so that (4) is valid for any such φ and ψ. The $(,)$ denotes the scalar product of the function before and after the comma, i.e., the integral over the product of both. Examples will be given later which show the way to find the adjoint M^{+} to a given M. If M is real, its characteristic values are in general the same as those of M^{+}. If M is complex, the characteristic values of M^{+} are conjugate complex to the characteristic values of M".

Wigner proceeds to show that

$$\lambda' = \frac{(N,(M+V)n')}{(N,n')} = \frac{(M^{+}N,n') + (N,Vn')}{(N,n')} = \frac{\lambda(N,n') + (N,Vn')}{(N,n')} = \lambda + \frac{(N,Vn')}{(N,n')} \tag{5}$$

and notes that "no approximation has been made to obtain (5) which gives an expression for $\lambda' - \lambda$", which, in Wigner's words: "is supposed to be a small quantity so that in the expression therefore one can replace n' by its unperturbed value n", to obtain

$$\lambda' - \lambda = \frac{(N,Vn)}{(N,n)} \tag{6}$$

Wigner's next remarks are fundamental to understanding the limitations of his perturbation-theory procedure, and will be reproduced here in their entirety: "It may be worth while to remark, for the sake of rigorous mathematics, that the extension of the full scope of the Rayleigh-Schrödinger theory is probably unjustified in general for arbitrary (e.g., not self-adjoint) operators M because it involves the assumption that the characteristic functions of M form a complete system. This is not true in general. On the other hand, the derivation of the first approximation (6) involved no such assumption. The only two assumptions that had to be made were that (N,n) shall not vanish and that n' approach n if V is made very small. The first assumption breaks down if λ is an elementary divisor and in this case, in fact, (6) is incorrect. One would notice this occurrence, however, when trying to use (6). For certain operators V, n' does not converge to n even if the coefficient of V converges to zero. This can occur for self adjoint M as well as in our case and examples for it are well known in quantum mechanics (action of weak uniform electric field on an atom). This possibility will be disregarded here, as it is not believed that it plays any role, just as it is quite customary to disregard it in quantum theory".

3. WIGNER'S EIGENFUNCTIONS EXPANSION METHOD FOR A CRITICAL REACTOR

Wigner also developed the fundamental experimental and computational methods for critical reactors, based on the use of the eigenfunctions of the adjoint operator M^+ introduced in Eq. (3); remarkably, Wigner's ideas and methods are still state-of-the-art today for critical reactors. It is convenient to present Wigner's eigenfunction expansion method in the general setting of the transport equation using, for convenience, the notation of Bell and Glasstone (1970), for the neutron flux with delayed neutrons:

$$\begin{aligned} &\frac{1}{\mathrm{v}}\frac{\partial}{\partial t}\varphi(\mathbf{r},E,\mathbf{\Omega},t)+\mathbf{\Omega}\cdot\nabla\varphi+\Sigma_t\varphi=\mathbf{S}\varphi+(1-\beta)\chi_p\mathbf{F}\varphi+\sum_i\chi_i\lambda_iC_i(\mathbf{r},t)+Q(\mathbf{r},E,\mathbf{\Omega},t)\\ &\frac{\partial C_i}{\partial t}+\lambda_iC_i=\beta_i\mathbf{F}\varphi \end{aligned} \quad (7)$$

where $Q(\mathbf{r},E,\mathbf{\Omega},t)$ is the external source, and where the scattering and fission operators are defined as

$$\begin{aligned} &\mathbf{S}\varphi\equiv\int_{\mathbf{\Omega}'}\int_{E'}\sum_{x\neq f}\Sigma_x(\mathbf{r},E'\to E,\mathbf{\Omega}'\to\mathbf{\Omega},t)\varphi(\mathbf{r},E',\mathbf{\Omega}',t)dE'\,d\mathbf{\Omega}'\\ &\chi_p(1-\beta)\mathbf{F}\varphi\equiv\frac{1}{4\pi}\int_{\mathbf{\Omega}'}\int_{E'}\chi_p(1-\beta)\nu(E')\Sigma_f(\mathbf{r},E',t)\varphi(\mathbf{r},E',\mathbf{\Omega}',t)dE'\,d\mathbf{\Omega}'\\ &\beta_i\mathbf{F}\varphi\equiv\frac{1}{4\pi}\int_{\mathbf{\Omega}'}\int_{E'}\beta_i\nu(E')\Sigma_f(\mathbf{r},E',t)\varphi(\mathbf{r},E',\mathbf{\Omega}',t)dE'\,d\mathbf{\Omega}' \end{aligned} \quad (8)$$

The equations for the adjoint flux and adjoint precursors corresponding to Eq. (7) are:

$$\begin{aligned} &-\frac{1}{\mathrm{v}}\frac{\partial}{\partial t}\varphi^+(\mathbf{r},E,\mathbf{\Omega},t)-\mathbf{\Omega}\cdot\nabla\varphi^++\Sigma_t\varphi^+=\mathbf{S}^+\varphi^++\left[\chi_p(1-\beta)\mathbf{F}\right]^+\varphi^+\\ &+\sum_i\beta_i\nu(E)\Sigma_f(\mathbf{r},E,t)C_i^+(\mathbf{r},t)+Q^+(\mathbf{r},E,\mathbf{\Omega},t)\\ &\frac{\partial C_i^+}{\partial t}+\lambda_iC_i^+=\lambda_i\int_{\mathbf{\Omega}}\int_{E}\chi_i(E)\varphi^+(\mathbf{r},E,\mathbf{\Omega},t)dE\,d\mathbf{\Omega} \end{aligned} \quad (9)$$

where $Q^+(\mathbf{r},E,\mathbf{\Omega},t)$ is an external source defined in terms of the specific response (e.g., multiplication factor, reaction rates, etc.) under consideration, and where

$$\begin{aligned} &\mathbf{S}^+\varphi^+\equiv\int_{\mathbf{\Omega}'}\int_{E'}\sum_{x\neq f}\Sigma_x(\mathbf{r},E\to E',\mathbf{\Omega}\to\mathbf{\Omega}',t)\varphi^+(\mathbf{r},E',\mathbf{\Omega}',t)dE'\,d\mathbf{\Omega}'\\ &\left[\chi_p(1-\beta)\mathbf{F}\right]^+\varphi^+\equiv\int_{\mathbf{\Omega}'}\int_{E'}\chi_p(E')(1-\beta)\nu(E)\Sigma_f(\mathbf{r},E,t)\varphi^+(\mathbf{r},E',\mathbf{\Omega}',t)dE'\,d\mathbf{\Omega}' \end{aligned} \quad (10)$$

Wigner introduced eigenfunction expansions for the neutron flux, external source, and precursors of the form:

$$\begin{aligned} &\varphi(\mathbf{r},E,\mathbf{\Omega},t)=\sum_j P_j(t)\,\varphi_j(\mathbf{r},E,\mathbf{\Omega})\;;\\ &C_i(\mathbf{r},E,\mathbf{\Omega},t)=\sum_j C_{ij}(t)\,\varphi_j(\mathbf{r},E,\mathbf{\Omega}); \end{aligned} \quad (11)$$

$$S(\mathbf{r}, E, \mathbf{\Omega}) = \sum_j S_j(t)\varphi_j(\mathbf{r}, E, \mathbf{\Omega});$$

where the quantities φ_j are eigenfunctions of an appropriate time-independent eigenvalue problem. In particular, Wigner discusses the use of: (i) the eigenfunctions of the homogeneous problem $L\varphi_j = \lambda_j \varphi_j$, obtained by considering time-dependent solutions of the form $\exp(\lambda_j t)$ for the transport equation, [cf. Eq. (1a); note that these "Wigner λ_j-modes" are nowadays called α_j-modes], and (ii) the eigenfunctions of the homogeneous problem

$$\mathbf{\Omega} \cdot \nabla \varphi_j + \Sigma_t \varphi_j - \mathbf{S}\varphi_j = \frac{1}{k_j} \chi \mathbf{F} \varphi_j \tag{12}$$

where the k_j-modes are the effective multiplication modes.

Wigner (see also Weinberg and Wigner, 1958) clearly states that neither the λ_j-modes nor the k_j-modes are necessarily complete or discrete; in particular, he clearly draws attention to the possible existence of continuum-modes. Assuming, however, that the expansion in Eq. (11) is formally valid, he forms the inner product of Eq.(7) with the eigenfunctions φ_j^+ of the adjoint homogeneous time-independent problem corresponding either to the eigenvalues k_j [i.e., the adjoint of Eq. (12)] or the eigenvalues λ_j of Eq. (3), and obtains the point kinetics equations:

$$\begin{aligned} \frac{dP_j(t)}{dt} &= \frac{\rho_j - \beta_{j,eff}}{\Lambda_j} P_j(t) + \sum_i \lambda_i C_{ij,eff}(t) + S_{j,eff}(t) \\ \frac{dC_{ij,eff}(t)}{dt} &+ \lambda_i C_{ij,eff}(t) = \beta_{ij,eff} P_j(t) \end{aligned} \tag{13}$$

where:

$$\begin{aligned} &\Lambda_j \equiv \frac{1}{F_j}\left\langle \varphi_j^+ \frac{1}{\mathrm{v}} \varphi_j \right\rangle; \quad \rho_j \equiv \frac{1}{F_j}\left\langle \varphi_j^+ \left(-\mathbf{\Omega} \cdot \nabla \varphi_j - \Sigma_t \varphi_j + \mathbf{I}\varphi_j + \chi \mathbf{F} \varphi_j \right) \right\rangle \\ &\beta_{j,eff} \equiv \frac{1}{F_j}\left\langle \varphi_j^+ \sum_i \chi_i \beta_i \mathbf{F} \varphi_j \right\rangle; \quad \beta_{ij,eff} \equiv \frac{1}{F_j}\left\langle \varphi_j^+ \chi_i \beta_i \mathbf{F} \varphi_j \right\rangle \\ &C_{ij,eff}(t) \equiv \frac{1}{\Lambda_j F_j}\left\langle \varphi_j^+ \chi_i C_i(\mathbf{r}, t) \right\rangle; \quad S_{j,eff} \equiv \frac{1}{\Lambda_j F_j}\left\langle \varphi_j^+ S \right\rangle; \quad F_j \equiv \left\langle \varphi_j^+ \chi \mathbf{F} \varphi_j \right\rangle \end{aligned} \tag{14}$$

The equations above form the basis of practically all of the computational and experimental methods currently used for analyzing issues pertinent to critical reactors; such applications include pulsed-source, reactor oscillator, neutron burst, neutron wave, source multiplication, and importance experiments.

