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Variational Principles for Functionals of the  
Solution to Linear Equations**

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***FUSION TECHNOLOGY INSTITUTE  
UNIVERSITY OF WISCONSIN  
MADISON WISCONSIN***

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E.T. Cheng and R.W. Conn

Fusion Technology Institute  
University of Wisconsin  
1500 Engineering Drive  
Madison, WI 53706

<http://fti.neep.wisc.edu>

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Principles for Functionals of the Solution to Linear Equations

by

Edward T. Cheng  
Robert W. Conn

Nuclear Engineering Department  
The University of Wisconsin  
Madison, Wisconsin 53706

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Abstract

A method is derived for using variational expressions to interpolate among known values of a functional of the solution to linear equations. For linear functionals of the solution to an inhomogeneous equation, the interpolation expression is exact at  $N$  distinct points when  $N$  distinct functions are used, each of which is the solution of the underlying Euler equation. Two point variational interpolation is derived to interpolate on the value of an eigenvalue using the Rayleigh quotient. Illustrative examples are given based on neutron transport studies of fusion reactor blanket systems and applications to sensitivity and optimization studies in reactor theory are discussed.

## I. Introduction

Variational theory has been widely used in mathematical physics to evaluate functionals or to derive approximate theories. In the former application, the motivation for using variational techniques is the fact that errors are second order with respect to inaccuracies in trial functions. An additional motivation is that one is often actually interested in a functional of the solution to an equation describing a physical system, rather than in the solution itself. Examples are the evaluation of transport coefficients for gases and plasmas and the evaluation of various scalar products of the neutron or gamma flux in fission and fusion reactor neutronics studies. In general, it is of interest to estimate inner products of the form

$$(S^\dagger, \phi) \tag{1}$$

where  $\phi$  satisfies a linear inhomogeneous equation

$$L\phi = S . \tag{2}$$

The adjoint equation is

$$L^\dagger \phi^\dagger = S^\dagger . \tag{3}$$

In neutron transport theory,  $L$  is the Boltzmann transport operator<sup>(1)</sup> and  $S$  is a source.

Two widely used variational principles to estimate linear functionals of the solution to an inhomogeneous equation are the Schwinger<sup>(2)</sup> and Roussopoulos<sup>(3)</sup> variational principles. Both these principles have been generalized by Pomraning<sup>(4)</sup> to provide an estimate of an arbitrary functional, rather than just a linear one. Several recent papers have also treated the problem of estimating changes in a functional of interest<sup>(5,6)</sup> using variational forms accurate to second order in the change.<sup>(7)</sup>

In this paper, a method for using variational expressions to interpolate among known values of a given functional is derived. The linear operator,  $L(\alpha)$ , is assumed to depend in some known way on a set of parameters,  $\alpha$ . To estimate the

effect of changes in  $\alpha$  on the functional of interest, e.g.,  $(S^\dagger, \phi)$ , the standard procedure has been to let  $\alpha = \alpha_1$ , be defined as a reference system and to use  $L(\alpha_1)$  and  $L^\dagger(\alpha_1)$  to determine solutions,  $\phi_1$  and  $\phi_1^\dagger$ . Then  $\phi_1$  and  $\phi_1^\dagger$  are used as trial functions in either the Schwinger or Roussopoulos functionals to assess the effect of changing  $\alpha$  on the response functional of interest. Often, the perturbation introduced is large and/or more than one reference system is appropriate. In such cases, the method of variational interpolation to be described here can be used to interpolate among several reference values. For linear functionals, an expression is derived which is exact at an arbitrary number of reference points and which can be used to interpolate among them. Two point variational interpolation is derived to interpolate on the value of an eigenvalue using the Rayleigh quotient. Some illustrative numerical examples are given based on neutron transport studies of fusion reactor blanket systems which have recently become of greatly increased interest.<sup>(8)</sup>

## II. Theory of Variational Interpolation

### a. Linear Functionals and Inhomogeneous Equations

The simplest illustration of the basic idea is to consider two point variational interpolation for linear functionals of the solution to a linear inhomogeneous equation. Letting  $(S^\dagger, \phi)$  be the linear functional of interest, the Roussopoulos functional,

$$I_R[\phi^\dagger, \phi; \alpha] = (S^\dagger(\alpha), \phi) + (\phi^\dagger, S(\alpha) - L(\alpha)\phi) \quad (4)$$

is stationary about the exact value of  $(S^\dagger(\alpha), \phi)$  with Euler equations

$$L(\alpha)\phi = S(\alpha) \quad (5)$$

$$L^\dagger(\alpha)\phi^\dagger = S^\dagger(\alpha) \quad (6)$$

As noted,  $\alpha$  represents parameters in the operator  $L$  (for example, cross sections or densities when  $L$  is the Boltzmann transport operator) and  $S$  and  $S^\dagger$  may depend on  $\alpha$ . Let us now characterize two reference systems by the parameters  $\alpha_1$  and  $\alpha_2$ . To estimate  $(S^\dagger(\alpha), \phi)$  at a point  $\alpha$  not the same as  $\alpha_1$  or  $\alpha_2$ , we chose trial functions  $\phi_1$  and  $\phi_2^\dagger$  which satisfy, respectively,

$$L(\alpha_1)\phi_1 = S(\alpha_1) \quad (7)$$

$$L^\dagger(\alpha_2)\phi_2^\dagger = S^\dagger(\alpha_2) \quad (8)$$

The simplest form of the method of variational interpolation follows from noting that the functional

$$I_R[\phi_2^\dagger, \phi_1; \alpha] = (S^\dagger(\alpha), \phi_1) + (\phi_2^\dagger, S(\alpha) - L(\alpha)\phi_1) \quad (9)$$

is exact at both reference points. Clearly, for  $\alpha = \alpha_1$ , the operator  $L$  is  $L(\alpha_1)$ , the source is  $S(\alpha_1)$  and  $S^\dagger$ . Thus, the second term in eq. (9) is zero and  $I_R[\phi_2^\dagger, \phi_1; \alpha_1]$  is exact. For a system with  $\alpha = \alpha_2$ , where  $L = L(\alpha_2)$ ,  $S = S(\alpha_2)$  and  $S^\dagger = S^\dagger(\alpha_2)$ , we use

$$(\phi_2^\dagger, L(\alpha_2)\phi_1) = (S^\dagger(\alpha_2), \phi_1) \quad (10)$$

from which it follows that  $I_R[\phi_2^\dagger, \phi_1; \alpha]$  is also exact. Thus, the functional  $I_R[\phi_2^\dagger, \phi_1; \alpha]$  can be used to interpolate in  $\alpha$  and thus estimate other values of the basic functional.

The Schwinger functional,

$$I_S[\phi_2^\dagger, \phi, \alpha] = \frac{(S^\dagger(\alpha), \phi)(\phi_2^\dagger, S(\alpha))}{(\phi_2^\dagger, L(\alpha)\phi)} \quad (11)$$

is also exact at  $\alpha = \alpha_1$  and  $\alpha = \alpha_2$  when  $\phi = \phi_1$  and  $\phi_2^\dagger = \phi_2^\dagger$  are used as input functions. The proof is equally straightforward. At  $\alpha = \alpha_1$ , use eq. (7) to show that  $I_S[\phi_2^\dagger, \phi_1; \alpha_1] = (S^\dagger(\alpha_1), \phi_1)$ . At  $\alpha = \alpha_2$ , again use

eqn. (10) to find  $I_S[\phi_2^\dagger, \phi_1; \alpha_2] = (\phi_2^\dagger, S(\alpha_2))$

which, of course, is equal to  $(S^\dagger(\alpha_2), \phi_2)$ . Thus, the Schwinger functional can equally well be employed to interpolate in  $\alpha$  and it can have advantages over the Roussopoulos functional, as has been discussed recently.<sup>(9)</sup> We will expand on this shortly.

A three point interpolation formula can readily be derived and it suggests the procedure to follow in constructing a general proof. Consider three reference systems,  $\alpha_1$ ,  $\alpha_2$ , and  $\alpha_3$ , and the trial functions

$$\phi_T(\alpha) = \phi_1 + a(\alpha)(\phi_2 - \phi_1) \quad (12)$$

$$\phi_T^\dagger(\alpha) = b(\alpha)\phi_3^\dagger \quad (13)$$

where  $\phi_1$ ,  $\phi_2$ , and  $\phi_3^\dagger$  are solutions to the appropriate equations for the subscripted reference points. Insert  $\phi_T(\alpha)$  and  $\phi_T^\dagger(\alpha)$  into  $I_R(\phi_T^\dagger, \phi_T; \alpha)$  and solve the equations  $\frac{\partial I_R}{\partial a} = 0$ ,  $\frac{\partial I_R}{\partial b} = 0$ . This yields

$$a(\alpha) = \frac{(\phi_3^\dagger, S(\alpha) - L(\alpha)\phi_1)}{(\phi_3^\dagger, L(\alpha)(\phi_2 - \phi_1))} \quad (14)$$

$$b(\alpha) = \frac{(S^\dagger(\alpha), \phi_2 - \phi_1)}{(\phi_3^\dagger, L(\alpha)(\phi_2 - \phi_1))} \quad (15)$$

Using these expressions in  $\phi_T$  and  $\phi_T^\dagger$  gives the functional

$$I_3[\phi_T^\dagger, \phi_T; \alpha] = (S^\dagger(\alpha), \phi_1) + \frac{(\phi_3^\dagger, S(\alpha) - L(\alpha)\phi_1)(S^\dagger(\alpha), \phi_2 - \phi_1)}{(\phi_3^\dagger, L(\alpha)(\phi_2 - \phi_1))} \quad (16)$$

which is exact when  $\alpha$  equals  $\alpha_1$ ,  $\alpha_2$ , or  $\alpha_3$ .