4. A PARADIGM ACCELERATOR DRIVEN SYSTEM (ADS) NEUTRON-KINETICS MODEL

Several authors (e.g.: M. Carta, and A. D'Angelo, 1999; TRADE Final Feasibility Report, 2002; I. Slessarev and A. Tchistiakov, 1997; M. Salvatores, et al, 1997, Gandini and Salvatores, 2002) have proposed investigations of Accelerator Driven Sub-Critical Systems (ADS) by using methods that are fundamentally based on the use of the eigenfunctions expansions and perturbation theory a la Wigner, as presented in the previous section. These authors postulate the existence of "an appropriate homogeneous fictitious steady-state eigenvalue problem", based on Eq. (9) or (in a simplified version) on the adjoint of Eq. (12), such that this fictitious problem can be adjusted to represent the adjoint of a sub-critical "fictitious steady state description of the ADS". In order to investigate the merits of these approaches, this section presents a paradigm ADS Neutron Kinetics Model that can be solved exactly. The exact solution obtained in this section will then be compared, in Sec. 5, with the solution that would be obtained by using the approaches advocated by the authors mentioned above.

Thus, consider a paradigm ADS-Model, in which the accelerator beam produces spallation neutrons in a cylindrical target of radius a and extrapolated height z_o, which is surrounded by a sub-critical multiplying core having the form of a bare cylindrical shell of inner radius a, extrapolated outer radius b, and extrapolated height z_o. For simplicity, the target is considered to consist of non-multiplying material (e.g., lead, tungsten, etc.) although multiplying material (e.g., depleted uranium) could equally well be considered. The protons from the accelerator beam give rise in the target to a volumetric source of (fast) neutrons, denoted by $Q(r,z,t)$. For the purposes of this paradigm ADS Model, it suffices to consider that the distribution of neutrons is described by the time-dependent, one-energy-group diffusion equation, which takes on the following forms:

- In the ADS-target region (superscript t):

$$\begin{cases} \dfrac{\partial N^t}{\partial t} = \mathrm{v}D^t\nabla^2 N^t(r,z,t) - \mathrm{v}\Sigma_a^t N^t(r,z,t) + Q(r,z,t); \quad 0 < r \le a, \quad t > 0 \\ N^t(r,z,t) = \text{finite everywhere, including at } r = 0, \quad t > 0 \\ N^t(r,0,t) = 0; \quad at\ z = 0, t > 0 \\ N^t(r,z_o,t) = 0; \quad at\ z = z_o, t > 0, \\ N^t(r,z,0) = 0, \quad at\ t = 0, \\ \nabla^2 \equiv \dfrac{\partial^2}{\partial r^2} + \dfrac{1}{r}\dfrac{\partial}{\partial r} + \dfrac{\partial^2}{\partial z^2} \end{cases} \tag{15}$$

- In the ADS sub-critical core region (superscript c):

$$\begin{cases} \dfrac{\partial N^c}{\partial t} = \mathrm{v}D^c\nabla^2 N^c(r,z,t) - \mathrm{v}\Sigma_a^c N^c(r,z,t) + \mathrm{v}(1-\beta)k_\infty^c\Sigma_a^c N^c(r,z,t) \\ + \sum_i \lambda_i C_i(r,z,t); \quad a \le r \le b, t > 0, \\ \dfrac{\partial C_i}{\partial t} + \lambda_i C_i(r,z,t) = \mathrm{v}\beta_i k_\infty^c \Sigma_a^c N^c(r,z,t), \quad i = 1,\ldots,I; \\ N^c(b,z,t) = 0, \quad t > 0, \\ N^c(r,0,t) = 0, \quad at\ z = 0, \quad t > 0, \\ N^c(r,z_o,t) = 0, \quad at\ z = z_o, \quad t > 0, \\ N^c(r,z,0) = 0, \quad C_i(r,z,0) = 0, \quad at\ t = 0. \end{cases} \tag{16}$$

- Interface conditions (continuity of flux and current) at $r = a$, between the target and the sub-critical core:

$$D^t \frac{\partial N^t}{\partial r} = D^c \frac{\partial N^c}{\partial r}, \quad and \quad N^t(r,z,t) = N^c(r,z,t), \quad at \ \ r = a, \quad t > 0 \tag{17}$$

The symbols in the above equations have their usual meanings, namely: D, v, and Σ_a are, respectively, the diffusion coefficient, neutron speed, and macroscopic absorption cross section; $k_\infty \equiv \nu^c \Sigma_f^c / \Sigma_a^c$ is the number of fission neutrons produced per neutron absorbed in the sub-critical assembly, λ_i is the decay constant and $C_i(r,z,t)$ is the density of the i^{th} emitter, while β_i is the delayed neutron fraction for the i^{th} emitter such that $\beta = \sum_i \beta_i$. Thus,

$$\begin{aligned}
&N(r,z,t)\,dV = number\ of\ neutrons\ in\ (the\ respective\ volume\ element)\ dV\ at\ time\ t;\\
&\mathrm{v}\,D\nabla^2 N(r,z,t)\,dV = number\ of\ neutrons\ diffusing\ in\ dV\ per\ unit\ time\ at\ time\ t;\\
&\mathrm{v}\,\Sigma_a N(r,z,t)\,dV = number\ of\ neutrons\ absorbed\ in\ dV\ per\ unit\ time\ at\ time\ t;\\
&Q(r,z,t)\,dV = number\ of\ neutrons\ produced\ in\ dV\ per\ unit\ time\ at\ time\ t.
\end{aligned}$$

It is important to note that the neutron balance equations in the sub-critical core, namely Eq. (16), do not formally contain an external volumetric neutron source. This is as it should be, since the sub-critical core would not be directly driven by a volumetric source.

4.1 EXACT SOLUTION FOR THE PARADIGM ADS MODEL

In the course of deriving the exact solution for the paradigm ADS-model represented by Eqs. (15)-(17), the following transformations will be used:

(a) Finite Fourier Sine Transform in the z-direction, defined as follows:

$$F_s\{f(z)\} \equiv f_s(n) \equiv \int_0^{z_o} f(z) \sin\frac{n\pi z}{z_o}\,dz \tag{18}$$

together with the inverse transform

$$F_s^{-1}\{f_s(n)\} \equiv f(z) = \frac{2}{z_o}\sum_{n=1}^{\infty} f_s(n) \sin\frac{n\pi z}{z_o} \tag{19}$$

Note that

$$F_s\{\partial^2 f/\partial z^2\} = -\left(\frac{n\pi}{z_o}\right)^2 f_s(n) + \frac{n\pi}{z_o}\left[f(0) + (-1)^{n+1} f(z_o)\right] \tag{20}$$

(b) Finite Hankel Transform of Order Zero, for the target region $0 < r \le a$, defined as

$$H_o\{g(r)\} \equiv \tilde{g}(B_j^t) \equiv \int_0^a g(r)\, r\, J_o(rB_j^t)\,dr \tag{21}$$

where B_j^t denote the (infinitely many) positive roots of the transcendental equation $J_o(aB_j^t) = 0$, together with the inverse transformation:

$$H_o^{-1}\left\{\tilde{g}\left(B_j^t\right)\right\} = g(r) = \frac{2}{a^2}\sum_{j=1}^{\infty}\tilde{g}\left(B_j^t\right)\frac{J_o\left(rB_j^t\right)}{J_1^2\left(aB_j^t\right)} \tag{22}$$

Note also the transformation

$$H_o\left\{\left(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}\right)g(r)\right\} = -\left(B_j^t\right)^2\tilde{g}\left(B_j^t\right) + ag(a)\left(B_j^t\right)J_1\left(aB_j^t\right) \tag{23}$$

(c) Generalized Finite Hankel Transform of Order Zero, for the sub-critical multiplying core region $a < r \le b$, defined as

$$H_o^G\{h(r)\} \equiv \tilde{h}\left(B_m^c\right) \equiv \int_a^b h(r)r\,A_o\left(rB_m^c\right)dr, \quad b > a, \tag{24}$$

where

$$A_o\left(rB_m^c\right) \equiv J_o\left(rB_m^c\right)Y_o\left(aB_m^c\right) - J_o\left(aB_m^c\right)Y_o\left(rB_m^c\right) \tag{25}$$

and where B_m^c denote the (infinitely many) positive roots of the transcendental equation $A_o\left(bB_m^c\right) = 0$. Note the corresponding inverse transformation:

$$\left(H_o^G\right)^{-1}\left\{\tilde{h}\left(B_m^c\right)\right\} = h(r) = \frac{\pi^2}{2}\sum_{m=1}^{\infty}\tilde{h}\left(B_m^c\right)\frac{A_o\left(rB_m^c\right)\left(B_m^c\right)^2 J_o^2\left(bB_m^c\right)}{J_o^2\left(aB_m^c\right) - J_o^2\left(bB_m^c\right)} \tag{26}$$

Note also the transformation

$$H_o^G\left\{\left(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}\right)h(r)\right\} = -\left(B_m^c\right)^2\tilde{h}\left(B_m^c\right) + \frac{2}{\pi}\left[h(b)\frac{J_o\left(aB_m^c\right)}{J_o\left(bB_m^c\right)} - h(a)\right] \tag{27}$$

Applying now the Finite Fourier Sine Transform, i.e., Eqs. (18) and (20), to the paradigm ADS-model described by Eqs. (15)-(17) yields the following Fourier-transformed problem:

- In the ADS-target region (superscript t):

$$\begin{cases} \dfrac{\partial N_s^t}{\partial t} = \mathrm{v}D^t\left[\dfrac{\partial^2}{\partial r^2}+\dfrac{1}{r}\dfrac{\partial}{\partial r}-\left(\dfrac{n\pi}{z_o}\right)^2\right]N_s^t(r,n,t) - \mathrm{v}\Sigma_a^t N_s^t(r,n,t) + Q_s(r,n,t); \quad 0 < r \le a, \quad t > 0 \\ N_s^t(r,n,t) = \text{finite everywhere, including at } r = 0, \quad t > 0 \\ N_s^t(r,n,0) = 0, \quad at\ t = 0, \\ N_s^t(r,n,t) \equiv F_s\left\{N^t(r,z,t)\right\}; \quad Q_s(r,n,t) \equiv F_s\{Q(r,z,t)\}, \end{cases} \tag{28}$$

- In the ADS sub-critical core region (superscript c):

$$\begin{cases} \dfrac{\partial N_s^c}{\partial t} = \mathrm{v}D^c\left[\dfrac{\partial^2}{\partial r^2} + \dfrac{1}{r}\dfrac{\partial}{\partial r} - \left(\dfrac{n\pi}{z_o}\right)^2\right]N_s^c(r,n,t) - \mathrm{v}\Sigma_a^c N_s^c(r,n,t) \\ + \mathrm{v}(1-\beta)k_\infty^c\Sigma_a^c N_s^c(r,n,t) + \sum_i \lambda_i C_i^s(r,n,t); \quad a \le r \le b,\ t > 0, \\ \dfrac{\partial C_i^s}{\partial t} + \lambda_i C_i^s(r,n,t) = \mathrm{v}\beta_i k_\infty^c \Sigma_a^c N_s^c(r,n,t), \quad i = 1,\ldots,I; \\ N_s^c(b,n,t) = 0, \quad t > 0; \quad N_s^c(r,n,0) = 0, \quad C_i^s(r,n,0) = 0, \quad at\ t = 0, \\ N_s^c(r,n,t) \equiv F_s\{N^c(r,z,t)\}; \quad C_i^s(r,n,t) \equiv F_s\{C_i(r,z,t)\} \end{cases} \tag{29}$$

- Interface conditions (continuity of flux and current) at $r = a$, between the target and the sub-critical core:

$$D^t\frac{\partial N_s^t}{\partial r} = D^c\frac{\partial N_s^c}{\partial r}, \quad and \quad N_s^t(r,n,t) = N_s^c(r,n,t), \quad at\ \ r = a, \quad t > 0 \tag{30}$$

Next, the Finite Hankel Transform of Order Zero is applied to Eqs. (28), in the target, and the Generalized Finite Hankel Transform of Order Zero is applied to Eqs. (29), in the sub-critical core, to obtain, respectively:

- In the ADS-target region (superscript t):

$$\begin{cases} \dfrac{d\widetilde{N}_s^t}{dt} = \mathrm{v}D^t\left[-\left(B_j^t\right)^2 - \left(\dfrac{n\pi}{z_o}\right)^2\right]\widetilde{N}_s^t\left(B_j^t,n,t\right) + \mathrm{v}D^t B_j^t J_1\left(aB_j^t\right)N_s^t(a,n,t) \\ \qquad - \mathrm{v}\Sigma_a^t \widetilde{N}_s^t\left(B_j^t,n,t\right) + \widetilde{Q}_s\left(B_j^t,n,t\right); \quad 0 < r \le a, \quad t > 0, \\ \widetilde{N}_s^t\left(B_j^t,n,0\right) = 0, \quad at\ t = 0, \\ \widetilde{N}_s^t\left(B_j^t,n,t\right) \equiv H_o\left\{N_s^t(r,n,t)\right\}; \quad \widetilde{Q}_s\left(B_j^t,n,t\right) \equiv H_o\left\{Q_s(r,n,t)\right\}, \end{cases} \tag{31}$$

- In the ADS sub-critical core region (superscript c):

$$\begin{cases} \dfrac{d\widetilde{N}_s^c}{dt} = \mathrm{v}D^c\left[-\left(B_m^c\right)^2 - \left(\dfrac{n\pi}{z_o}\right)^2\right]\widetilde{N}_s^c\left(B_m^c,n,t\right) - \mathrm{v}D^c\dfrac{2}{\pi}N_s^c(a,n,t) - \mathrm{v}\Sigma_a^c\widetilde{N}_s^c\left(B_m^c,n,t\right) \\ \qquad + \mathrm{v}(1-\beta)k_\infty^c\Sigma_a^c\widetilde{N}_s^c\left(B_m^c,n,t\right) + \sum_i \lambda_i\widetilde{C}_i^s\left(B_m^c,n,t\right); \quad a \le r \le b,\ t > 0, \\ \dfrac{d\widetilde{C}_i^s}{dt} + \lambda_i\widetilde{C}_i^s\left(B_m^c,n,t\right) = \mathrm{v}\beta_i k_\infty^c\Sigma_a^c\widetilde{N}_s^c\left(B_m^c,n,t\right), \quad i = 1,\ldots,I; \\ \widetilde{N}_s^c\left(B_m^c,n,0\right) = 0, \quad \widetilde{C}_i^s\left(B_m^c,n,0\right) = 0, \quad at\ t = 0, \\ \widetilde{N}_s^c\left(B_m^c,n,t\right) \equiv H_o^G\left\{N_s^c(r,n,t)\right\}; \quad \widetilde{C}_i^s\left(B_m^c,n,t\right) \equiv H_o^G\left\{C_i^s(r,n,t)\right\} \end{cases} \tag{32}$$

Once the solution of the system of coupled differential equations (30) through (32) has been solved, the neutron distributions in the target and sub-critical core are obtained from the respective inverse Fourier and Hankel transforms as

$$N^t(r,z,t) = F_s^{-1}\left\{H_o^{-1}\left\{\widetilde{N}_s^t\left(B_j^t,n,t\right)\right\}\right\} = \frac{2}{z_o}\left(\sum_{n=1}^{\infty}\sin\frac{n\pi z}{z_o}\right)\frac{2}{a^2}\sum_{j=1}^{\infty}\widetilde{N}_s^t\left(B_j^t,n,t\right)\frac{J_o\left(rB_j^t\right)}{J_1^2\left(aB_j^t\right)} \tag{33.t}$$

and

$$N^c(r,z,t) = F_s^{-1}\left\{\left(H_o^G\right)^{-1}\left\{\widetilde{N}_s^c\left(B_m^c,n,t\right)\right\}\right\}$$
$$= \frac{2}{z_o}\left(\sum_{n=1}^{\infty}\sin\frac{n\pi z}{z_o}\right)\frac{\pi^2}{2}\sum_{m=1}^{\infty}\widetilde{N}_s^c\left(B_m^c,n,t\right)\frac{A_o\left(rB_m^c\right)\left(B_m^c\right)^2 J_o^2\left(bB_m^c\right)}{J_o^2\left(aB_m^c\right)-J_o^2\left(bB_m^c\right)} \tag{33.c}$$

Note that Eqs. (30)-(32) actually constitute the ADS-Point-Kinetics-Model for the time-dependent amplitudes of the $(j,n)^{th}$-spatial mode $\widetilde{N}_s^t\left(B_j^t,n,t\right)$ in the target region, and the $(m,n)^{th}$-spatial mode $\widetilde{N}_s^c\left(B_m^c,n,t\right)$ in the sub-critical core region, respectively. These equations can be recast into a form that resembles the more familiar point-kinetics equations for a critical reactor, by defining the following quantities:

- In the ADS-target region (superscript t):

(a) infinite medium neutron life-time: $l_\infty^t \equiv \left(\mathrm{v}\Sigma_a^t\right)^{-1}$;

(b) diffusion (migration) area: $\left(L^t\right)^2 \equiv D^t/\Sigma_a^t$;

(c) geometrical buckling for the $(j,n)^{th}$-spatial mode: $\left(B_{jn}^t\right)^2 \equiv \left(B_j^t\right)^2 + \left(\frac{n\pi}{z_o}\right)^2$

(d) effective neutron life-time for the $(j,n)^{th}$-spatial mode: $l_{jn}^t \equiv l_\infty^t \Big/ \left[1+\left(L^t B_{jn}^t\right)^2\right]$

- In the ADS sub-critical core region (superscript c):

(a) infinite medium neutron life-time: $l_\infty^c \equiv \left(\mathrm{v}\Sigma_a^c\right)^{-1}$;

(b) diffusion (migration) area: $\left(L^c\right)^2 \equiv D^c/\Sigma_a^c$;

(c) geometrical buckling for the $(m,n)^{th}$-spatial mode: $\left(B_{mn}^c\right)^2 \equiv \left(B_m^c\right)^2 + \left(\frac{n\pi}{z_o}\right)^2$

(d) effective neutron reproduction factor for the $(m,n)^{th}$-spatial mode: $k_{mn}^c \equiv k_\infty^c \Big/ \left[1+\left(L^c B_{mn}^c\right)^2\right]$

(e) effective neutron life-time for the $(m,n)^{th}$-spatial mode: $l_{mn}^c \equiv l_\infty^c \Big/ \left[1+\left(L^c B_{mn}^c\right)^2\right]$

(f) effective neutron generation-time in the sub-critical core: $l^c \equiv l^c_{mn} / k^c_{mn} = l^c_\infty / k^c_\infty$

(g) the reactivity for the $(m,n)^{th}$-spatial mode: $\rho_{mn} \equiv \left(k^c_{mn} - 1\right) / k^c_{mn}$

The above definitions are now introduced in Eqs. (31) and (32) to recast them into the following forms:

- In the ADS-target region (superscript t):

$$\begin{cases} \dfrac{d\widetilde{N}^t_s}{dt} = -\dfrac{1}{l^t_{jn}} \widetilde{N}^t_s\left(B^t_j, n, t\right) + \widetilde{Q}_s\left(B^t_j, n, t\right) + \dfrac{\left(L^t\right)^2}{l^t_\infty} B^t_j J_1\left(aB^t_j\right) N^t_s(a,n,t); \quad 0 < r \le a, \quad t > 0, \\ \widetilde{N}^t_s\left(B^t_j, n, 0\right) = 0, \quad at\ t = 0, \\ where \quad B^t_j \quad are \quad the \quad positive \quad roots \quad of \quad J_o\left(aB^t_j\right) = 0, \\ for\ all\ j = 1, \ldots, \quad and \quad n = 1, \ldots, \end{cases} \tag{34}$$

- In the ADS sub-critical core region (superscript c):

$$\begin{cases} \dfrac{d\widetilde{N}^c_s}{dt} = \dfrac{\rho_{mn} - \beta}{l^c} \widetilde{N}^c_s\left(B^c_m, n, t\right) + \sum_i \lambda_i \widetilde{C}^s_i\left(B^c_m, n, t\right) - \dfrac{2}{\pi} \dfrac{\left(L^c\right)^2}{l^c_\infty} N^c_s(a,n,t); \quad a \le r \le b, t > 0, \\ \dfrac{\partial \widetilde{C}^s_i}{\partial t} + \lambda_i \widetilde{C}^s_i\left(B^c_m, n, t\right) = \dfrac{\beta_i}{l^c} \widetilde{N}^c_s\left(B^c_m, n, t\right), \quad i = 1,2,\ldots, I; \quad m = 1,2,\ldots; \quad n = 1,2,\ldots; \\ \widetilde{N}^c_s\left(B^c_m, n, 0\right) = 0, \quad \widetilde{C}^s_i\left(B^c_m, n, 0\right) = 0, \quad at\ t = 0, \\ where \quad B^c_m \quad are \quad the \quad roots \quad of \quad A_o\left(bB^c_m\right) \equiv J_o\left(bB^c_m\right) Y_o\left(aB^c_m\right) - J_o\left(aB^c_m\right) Y_o\left(bB^c_m\right) = 0, \end{cases} \tag{35}$$

Thus, the ADS Point-Kinetics Model, represented by Eqs. (34) and (35), together with the target/sub-critical core interface conditions given in Eq. (30), comprises a set of (I+4)-coupled differential equations for the time-evolution of the unknowns $\widetilde{N}^t_s\left(B^t_j, n, t\right)$, $\widetilde{N}^c_s\left(B^c_m, n, t\right)$, $N^t_s(a,n,t)$, and $N^c_s(a,n,t)$, for each spatial mode (m, n) in the sub-critical core and spatial mode (j, n) in the target.