A general proof can be constructed for N forward trial functions and N-1, N, or N+1 distinct adjoint trial functions (or N adjoint functions and N-1, N, or N+1 distinct forward functions.) The proof for 2N distinct reference



systems proceeds as follows. Let

$$\phi_T(\alpha) = \phi_1 + \sum_{i=2}^N a_i(\alpha) (\phi_i - \phi_1) \quad (17)$$

and

$$\phi_T^\dagger(\alpha) = \phi_{N+1}^\dagger + \sum_{i=N+2}^{2N} b_i(\alpha) (\phi_i^\dagger - \phi_{N+1}^\dagger) \quad (18)$$

where the  $\phi_i$  satisfy

$$L(\alpha_i)\phi_i = S(\alpha_i) \quad (19)$$

and the  $\phi_i^\dagger$  satisfy

$$L^\dagger(\alpha_i)\phi_i^\dagger = S^\dagger(\alpha_i) \quad (20)$$

All  $\alpha_i$  are distinct and the indices can clearly be arbitrarily assigned.

Inserting eqns. (17) and (18) into  $I_R[\phi_T^\dagger, \phi_T; \alpha]$  and carrying out a Rayleigh-Ritz procedure, ( $\frac{\partial I_R}{\partial a_i} = 0$ ,  $\frac{\partial I_R}{\partial b_i} = 0$ ), the following set of coupled algebraic equations are obtained:

For the coefficients,  $a_i(\alpha)$ :

$$\begin{aligned} & a_2(\alpha) ((\phi_i^\dagger - \phi_{N+1}^\dagger), L(\alpha)(\phi_2 - \phi_1)) \\ & + a_3(\alpha) ((\phi_i^\dagger - \phi_{N+1}^\dagger), L(\alpha)(\phi_3 - \phi_1)) + \dots \\ & + a_N(\alpha) ((\phi_i^\dagger - \phi_{N+1}^\dagger), L(\alpha)(\phi_N - \phi_1)) = ((\phi_i^\dagger - \phi_{N+1}^\dagger), S(\alpha) - L(\alpha)\phi_1) \end{aligned} \quad (21)$$

$$i = N + 2, N + 3, \dots, 2N$$

For the coefficients,  $b_i(\alpha)$ :

$$\begin{aligned} & b_{N+2}(L^\dagger(\alpha)(\phi_{N+2}^\dagger - \phi_{N+1}^\dagger), (\phi_i - \phi_1)) \\ & + b_{N+3}(L^\dagger(\alpha)(\phi_{N+3}^\dagger - \phi_{N+1}^\dagger), (\phi_i - \phi_1)) + \dots \\ & + b_{2N}(L^\dagger(\alpha)(\phi_{2N}^\dagger - \phi_{N+1}^\dagger), (\phi_i - \phi_1)) = (S^\dagger(\alpha) - L^\dagger(\alpha)\phi_{N+1}^\dagger, (\phi_i - \phi_1)) \end{aligned} \quad (22)$$

$$i = 2, 3, \dots, N$$

The functional  $I_{2N}[\phi_T^\dagger, \phi_T; \alpha]$  is formed by using eqns. (17) and (18) as trial functions with coefficients  $\{a_i(\alpha)\}$  and  $\{b_i(\alpha)\}$  determined by solving eqns. (21) and (22). To prove that  $I_{2N}[\phi_T^\dagger, \phi_T; \alpha]$  is exact whenever  $\alpha = \alpha_i$ ,  $i = 1, 2, \dots, 2N$  is equivalent to proving that at  $\alpha = \alpha_p$ , one of the trial functions equals the exact solution, i.e., either  $\phi_T = \phi_p$  or  $\phi_T^\dagger = \phi_p^\dagger$ .

For  $\alpha = \alpha_1$  the right hand side of eqn. (21) vanishes. Since the coefficients are linearly independent (the  $\alpha_i$  are distinct), it follows that  $a_i(\alpha_1) = 0$  for  $i = 2, 3, \dots, N$ . Thus,  $\phi_T(\alpha_1) = \phi_1$  and  $I_{2N}[\phi_T^\dagger, \phi_T; \alpha_1]$  is exact. For  $\alpha = \alpha_k \neq \alpha_1$ , rewrite the right hand side of eqn. (21) as

$$((\phi_1^\dagger - \phi_{N+1}^\dagger), S(\alpha_k) - L(\alpha_k)\phi_1) = ((\phi_1^\dagger - \phi_{N+1}^\dagger, L(\alpha_k)(\phi_k - \phi_1)). \quad (23)$$