4.2 FUNDAMENTAL CHARACTERISTICS OF THE PARADIGM ADS-NEUTRON KINETICS MODEL

In the Paradigm ADS neutron kinetics model presented in the previous section features the following fundamental characteristics expected to be representative of the time- and space-behavior of ADS:

1. The neutron kinetics/dynamics processes in the target are driven by the volumetric source term $\widetilde{Q}_s\left(B^t_j, n, t\right)$, which originates directly from the spallation neutrons, and the term $B^t_j J_1\left(aB^t_j\right) N^t_s(a,n,t) \left(L^t\right)^2 / l^t_\infty$, which arises from the neutronic coupling between the target and the ADS sub-critical core. Since the target consisted of non-fissionable material, there are no reactivity changes or reactivity control in the target. Of course, feedback effects in the

target will arise from thermal-hydraulic considerations, but the discussion of such effects is beyond the scope of this Wigner Keynote Lecture.

2. Consider the first of the source terms for the target kinetics equations, namely

$$\tilde{Q}_s\left(B_j^t,n,t\right) \equiv H_o\{F_s\{Q(r,z,t)\}\} \equiv \int_0^a r\,J_o\left(rB_j^t\right)dr \int_0^{z_o} Q(r,z,t)\sin\frac{n\pi z}{z_o}\,dz \tag{36}$$

This term originates directly from the spallation neutrons, and the above expression clearly indicates that it must depend on the material properties of the target. In fact, the source term $\tilde{Q}_s\left(B_j^t,n,t\right)$ is independent of the material properties of the sub-critical ADS-core. Therefore, this source term (which originates directly from the spallation neutrons) cannot be possibly expressed in terms of any expansion containing solely the eigenfunction of the sub-critical core (regardless of whether they are k-eigenfunctions, or λ-eigenfunctions, or α-eigenfunctions, or ω-eigenfunctions, etc.). This fact, therefore, will invalidate any attempt to express the "ADS Source" exclusively in terms of eigenfunctions of the sub-critical core. Furthermore, it is not possible to construct "k-eigenfunctions expansions" for the target, since there are no fissions in the target (unless the target were made of depleted uranium, for example, but even in such a case, the respective "k-eigenfunctions expansions" would be artificial and practically useless).

To illustrate the foregoing statements by a specific example, consider the axial and radial distributions of primary spallation neutrons presented recently by Seltborg at the 2002 Frederic Joliot / Otto Hahn Summer School (see Seltborg, 2002): a back-of-the envelope calculation readily shows that these distributions can be roughly approximated in the radial direction by the function $\left(a^2-r^2\right)$ and in the axial direction by the function $\left[z\left(z_o^2-z^2\right)\right]$. Inserting these functional expressions in Eq. (36) yields:

$$\begin{aligned}\tilde{Q}_s\left(B_j^t,n,t\right) &= \int_0^a r\,J_o\left(rB_j^t\right)\left(a^2-r^2\right)dr \int_0^{z_o} q(t)\left[z\left(z_o^2-z^2\right)\right]\sin\frac{n\pi z}{z_o}\,dz \\ &= q(t)\frac{4a}{\left(B_j^t\right)^3}J_1\left(aB_j^t\right)(-1)^{n+1}6z_o\left(\frac{z_o}{n\pi}\right)^3\end{aligned}\,, \tag{37}$$

where $q(t)$ contains the time-variation of the spallation neutron source. Clearly, the representation of the spallation neutron source depends on the geometric bucklings of the target. Of course, the proton source energy and spatial distribution also determine to a large extent the spatial distribution of the neutrons in the target. The important point to note here, though, is that the representation of the spallation neutron source does not depend on the sub-critical ADS-core.

Note also that the time variation of the spallation neutron source, represented here by the quantity $q(t)$, depends decisively upon the future ability to build reliable accelerators, capable of sustaining the beam at full power for long operating times, without beam interruptions. At the present time, however, the beam interruptions are very frequent, as typified by the SINQ-Accelerator beam, which has a very "lively" time variation!

3. Consider now the second source term for the target equations, namely the term

$$\frac{\left(L^t\right)^2}{l_\infty^t}B_j^tJ_1\left(aB_j^t\right)N_s^t(a,n,t) \tag{38}$$

Note that the quantity $N_s^t(a,n,t)$ does not arise directly from the spallation neutron source, but arises because of the coupling between the ADS target and the ADS sub-critical core. Thus, this quantity must be determined as part of the overall solution for the entire (ADS target-core) coupled system. On the other hand, the quantity $B_j^t J_1\left(aB_j^t\right)\left(L^t\right)^2/l_\infty^t$ clearly depends solely on the material properties of the target.

4. Consider now the quantity $\frac{2}{\pi}\frac{\left(L^c\right)^2}{l_\infty^c}N_s^c(a,n,t)$, which appears as a source-term in Eq. (35), pertaining to the sub-critical core. Clearly, the term $\frac{2}{\pi}\frac{\left(L^c\right)^2}{l_\infty^c}$ depends solely on the material properties of the sub-critical core target, while the term $N_s^c(a,n,t)$ must be determined as part of the overall solution for the entire (ADS target-core) coupled system.

5. The coupling between the target and the sub-critical core takes place not only through the quantities $N_s^c(a,n,t)$ and $N_s^t(a,n,t)$, which appear both as source source-terms in Eqs. (34) and (35) and surface interface terms in Eq. (30), but also through the derivative terms involved in the target/sub-critical core interface conditions given in Eq. (30), namely

$$D^t \frac{\partial N_s^t(r,n,t)}{\partial r} = D^c \frac{\partial N_s^c(r,n,t)}{\partial r}, \quad at \ \ r=a, \quad t>0 \tag{39}$$

It is very important to note here that these derivative terms could be controlled by design measures (involving use of materials, thermal-hydraulic target cooling considerations, etc.) which will also influence the coupling between the target and the sub-critical core regions.

6. As clearly highlighted by the ADS-Point-Kinetics Model presented here, the intimate coupling between the ADS target-region and the ADS sub-critical core cannot be represented through some eigenfunction expansion involving solely the properties of the sub-critical core. Actually, this is as it should be for an externally (e.g., accelerator-) driven sub-critical core, for otherwise the very purpose of an ADS would be defeated!

7. Note that the reactivity for the $(m,n)^{th}$-spatial mode is defined as $\rho_{mn} \equiv \left(k_{mn}^c - 1\right)/k_{mn}^c$. This definition does not arise as a result of using some first-order perturbation theory. Furthermore, these reactivity coefficients depend solely on the material properties and geometry of the sub-critical core, and are independent of the external source of spallation neutrons in the target. Therefore, these reactivity coefficients cannot be artificially "perturbed" in order to simulate time- and/or spatial variation of the external spallation neutron source, by analogy to the case of critical reactors. These reactivity coefficients would change solely by changing the material properties and/or geometry of the sub-critical core, independently of the external source. If such changes would be actuated within the sub-critical core (for example, by adjusting some control rod) and, in addition, if the respective variations around some operating condition were small, then the effects of the respective perturbations on the ADS operating design parameters could be estimated by perturbation theory, as discussed in Sec. 6, in the sequel.

8. From a mathematical point of view, both an ADS and a critical reactor with an external source can be described by the following (compact) operator equation (in a Hilbert space H)

$$(\lambda I - L)f = g, \quad g \in H, \quad . \tag{F}$$

However, the physics underlying an ADS is distinct from the physics underlying a critical reactor with an external source, and this distinction between the two systems is expressed mathematically unambiguously by the Fredholm Alternative Theorem, which states that only one of the following alternatives can hold for Eq. (F) above: either

(i) The homogeneous equation has only the zero solution; in this case, $\lambda \in \rho(L)$, where $\rho(L)$ denotes the resolvent set of L (thus, λ cannot be an eigenvalue of L); furthermore, $(\lambda I - L)^{-1}$ is bounded, and the inhomogeneous equation has exactly one solution $f = (\lambda I - L)^{-1} g,$ for each $g \in H$, or

(ii) The homogeneous equation has a non-zero solution; in this case, the inhomogeneous equation has a solution, necessarily non-unique, if and only if $\langle g, \varphi^+ \rangle = 0$, for every solution φ^+ of the adjoint equation $\lambda \varphi^+ = L^+ \varphi^+$, where L^+ denotes the operator adjoint to L, and $\langle , \rangle$ denotes the inner product in the respective Hilbert space H.

Clearly, an ADS falls within alternative (i) while a critical reactor with an external source falls within alternative (ii); these two alternatives cannot be substituted for (and should not be confused with) one another. For this reason, the computational methods and experiments designed for critical reactors cannot be simply taken over for designing, operating and controlling an ADS; new methods and experiments would need to be developed for this purpose.

5. INVESTIGATION OF RESULTS PRODUCED BY METHODS BASED ON "EXPANSIONS IN EIGENFUNCTIONS OF AN APPROPRIATE HOMOGENEOUS STEADY-STATE K-EIGENVALUE PROBLEM"

In this section, we investigate the leading methods currently proposed for treating the space- and time-behavior of an ADS. These methods were proposed by the following authors: (i) Carta, and D'Angelo, (1999; see also TRADE Final Feasibility Report, 2002); (ii) Slessarev and Tchistiakov (1997), see also Salvatores et. al. (1997), and (iii) Gandini and Salvatores (2002). Note that all of these authors propose the use of perturbation theory in conjunction of eigenfunction expansion methods a la Wigner around a "fictitious ADS steady-state".

To begin with, consider the method of Carta and D'Angelo (see M. Carta, and A. D'Angelo, 1999; see also TRADE Final Feasibility Report, 2002); these authors propose that Eqs. (11) and (12) be used as the representative "fictitious steady-state k-eigenvalue problem" for developing a point-kinetics model representative of an ADS. Subsequently, they propose that classical experiments (harmonic source, pulsed source, source multiplication methods) be performed for simulating the space- and time-behavior of a TRIGA reactor coupled to an accelerator (see TRADE, 2002).

Obviously, the method of Carta and D'Angelo (1999) cannot be applied to the target region, since even if a "fictitious steady-state source" could be somehow postulated for the accelerator beam, the neutron transport problem in the target region is a source-driven, rather than an eigenvalue problem. Thus, based on physical considerations, the "fictitious homogeneous steady-state problem" required by the method of Carta and D'Angelo (1999) can only have the identically-zero flux solution, since in the absence of the accelerator beam, the only steady-state flux in the target is the identically-zero flux. From a mathematical point of view, this result is entirely consistent with the Fredholm Alternative Theorem, which guarantees mathematically that the only solution of Eq. (15) with $Q(r,z,t) \equiv 0$ is $N^t(r,z,t) \equiv 0$. (see Sec. 4.2, above)

Consider now the sub-critical core region: the method of Carta and D'Angelo (1999) would require expansions of the types shown in Eq. (11), where the eigenfunctions would be those of Eq. (11), considered within the core region. Noting that the operators in Eq. (12) are self-adjoint, it follows that application of the method of Carta and D'Angelo (1999) commences with calculating the eigenfunctions of the steady-state version of Eq.(16), but without the precursors, namely:

$$\begin{cases} 0 = D^c\nabla^2 N_j^c(r,z,t) - \Sigma_a^c N_j^c(r,z,t) + \dfrac{1}{K_j}\nu\Sigma_f^c N_j^c(r,z,t); \quad a \le r \le b, t > 0, \\ N_j^c(b,z,t) = 0, \quad N_j^c(a,z,t) = 0, \quad t > 0, \\ N_j^c(r,z_o,t) = 0, \quad N_j^c(r,0,t) = 0, \quad t > 0, \\ N_j^c(r,z,0) = 0, \quad at\ t = 0. \end{cases} \tag{40}$$

The eigenvalues K_j and the corresponding eigenfunctions are readily obtained by using Eqs. (18) and (24) to Eq. (40), to obtain

$$K_{mn}^c = k_\infty^c \Big/ \left(L^c B_{mn}^c\right)^2 \tag{41}$$

and corresponding eigenfunctions

$$\varphi_{mn}(r,z) = A_o\left(rB_m^c\right)\sin\frac{n\pi z}{z_o} \tag{42}$$

It is important to note here that the neutron balance equations in the sub-critical core, namely Eq. (16), do not formally contain a volumetric neutron source. Thus, there is no volumetric source to expand in the eigenfunctions obtained in Eq. (42), and this is as it should be if the physical problem is to be modeled correctly.

The next step is to consider expansions for the flux and precursors of the type shown in Eq. (11), namely

$$\varphi(r,z,t) = \sum_m\sum_n p_{mn}(t)\ \varphi_{mn}(r,z)\,; C_i(r,z,t) = \sum_m\sum_n C_{mn}^i(t)\ \varphi_{mn}(r,z) \tag{43}$$

and substitute the above expansions into Eq. (16). Using on the resulting equations the orthogonality relationships for the functions $\sin n\pi z/z_o$ and $A_o\left(rB_n^c\right)$ leads to a traditional (see the textbooks mentioned in the reference section) set of homogeneous point-kinetics equations for the amplitudes $p_{mn}(t)$ and $C_{mn}^i(t)$:

$$\begin{cases} \dfrac{dp_{mn}}{dt} = \dfrac{\rho_{mn} - \beta}{l^c} p_{mn}(t) + \sum_i \lambda_i C_{mn}^i(t); \quad a \le r \le b, t > 0, \\ \dfrac{\partial C_{mn}^i}{\partial t} + \lambda_i C_{mn}^i(t) = \dfrac{\beta_i}{l^c} p_{mn}(t), \quad i = 1,2,\ldots,I; \quad m = 1,2,\ldots; \quad n = 1,2,\ldots; \\ p_{mn}(0) = 0, \quad C_{mn}^i(0) = 0, \quad at\ t = 0, \end{cases} \tag{44}$$

where the quantities ρ_{mn}, l^c, λ_i, β_i, β, have the same meaning as in the exact model provided by Eq. (35).

The method proposed by Slessarev and Tchistiakov (1997) is actually a simplified version of the method proposed by Carta and D'Angelo (1999). Slessarev and Tchistiakov use the eigenvalue problem

$$\begin{cases} 0 = D^c \nabla^2 N_j^c(r,z,t) - \Sigma_a^c N_j^c(r,z,t) + \dfrac{1}{K_{eff}} \nu \Sigma_f^c N_j^c(r,z,t); \quad a \le r \le b, t > 0, \\ N_j^c(b,z,t) = 0, \quad N_j^c(a,z,t) = 0, \quad t > 0, \\ N_j^c(r,z_o,t) = 0, \quad N_j^c(r,0,t) = 0, \quad t > 0, \\ N_j^c(r,z,0) = 0, \quad at\ t = 0. \end{cases}$$

The above eigenvalue problem leads to

$$K_{eff}^c = k_\infty^c \Big/ \left(L^c B_{11}^c\right)^2 ;\ \varphi_{11}(r,z) = A_o\left(rB_1^c\right)\sin\frac{\pi z}{z_o}, \quad \varphi_{mn}(r,z) = 0,\ m,n \ne 1,$$

with corresponding expansions consisting of the fundamental term only, namely:

$$\varphi(r,z,t) = p_{11}(t)\ \varphi_{11}(r,z); C_i(r,z,t) = C_{11}^i(t)\ \varphi_{11}(r,z). \tag{45}$$

Thus, the resulting point-kinetics equations produced by the Slessarev and Tchistiakov (1997) method consist of just the (1,1)-term of Eq. (44) of Carta and D'Angelo.(1999).

Finally, the recent method proposed by Gandini and Salvatores (2002) is based on a simplified, time-independent version of Eq. (9) that (i) neglects the delayed neutrons and (ii) uses an adjoint source which attempts to describes the equivalent number of fissions that would correspond to the accelerator beam proton "steady-state" power. The specific form of this equation is

$$-\mathbf{\Omega} \cdot \nabla n_o^* + \Sigma_t n_o^* = \mathbf{S}^+ n_o^* + \left[\chi_p(1-\beta)\mathbf{F}\right]^+ n_o^* + \gamma \Sigma_f / W_o \tag{46}$$

where γ represents the energy released per fission and W_o would represent a "steady-state power" of the sub-critical core. They use n_o^* in the classical manner, a la Wigner, to obtain perturbation-theory-type expressions for the point-kinetic equations in a "subcritical system", which is essentially leads to the same results as obtained by Carta and D'Angelo (1999). Thus, all of these methods ultimately yield perturbation theory-type results, which are valid for critical reactors as originally derived by Wigner (see Weinberg and Wigner, 1957, and Bell and Glasstone, 1970). As shall be shown in the next section, such results cannot be used to describe the global behavior of an ADS, but may be used, as will be shown in a much more general setting in Sec. 6, for assessing the effects of small control rod adjustments in the sub-critical ADS core.

5.1 COMPARISON OF THE EXACT SOLUTION FOR THE ADS NEUTRON KINETICS PARADIGM MODEL WITH RESULTS PRODUCED BY "EIGENFUNCTIONS EXPANSIONS OF AN APPROPRIATE HOMOGENEOUS STEADY-STATE K-EIGENVALUE PROBLEM"

Comparison of Eq. (44) with the exact ADS Point-Kinetics Model specified by Eqs. (30), (34), and (35), and consideration of items 1-7 discussed in Section 4.2 underscores the main reasons why the methods based on "eigenfunctions expansion of a fictitious steady-state k-eigenvalue problem" and classical perturbation theory a la Wigner cannot describe the kinetic and/or dynamic behavior of an ADS. These reasons are summarized below:

(i) The caveats (regarding existence, completeness, etc.) expressed originally by Wigner regarding the use of eigenfunction expansions (see Sections 1 and 2, above) also apply to sub-critical systems. Furthermore, k-eigenfunction expansions cannot be reasonably postulated for the ADS target region (since they do not exist at all, unless there are fissions in the target). For this reason, the target region cannot be properly taken into account by any k-eigenfunction expansion.

(ii) It is not possible to obtain a realistically useful "steady-state problem" to use as a basis for an "eigenfunction expansion" applicable to an ADS. A typical time evolution of a state-of-the-art accelerator beam is provided by the SINQ-Accelerator of the Paul Scherer Institute in Switzerland. For example, during the week of August 23-30, 2000, there were a total of 1700 beam interruptions, with 380 of them lasting for longer than 1 second; 5 interruptions lasted, respectively, for 4 hours, 15, 20, 25 minutes, and 11 hours. The behavior of the SINQ accelerator is obviously relevant, since it is the driver for the MEGAPIE Target Experiment, which is supposed to be prototypical for ADS operation (see, e.g., Groeschel, 2002). Although a "fictitious steady-state" could be concocted for the time-behavior of SINQ, such a fictitious steady-state would be irrelevant to the actual behavior of an ADS.

(iii) Comparison of Eq. (44) with the exact ADS Point-Kinetics Model specified by Eqs. (30), (34), and (35), clearly indicates that the "k-eigenfunctions expansion based on a "fictitious ADS-steady-state" describes inadequately both (a) the kinetic/dynamic behavior of the spallation neutron source in the target and in the sub-critical core, and (b) the space-time behavior of the interface coupling between the spallation target and the sub-critical ADS core, which is supposed to "be driven" by the target.

(iv) The exact derivations in Sec. 4 have underscored the non-perturbative nature of the ADS Point-Kinetics Equations. Furthermore, an ADS accelerator source cannot be simply characterized by "small perturbations"; consequently, perturbation theory (as customarily used for treating small reactivity changes in a critical reactor) cannot be expected to yield accurate results for characterizing accelerator-induced power variations in an ADS. Classical perturbation theory certainly cannot be used for optimal operation and control of an ADS.

6. AN OPTIMIZATION/CONTROL-THEORY FRAMEWORK FOR DEVELOPING NEW COMPUTATIONAL METHODS AND EXPERIMENTS FOR ADS CONTROL AND OPERATION

The exact treatment of the ADS Point Kinetics Paradigm Model presented in Sec. 4 clearly highlights the fundamental distinctions between the target and the sub-critical core regions. Furthermore, it is also apparent that the coupling in time and space between the target and the sub-critical core region is crucial and must therefore be treated accurately. This has been accomplished in Sec. 4.2 by applying Fourier and Hankel Transforms in the spatial variables, which is similar to inverting the Laplacian-operator in the spatial variables by using the eigenfunctions of the homogeneous Helmholtz equation

$$\begin{cases} \nabla^2 \psi_{lmn}\left(B_{lmn}^g, \mathbf{r}\right) + B_{lmn}^g \psi_{lmn}\left(B_{lmn}^g, \mathbf{r}\right) = 0, & \mathbf{r} \in V, t > 0 \\ \psi_{lmn}\left(B_{lmn}^g, \mathbf{r}\right) = 0, \text{for } \mathbf{r} \in \partial V, t > 0 & \end{cases} \tag{47}$$

where the eigenvalues B_{lmn}^g correspond to the geometrical bucklings of the respective assembly. Note, however, that the transform technique automatically incorporates the correct boundary conditions into the transformed problem, while eigenfunction expansions based on the homogeneous Helmholtz equation do not necessarily accomplish this automatically. Although the eigenfunctions of an appropriate Helmholtz equation may be useful for certain applications (for example, within an analytical nodal method-like approach to solving the spatial part of the equations describing an ADS), they are not mandatory for solving the ADS equations; in practice, more efficient methods, based on collocation, weighted residuals, etc, would be recommended for treating the respective spatial dependence.

As is well-known from illustrative examples from classical mechanics, the "self-sustaining oscillators" (which would correspond to critical reactors) are fundamentally distinct from the "externally driven oscillators" (which would correspond to an ADS). Thus, self-sustaining oscillators are described mathematically by a homogeneous eigenvalue problem, in which small departures from equilibrium can be adequately described by perturbation theory, as Wigner originally did (see Sec. I). By contrast, driven oscillators are mathematically described by inhomogeneous problems, where perturbation theory has only limited applicability. In particular, an ADS would correspond to a driven oscillator which should admit only the trivial, identically-zero, (flux) solution in the absence of the external driving source. As is well known, externally driven systems may exhibit behavior that is completely different than that of a self-sustaining oscillator. For example, large oscillations near a (perhaps hidden) resonance may occur even when the respective system is described by linear equations without feedback. For instance, the left-side (i.e., "driven" part) of the equation

$$\begin{bmatrix} dx/dt \\ dy/dt \end{bmatrix} - \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 0 \\ \sin \omega t \end{bmatrix}$$

admits the (purely imaginary, and therefore not immediately obvious) eigenvalues $\pm i$; thus, whenever ω is close to ± 1, the solutions of this equation exhibit large oscillations that become divergent at $\omega = \pm 1$. Since the time-dependent current (and, consequently, power) oscillations of the driving accelerator may be of large amplitude, they could cause a diverging power oscillation of the ADS. Of course, additional feedback mechanisms (such as provided, for example, by the ADS thermal-hydraulics equations) would introduce additional complications, which at least theoretically, could include chaotic behavior.

For all of the above reasons, and many other practical ones which cannot be discussed in here in detail, it appears that the space-time behavior of an ADS should not be artificially described in terms of "eigenfunction expansions around a fictitious steady-state". Instead, it is hereby proposed that the ADS be treated from the point of view of optimization theory and optimal control, so that the time- and space-dependent ADS equations (i.e., neutron transport equations with delayed neutrons, thermal-hydraulics equations) are solved with the goal of controlling the ADS in an optimal manner for attaining predetermined objectives. Examples of such objectives would include minimization of possible flux tilts in the ADS core, optimal load following, minimum response time to power variations. The remainder of this Section suggests a global optimization framework for attaining such objectives, including the calculation of sensitivities around optimal configurations. In particular, this new conceptual framework unambiguously indicates that the optimal "weighting" functions to be used are the solutions of adjoint equations appropriate to the actual objective to be optimized (rather than some "adjoint equation" driven by a "fission source" or "accelerator power source" as proposed in the previous works by Slessarev and Tchistiakov, 1997; Carta and d'Angelo, 1999; Gandini and Salvatores, 2002).

6.1 CONCEPTUAL FRAMEWORK BASED ON GLOBAL OPTIMIZATION THEORY FOR ADS OPERATION AND CONTROL

To simplify the ensuing mathematical manipulations without, however, detracting from the conceptual generality of the underlying methodology, consider that the neutron balance and thermal hydraulics equations that describe the time-space behavior of an ADS have been discretized consistently to obtain algebraic relationships as required in preparation for numerical solution. Then, the canonical discretized mathematical representation of the ADS would comprise m linear and/or nonlinear equations of the form:

$$\mathbf{N}(\boldsymbol{\varphi},\boldsymbol{\alpha}) = \mathbf{0}\,, \quad \mathbf{N} : D_N \subset D_\varphi \times R^i \rightarrow R^m\,, \tag{48}$$

where

$$\mathbf{N} \equiv \left[N_1(\boldsymbol{\varphi},\boldsymbol{\alpha}),\ldots,N_m(\boldsymbol{\varphi},\boldsymbol{\alpha})\right], \tag{49}$$

is an m-component column vector whose components are linear and/or nonlinear operators; $\mathbf{N}$ is here defined on a domain D_N and takes values in the Euclidean space R^m. Each component of $\mathbf{N}$ is considered to operate on the vectors $\boldsymbol{\alpha}$ and $\boldsymbol{\varphi}$, where

$$\boldsymbol{\alpha} \equiv (\alpha_1,\ldots,\alpha_i)\,, \quad \boldsymbol{\alpha} \in R^i \tag{50}$$

is an i-component column vector, comprising the system parameters, and

$$\boldsymbol{\varphi} \equiv (\varphi_1,\ldots,\varphi_m)\,, \quad \boldsymbol{\varphi} : D_\varphi \subset R^m\,, \tag{51}$$

is an m-component column vector, comprising the system's dependent variables, defined on a domain $D_\varphi \subset R^m$. Note that the components of both $\boldsymbol{\alpha}$ and $\boldsymbol{\varphi}$ are considered here to be scalar quantities, taking on values in the real Euclidean spaces R^i and R^m, respectively. Since Eq. (48) is a canonical representation for problems that have been fully discretized in preparation for a numerical solution, it automatically comprises all initial and/or boundary conditions that may have appeared in the originally continuous-variable description of the ADS.

In addition, the mathematical description of ADS operation and control may be characterized by k inequality and/or equality constraints of the form:

$$\mathbf{g}(\boldsymbol{\alpha}) \leq \mathbf{0}\,, \quad \mathbf{g} : D_g \subset R^i \subset R^k\,, \tag{52}$$

where $\mathbf{g}(\boldsymbol{\alpha}) \equiv [g_1(\alpha),\ldots,g_k(\alpha)]$ is a k-component column vector, defined on a domain D_g that delimits, directly or indirectly, the range of the parameters α_i. Finally, the ADS performance objective (i.e., system response) to be optimized (while optimally operating/controlling the ADS) can be represented as a real-valued functional of $\boldsymbol{\alpha}$ and $\boldsymbol{\varphi}$, defined on a domain D_P and range in R^1, namely:

$$P(\boldsymbol{\varphi},\boldsymbol{\alpha})\,, \quad P : D_P \subset D_\varphi \times R^i \rightarrow R^1\,. \tag{53}$$

The problem of optimally operating/controlling the ADS is mathematically equivalent to an optimization problem that determines the minima and/or maxima of the system response $P(\boldsymbol{\varphi},\boldsymbol{\alpha})$ subject to the equality and inequality constraints represented by Eqs. (48) and (52). This problem is typically handled by introducing the Lagrange functional $L(\boldsymbol{\varphi},\, \mathbf{y},\, \boldsymbol{\alpha},\, \mathbf{z})$, defined as

$$L(\boldsymbol{\varphi},\, \mathbf{y},\, \boldsymbol{\alpha},\, \mathbf{z}) \equiv P(\boldsymbol{\varphi},\boldsymbol{\alpha}) + \langle \mathbf{y},\, \mathbf{N}(\boldsymbol{\varphi},\boldsymbol{\alpha})\rangle_m + \langle \mathbf{z},\, \mathbf{g}(\boldsymbol{\alpha})\rangle_k\,, \tag{54}$$

where the angular brackets denote inner products in R^m and R^k, respectively, namely:

$$\langle a,\, b\rangle_n = a \bullet b = \sum_{i=1}^{n} a_i b_i \;; \quad a,\, b \in R^n; \quad (n = m \;\; or \;\; k), \tag{55}$$

and where

$$\boldsymbol{y} = (y_1, \ldots, y_m) \tag{56}$$

and

$$\boldsymbol{z} = (z_1, \ldots, z_k) \tag{57}$$

are column vectors of Lagrange multipliers.

The critical points (extrema) of P are obtained by requiring the first Gateaux-variation δL of L to vanish for arbitrary variations $\delta\boldsymbol{\varphi}, \delta\boldsymbol{y}, \delta\boldsymbol{z}$ and $\delta\boldsymbol{\alpha}$. From Eq. (54), δL is obtained as

$$\delta L(\varphi,\; \boldsymbol{y},\; \boldsymbol{\alpha},\; z) = \delta\boldsymbol{\varphi} \bullet \boldsymbol{N}^*(\varphi, \boldsymbol{y}, \boldsymbol{\alpha}) + \delta\boldsymbol{y} \bullet \boldsymbol{N}(\varphi, \boldsymbol{\alpha}) + \delta\boldsymbol{z} \bullet \boldsymbol{g}(\boldsymbol{\alpha}) + \delta\boldsymbol{\alpha} \bullet \boldsymbol{S}(\varphi,\; \boldsymbol{y},\; \boldsymbol{\alpha},\; z), \tag{58}$$

where the column vectors $\boldsymbol{N}^*$ and $\boldsymbol{S}$ are defined as

$$\boldsymbol{N}^*(\varphi, \boldsymbol{y}, \boldsymbol{\alpha}) \equiv \nabla_\varphi P + (\nabla_\varphi \boldsymbol{N})\boldsymbol{y} \tag{59}$$

and

$$\boldsymbol{S}(\varphi,\; \boldsymbol{y},\; \boldsymbol{\alpha},\; z) \equiv \nabla_\alpha P + (\nabla_\alpha \boldsymbol{N})\boldsymbol{y} + (\nabla_\alpha \boldsymbol{g})\boldsymbol{z}\,, \tag{60}$$

respectively. The various gradients vectors and matrices appearing in Eqs. (59) and (60) are defined as follows:

$$\nabla_\varphi P \equiv \left(\partial P / \partial \varphi_p\right)_{m\times 1}, \quad \nabla_\alpha P \equiv \left(\partial P / \partial \alpha_q\right)_{i\times 1}, \tag{61}$$

$$\nabla_\varphi \boldsymbol{N} \equiv \left(\partial N_r / \partial \varphi_p\right)_{m\times m}, \quad \nabla_\alpha \boldsymbol{N} \equiv \left(\partial N_r / \partial \alpha_q\right)_{i\times m}, \tag{62}$$

$$\nabla \boldsymbol{g} \equiv \left(\partial g_s / \partial \alpha_q\right)_{i\times k}. \tag{63}$$

The requirements that the first variation δL of L vanish, for arbitrary $\delta\boldsymbol{\varphi}, \delta\boldsymbol{y}, \delta\boldsymbol{z}$ and $\delta\boldsymbol{\alpha}$, together with the constraints $\boldsymbol{g} \le \boldsymbol{0}$ leads to the following conditions:

$$\boldsymbol{N}^*(\varphi, \boldsymbol{y}, \boldsymbol{\alpha}) = \boldsymbol{0}\,, \quad \boldsymbol{S}(\varphi,\; \boldsymbol{y},\; \boldsymbol{\alpha},\; z) = \boldsymbol{0}\,, \quad \boldsymbol{N}(\varphi, \boldsymbol{\alpha}) = \boldsymbol{0}\,, \quad \boldsymbol{z} \bullet \boldsymbol{g} = \boldsymbol{0}, \quad \boldsymbol{g} \le \boldsymbol{0}\,, \quad \boldsymbol{z} \ge \boldsymbol{0}\,, \tag{64}$$

for the minima of $P(\varphi, \boldsymbol{\alpha})$ and similar conditions (except that $\boldsymbol{z} \le \boldsymbol{0}$) for the maxima of $P(\varphi, \boldsymbol{\alpha})$. The inequalities in Eq. (64) imply a lack of global differentiability so attempts at solving Eq.(64) directly are usually hampered by computational difficulties. These difficulties can be mitigated by recasting the last three conditions in Eq. (64) into the equivalent single relationship

$$\boldsymbol{K} \equiv \left(K_1, \ldots, K_k\right) = \boldsymbol{0}, \tag{65}$$

where the components K_i of the column vector $\boldsymbol{K}$ are defined as

$$K_i \equiv \left(g_i + z_i\right)^2 + g_i\left|g_i\right| - z_i\left|z_i\right| . \tag{66}$$

Thus, Eq. (64) can be recast into the form

$$\boldsymbol{F}(\boldsymbol{u}) \equiv \left[\boldsymbol{N}^*(\boldsymbol{u}), \boldsymbol{N}(\boldsymbol{u}), \boldsymbol{S}(\boldsymbol{u}), \boldsymbol{K}(\boldsymbol{u})\right] = \boldsymbol{0}, \tag{67}$$

where the components of the column vector

$$\boldsymbol{u} \equiv (\boldsymbol{\varphi}, \boldsymbol{y}, \boldsymbol{\alpha}, \boldsymbol{z}), \quad \boldsymbol{u} \in R^{2m+i+k} \tag{68}$$

are the dependent variables $\boldsymbol{\varphi}$, their corresponding Lagrange multipliers $\boldsymbol{y}$, the parameters $\boldsymbol{\alpha}$, and the Lagrange multipliers $\boldsymbol{z}$ corresponding to the inequalities constraints $\boldsymbol{g}$. The above structure of $\boldsymbol{F}$ has been deliberately selected, since it simplifies considerably the numerical procedure (see, e.g., Cacuci, 1990) for finding globally the roots and critical points of Eq. (67).

It is important to note that $\boldsymbol{F}$ is globally differentiable if $P, \boldsymbol{N}$ and $\boldsymbol{g}$ are differentiable twice globally, as indicated by the Jacobian matrix $\boldsymbol{F}'(\boldsymbol{u})$ of $\boldsymbol{F}(\boldsymbol{u})$, which has the block matrix structure

$$\boldsymbol{F}'(\boldsymbol{u}) = \begin{bmatrix} \nabla_\varphi \boldsymbol{N}^* & \nabla_\varphi \boldsymbol{N} & \nabla_\varphi \boldsymbol{S} & \boldsymbol{0} & \boldsymbol{0} \\ \left(\nabla_\varphi \boldsymbol{N}\right)^T & \boldsymbol{0} & \left(\nabla_\alpha \boldsymbol{N}\right)^T & \boldsymbol{0} & \boldsymbol{0} \\ \left(\nabla_\varphi \boldsymbol{S}\right)^T & \nabla_\alpha \boldsymbol{N} & \nabla_\alpha \boldsymbol{S} & \nabla \boldsymbol{g}_A & \nabla \boldsymbol{g}_I \\ \boldsymbol{0} & \boldsymbol{0} & 2\boldsymbol{Z}_A\left(\nabla \boldsymbol{g}_A\right)^T & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{0} & 2\boldsymbol{C}_I \end{bmatrix}, \tag{69}$$

where $A \equiv \left\{j \,\middle|\, g_j = 0\right\}$ and $I \equiv \left\{j \,\middle|\, g_j < 0\right\}$ denote the set of indexes corresponding to the active and inactive constraints, respectively, and

$$\nabla_\varphi \boldsymbol{N}^* \equiv \left(\partial^2 P / \partial\varphi_p \partial\varphi_r + \left\langle \boldsymbol{y}, \partial^2 \boldsymbol{N} / \partial\varphi_p \partial\varphi_r \right\rangle_m \right)_{m\times m}, \tag{70}$$

$$\nabla_\varphi \boldsymbol{S} \equiv \left(\partial^2 P / \partial\varphi_p \partial\alpha_q + \left\langle \boldsymbol{y}, \partial^2 \boldsymbol{N} / \partial\varphi_p \partial\alpha_q \right\rangle_m \right)_{m\times i}, \tag{71}$$

$$\nabla_\alpha \boldsymbol{S} \equiv \left(\partial^2 P / \partial\alpha_q \partial\alpha_r + \left\langle \boldsymbol{y}, \partial^2 \boldsymbol{N} / \partial\alpha_q \partial\alpha_r \right\rangle_m + \left\langle \boldsymbol{z}, \partial^2 \boldsymbol{g} / \partial\alpha_q \partial\alpha_r \right\rangle_k \right)_{i\times i}, \tag{72}$$

$$\boldsymbol{Z}_A \equiv diag\left(z_j\right)_{j\in A}, \tag{73}$$

$$\boldsymbol{C}_I \equiv diag\left(g_j\right)_{j\in I}\ , \tag{74}$$

$$\nabla \boldsymbol{g}_A \equiv \left(\partial g_j / \partial \alpha_q\right)_{(j\in A)\times i}\ , \tag{75}$$

$$\nabla \boldsymbol{g}_I \equiv \left(\partial g_j / \partial \alpha_q\right)_{(j\in I)\times i}\ . \tag{76}$$

Note that in the two extreme situations when the constraints are either all inactive or all active, the matrices $\nabla \boldsymbol{g}_A$ and $2\boldsymbol{Z}_A\left(\nabla \boldsymbol{g}_A\right)^T$ or, respectively, the matrices $\nabla \boldsymbol{g}_I$ and $\boldsymbol{C}_I$ disappear from the structure of $\boldsymbol{F}'(\boldsymbol{u})$ in Eq. (69). Note also that in the equivalence (64) $\Leftrightarrow$ (67), all inequalities have disappeared from $\boldsymbol{F}(\boldsymbol{u}) = \boldsymbol{0}$. Furthermore, it can be shown that the Jacobian $\boldsymbol{F}'(\boldsymbol{u})$ is nonsingular at the zeros of $\boldsymbol{F}(\boldsymbol{u})$ so efficient numerical methods, such as locally superlinearly convergent quasi-Newton methods, can be used to find these zeros. The Jacobian $\boldsymbol{F}'(\boldsymbol{u})$ vanishes, though, at the bifurcation and limit/turning points present in our system. Such critical points need to be located by using global methods that are capable of avoiding local non-convergence problems (a class of such methods has been suggested by Cacuci, 1990).

The optimization theory framework operating and controlling an ADS leads to Eq. (64) or, alternatively, Eq. (67), which imposes the following requirements:

1. δL be stationary with respect to $\delta \boldsymbol{y}$, implying that $N(\varphi^*,\alpha^*) = \boldsymbol{0}$ at the optimal operating point (φ^*,α^*). Note that $N(\varphi^*,\alpha^*) = \boldsymbol{0}$ is the mathematical expression of the fact that the coupled neutronics/thermal hydraulic balance equations must properly describe the ADS time-space behavior at the optimal operating point (φ^*,α^*).
2. δL be stationary with respect to $\delta \varphi$, implying that $\boldsymbol{y}^*$ must satisfy at (φ^*,α^*) the adjoint equation $\boldsymbol{N}^*(\varphi^*,\boldsymbol{y}^*,\alpha^*) \equiv \left\{\nabla_\varphi \boldsymbol{N}\right\}_{(\varphi^*,\alpha^*)} \boldsymbol{y}^* + \left\{\nabla_\varphi P\right\}_{(\varphi^*,\alpha^*)} = \boldsymbol{0}$. Note that this equation is actually the proper adjoint equation (including the adjoint prompt neutron equation, the adjoint precursors equations, and the adjoint thermal-hydraulics equations, etc.) that must be solved at the optimal operating point (φ^*,α^*). It is thus clear that the appropriate source-term for the ADS adjoint equation is not some fission reaction rate or accelerator power, etc., but is (mathematically speaking), the partial Gateaux-derivative of the ADS design objectives, $P(\varphi,\alpha)$, evaluated at the optimal operating point (φ^*,α^*). Note that $P(\varphi,\alpha)$ incorporates all ADS relevant parameters, including those from neutron physics and thermal-hydraulics considerations.
3. δL be stationary with respect to δz, implying that the respective constraints must be satisfied at the optimal operating point (φ^*,α^*).

4. δL be stationary with respect to $\delta\alpha$, implying that the relationship $S(\varphi^*,y^*,\alpha^*,z^*) \equiv \{\nabla_\alpha P\}_{(\varphi^*,\alpha^*)} + \{\nabla_\alpha N\}_{(\varphi^*,\alpha^*)} \; y^* + \{\nabla_\alpha g\}_{(\varphi^*,\alpha^*)} z^* = \mathbf{0}$ must be satisfied at the optimal operating point (φ^*,α^*). Note that this requirement is in contradistinction to the framework of first-order perturbation theory, which would require that $S(\varphi^*,y^*,\alpha^*,z^*) \neq \mathbf{0}$

Conditions (1) through (4) above constitute a system of $2m+i+k$ equations whose solutions yield the optimal operating point(s) (φ^*,α^*), which optimize the performance parameters (responses) $P(\varphi^*,\alpha^*)$ envisaged for optimal operation and control of the ADS. Note the important fact that condition (4) above cannot be imposed in the framework of perturbation theory, since δL cannot be required to vanish for arbitrary variations $\delta\alpha$ around a predetermined, fixed point, (φ_o,α_o), which is considered to be a priori known within the framework of perturbation theory. Clearly, δL will vanish for arbitrary variations $\delta\alpha$ only if the point (φ_o,α_o), considered to be "known" within the framework of perturbation theory, happens to coincide with the optimal operating point (φ^*,α^*).

6.2 MAIN CHARACTERISTICS OF THE NEW CONCEPTUAL FRAMEWORK FOR ADS OPTIMAL OPERATION AND CONTROL

As has been indicated in items 1 through 4 above, the new conceptual framework for ADS operation and control unambiguously specifies the optimal state for the ADS, once the objective has been specified. In particular, there is no need to concoct any "fictitious ADS steady-state", or to argue about the form and sources of the adjoint equations, since they are also unambiguously and optimally specified.

Furthermore, the new conceptual framework for ADS operation and control proposed in the foregoing also incorporates sensitivity analysis of response changes caused by small variations in ADS parameters, including variations such as would be induced by control rod adjustment in the sub-critical core, around any ADS operating point in phase space. Thus, if some parameters were changed (e.g., small changes in the absorption or fission cross sections, or coolant properties, or target properties, or source properties) from their nominal values α_o to "perturbed" values $\alpha = \alpha_o + \delta\alpha$, then the first order sensitivities of the response $P(\varphi,\alpha)$ can be routinely obtained within the general optimization-theory conceptual framework proposed here, as follows:

(a) To begin with, all of the constraints $g(\alpha)$ which are to remain strict equalities over the considered range of variations $\delta\alpha$ of the parameters α are to be included formally within the definition of $N(\varphi,\alpha)$, thereby redefining (i) the parameters α that are to be considered as independent variables; hence, the inequality constraints $g_j(\alpha)$ which remain inactive at α_0; i.e., $g_j(\alpha_0) < 0$ produce, by definition, inactive corresponding Lagrange multipliers, namely $z_0 = \mathbf{0}$ (ii) the definition and structure of the vector φ of dependent variables, to an augmented vector, say $\boldsymbol{\psi} \equiv (\varphi,\boldsymbol{\beta})$, where $\boldsymbol{\beta}$ denotes the ADS parameters which are determined by the active equality constraints $g(\alpha)$, and (iii) the definition of the operator $N(\varphi,\alpha)$, which will change to the concatenated operator $M(\boldsymbol{\psi},\boldsymbol{\sigma}) \equiv (N(\varphi,\alpha), g(\alpha))^T$, where $\boldsymbol{\sigma}$ denotes the parameters for which sensitivity analysis is envisaged, and where the symbol T denotes "transposition".

(b) Next, obtain the corresponding nominal values $\boldsymbol{\psi}_o$, of the state variables $\boldsymbol{\psi}$, by solving the (forward) ADS-equations $M(\boldsymbol{\psi},\boldsymbol{\sigma}) = \mathbf{0}$.

(c). Obtain the nominal values $\mathbf{w}_o$, of the corresponding adjoint functions $\mathbf{w}$, by solving the adjoint equations

$$\boldsymbol{M}^*\left(\boldsymbol{\psi}_o,\boldsymbol{\sigma}_o,\mathbf{w}_o\right)\equiv\left\{\nabla_\psi \boldsymbol{N}\right\}_{(\psi_o,\sigma_o)}\mathbf{w}_o+\left\{\nabla_\psi P\right\}_{(\psi_o,\sigma_o)}=\mathbf{0}. \tag{77}$$

Note, once again, that the adjoint equations, including their appropriate source terms are unambiguously defined.

(d) Finally, compute the first-order sensitivities of the response $P(\varphi,\alpha)$ around the desired operating point $(\boldsymbol{\psi}_o,\boldsymbol{\sigma}_o,\mathbf{w}_o)$ by using the resulting expression

$$\boldsymbol{S}(\varphi_o,\boldsymbol{y}_o,\alpha_o,z_o)=\left\{\nabla_\alpha P\right\}_{(\varphi_o,\alpha_o)}+\left\{\nabla_\alpha \boldsymbol{N}\right\}_{(\varphi_o,\alpha_o)}\boldsymbol{y}_o+\left\{\nabla_\alpha \boldsymbol{g}\right\}_{(\varphi_o,\alpha_o)}\boldsymbol{z}_o\ , \tag{78}$$

where the contributions from the active constraints have been explicitly written out as the last term on the right-side of the above equation.

(e) once the sensitivities $\boldsymbol{S}(\varphi_o,\boldsymbol{y}_o,\alpha_o,z_o)$ have been obtained, they can be used for a variety of purposes, including uncertainty analysis or calculation of predicted response variations (a la first-order perturbation-theory), by using the formula

$$\Delta P(\varphi_o,\boldsymbol{y}_o,\alpha_o,z_o)=\delta\alpha\bullet\boldsymbol{S}(\varphi_o,\boldsymbol{y}_o,\alpha_o,z_o)+O\left(\|\Delta\alpha\|^2,\|\Delta\varphi\|^2\right), \tag{79}$$

Last, but not least, it should be noted that the conceptual framework for ADS operation and control proposed here is modular, in that it allows step-by-step introduction of as many equations (describing as many physical phenomena) as desired. Thus, for example, the transport equations describing the neutron distribution in the ADS could constitute the starting point; thermal-hydraulics equations, including heat transfer through the ADS structure could be added next, etc. The respective adjoint equations would also be introduced gradually, via an augmentation procedure, by taking advantage of the block-matrix structure of the proposed conceptual framework, cf. Eqs. (47)-(79), and using the same conceptual procedure as recently used by Cacuci et al (2002) for the reactor safety code system RELAP V/MOD 3.3.

7. CONCLUSIONS

The purpose of this Eugene P. Wigner Lecture at PHYSOR 2002 has been to review the current methods and experiments proposed for the dynamic operation and control of future ADS. It has been shown that the currently proposed methods are based on the original ideas of Wigner, which are eminently applicable to critical reactors, where reactivity changes can be described by perturbation theory around a physically meaningful steady-state (namely, the reactor's critical state) around which the spatial shape functions are expected to vary slowly. However, the Paradigm ADS Neutron Kinetics Model formulated in Sec. 4 has underscored the fact that the effects of the driving (spallation neutron) source in an ADS cannot be described by perturbation theory as developed for critical reactors. It has also been shown that the interface coupling between the target and the sub-critical core region plays a key role in controlling and operating the respective ADS and it, too, cannot de adequately described by perturbation theory or k-eigenfunctions expansion in the traditional manner (as done for critical reactors). This is because, conceptually, the paradigm describing a critical reactor is that of maintaining and controlling a self-sustained reaction, whereas the paradigm describing an ADS should be that of optimal control of an externally driven system. Not only physically, but also mathematically, the two problems are fundamentally distinct: mathematically, the critical reactor is a described by a homogeneous eigenvalue problem for the non-zero (self-sustaining) flux solution, whereas the ADS is described by an inhomogeneous problem where the corresponding homogeneous problem should by design admit only the identically zero flux solution. This is the basic reason why, for example, it is quite difficult to find a practically useful "fictitious ADS steady-state", which is required by the traditional perturbation-theory-based methods to work.

Therefore, a new conceptual framework has been proposed here for describing an ADS, by adopting an optimal control theory point of view rather than the traditional perturbation theory point of view. This new conceptual framework encompasses not only the time- and space-behavior of the coupled neutron kinetics but also the ADS thermal-hydraulic balance equations, and is based on optimization and optimal control of ADS operational objectives, which would include minimization of local flux disturbances, load and source following, etc. In particular, this new conceptual framework makes no use of a "fictitious ADS steady-state", as required by the traditional approaches, and, also in contradistinction to the traditional approaches, delivers the correct and complete (i.e., including sources) adjoint equations, without leaving any room for ambiguities. Thus, the optimal-control conceptual framework proposed in Sec. 6 provides a natural basis for developing the new computational code systems needed for realistic operation and control of ADS.

The considerations highlighted in this Wigner Keynote Lecture should be viewed as emphasizing the need for developing new, dedicated computational procedures, based on principles of control theory (rather than criticality), for describing the space-time behavior of ADS. Thus, the experimental program MUSE (see, e.g., Salvatores at al, 1996) is very useful for measuring the material properties of various configurations of sub-critical cores. Similarly, the experiments proposed within the TRADE Project are useful to obtain preliminary information about the respective sub-critical core configuration in the TRIGA reactor. However, the currently proposed TRADE experiments cannot elucidate the time-space coupling between the driver (spallation target) and the driven sub-critical TRIGA core. Additional experiments, truly relevant for an ADS, still remain to be conceived; our current research also aims at suggesting such experiments based on the conceptual framework presented in this Wigner Keynote Lecture.

In parting, it is perhaps appropriate to note that Wigner holds 37 US Patents on nuclear reactors, including: graphite-moderated reactors; air-cooled graphite-moderated reactors; D_2O-moderated reactors; molten salt and slurry-circulating reactors; thermal and fast breeders and converters; including the basic patents on liquid-metal fast breeders, (with Na, Na-Ka, Bi, and Pb-Bi coolants), material testing reactors, as well as numerous designs of separation methods, shaped fissionable bodies, shields and components. Remarkably, though, Wigner has never considered accelerator driven sub-critical systems, and has therefore not provided solutions for such systems, too, in addition to all of the other fundamental contributions he made to physical and engineering sciences! The development of experiments and computational tools appropriate for designing and controlling ADS remains, therefore, a challenge for future research.

ACKNOWLEDGEMENTS

The topic of this PHYSOR 2002 Wigner Keynote Lecture has been motivated by the lectures and discussions attended by the author within the framework of the 2002 Frederic Joliot / Otto Hahn Summer School on the Modern Reactor Physics and the Modeling of Complex Systems, held August 21-30, 2002, in Cadarache, France (2002), which was dedicated to ADS. The support of the Forschungszentrum Karslruhe (Germany), through the Energy Research Division directed by Dr.

Peter Fritz, and of the Commissariat a L'Energie Atomique (France), through the Nuclear Energy Directorate directed by Dr. Jacques Bouchard, is gratefully acknowledged.

REFERENCES

1. E.P. Wigner, "Effect of Small Perturbations on Pile Period", The Collected Works of Eugene Paul Wigner, page 540, Springer Verlag, Berlin (1992).
2. A.M. Weinberg and E.P. Wigner, The Physical Theory of Neutron Chain Reactors, University of Chicago Press, Chicago, Ill, USA (1958).
3. G.I. Bell and S. Glasstone, Nuclear Reactor Theory", Van Nostrand Reinhold Company, New York (1970).
4. A.F. Henry, Nuclear-Reactor Analysis, MIT Press, Boston, USA, Fourth printing (1986).
5. W.M. Stacey, Jr., Space-Time Nuclear Reactor Kinetics, Academic Press, New York, USA (1969).
6. M. Ash, Nuclear Reactor Kinetics, McGraw-Hill, New York, USA (1979).
7. K.O. Ott, R.J. Neuhold, Introductory Nuclear Reactor Dynamics, American Nuclear Society, LaGrange Park, Ill, USA (1985).
8. P. Seltborg, "The Sub-Critical Core and the Simulation Tools", Frederic Joliot / Otto Hahn Summer School on the Modern Reactor Physics and the Modelling of Complex Systems, August 21-30, 2002, Cadarache, France (2002).
9. M. Carta, and A. D'Angelo, "Subcriticality Level Evaluation in Accelerator Driven Systems by Harmonic Modulation of the External Source", Nucl. Sci. Eng., 133, 282-292 (1999).
10. TRADE Final Feasibility Report, prepared by the Working Group on TRADE, p. 127-134, March (2002).
11. I. Slessarev and A. Tchistiakov, "IAEA-ADS Benchmark, Stage 1: Results and Analysis", TCM-Meeting, September 17-19, 1997, Madrid, Spain (1997); see also: M. Salvatores, et al, "The Potential of Accelerator-Driven Systems for Transmutation of Power Production Using Thorium or Uranium Fuel Cycles", Nucl. Sci. Eng., 126, 333-340 (1997).
12. A. Gandini and M. Salvatores, "The Physics of Subcritical Multiplying Systems", J. Nucl. Sci. Eng. (Japan), 39, 673-686, (2002).
13. D. G. Cacuci, "Global Optimization and Sensitivity Analysis", Nucl. Sci. Eng., 104, 78-88 (1990).
14. F. Groeschel, "The MEGAPIE Project: An Overview", MEGAPIE Technical Review Meeting, Bologna, March 5-6, 2002 (2002).
15. D.G. Cacuci, M. Ionescu-Bujor, and X. Jin, "Sensitivity Analysis Of The Quench-04 Nuclear Safety Experiment Using The Adjoint Sensitivity Analysis Procedure (ASAP) In Relap5/Mod3.2 Code System", Physor 2002 International Conference on the New Frontiers of Nuclear Technology : Reactor Physics, Safety and High-Performance Computing, October 7-10, 2002, Seoul, Korea (2002).