Then the coupled algebraic equations become

$$\begin{aligned} & a_2((\phi_1^\dagger - \phi_{N+1}^\dagger), L(\alpha_k)(\phi_2 - \phi_1)) + \dots \\ & + (a_k - 1)((\phi_1^\dagger - \phi_{N+1}^\dagger), L(\alpha_k)(\phi_k - \phi_1)) + \dots \\ & + a_N((\phi_1^\dagger - \phi_{N+1}^\dagger), L(\alpha_k)(\phi_N - \phi_1)) = 0. \end{aligned} \quad (24)$$

In this form, we see that the linear independence of the inner product coefficients again implies

$$a_2 = a_3 = \dots = a_{k-1} = \dots = a_N = 0. \quad (25)$$

Thus,  $a_i = \delta_{ik}$ ,  $\phi_T(\alpha_k) = \phi_k$ , and this guarantees that  $I_{2N}[\phi_T^\dagger, \phi_T; \alpha_k]$  is exact for any  $k = 2, 3, \dots, N$ . Therefore, we have proven that  $I_{2N}[\phi_T^\dagger, \phi_T; \alpha]$  is exact whenever  $\alpha = \alpha_1, \alpha_2, \dots, \alpha_N$ .

Similar arguments applied to eqn. (22) prove that for  $\alpha = \alpha_k$ ,  $k = N+1, N+2, \dots, 2N$ ,  $I_{2N}[\phi_T^\dagger, \phi_T; \alpha_k]$  is also exact. Thus,  $I_{2N}[\phi_T^\dagger, \phi_T; \alpha]$  involves  $2N$  distinct trial functions and takes on the exact value for the

corresponding  $2N$  distinct reference systems. This functional can therefore be used to interpolate in  $\alpha$  among these exact values and constitutes a multipoint variational interpolation. A proof for  $N$  reference  $\phi$  functions and  $N-1$  or  $N+1$  distinct reference adjoint functions can be carried through following the same procedure.

The form of the error term in variational interpolation can be illustrated by examining the two point formula. Again consider the linear functional,  $R(\alpha) = (S^\dagger(\alpha), \phi)$ , of the solution of a linear inhomogeneous equation. When an altered  $S^\dagger = S_T^\dagger$  and an altered  $\phi = \phi_T$  are used, the first order change relative to the reference point in  $R$  is given by

$$\delta R = (\delta S^\dagger, \phi) + (S^\dagger, \delta \phi) \quad (26)$$

where  $\delta S^\dagger = S_T^\dagger - S^\dagger$  and  $\delta \phi = \phi_T - \phi$ . This expression is the sum of an error term due to the perturbation itself, which changes  $S^\dagger$ , and the error induced because the perturbation in turn effects the solution. The change,  $\delta R$ , can be rewritten using  $L\delta\phi = -\delta L\phi + \delta S$  where the operator  $L_T$  has been written as  $L + \delta L$  and  $S_T$  as  $S + \delta S$ .  $\delta R$  becomes

$$\delta R = (\delta S^\dagger, \phi) + (\phi^\dagger, \delta S) - (\phi^\dagger, \delta L\phi). \quad (27)$$

Assume  $\delta S$ ,  $\delta S^\dagger$ , and  $\delta L$  depend linearly on the change in a parameter  $\alpha$  so that

$$\delta S = s\delta\alpha, \quad (28-a)$$

$$\delta S^\dagger = s^\dagger\delta\alpha, \quad (28-b)$$

and

$$\delta L = H\delta\alpha. \quad (29)$$

Then the derivative of  $R$  with respect to  $\alpha$  at the reference value  $\alpha_1$  is

$$\left. \frac{\delta R}{\delta \alpha} \right|_{\alpha_1} = (s^\dagger, \phi_1) + (\phi_1^\dagger, s) - (\phi_1^\dagger, H\phi_1). \quad (30)$$

It is easily shown that both the Roussopoulos functional, eqn. (4), and the Schwinger functional, eqn. (11), also preserve the exact slope at  $\alpha = \alpha_1$  if

trial functions  $\phi_1$  and  $\phi_1^\dagger$  are used.

In the method of variational interpolation, the trial functions are taken at distinct reference points, for example,  $\phi_1$  at  $\alpha = \alpha_1$  and  $\phi_2^\dagger$  at  $\alpha = \alpha_2$ . The slope of the functional does not, however, preserve the exact slope at either  $\alpha_1$  or  $\alpha_2$ . Indeed, for two point interpolation where the changes depend linearly on  $\alpha$ , the Roussopoulos form, eqn. (9) yields a straight line interpolation between  $(S^\dagger(\alpha_1), \phi_1)$  and  $(S^\dagger(\alpha_2), \phi_2)$ . The difference between the slope using eqn. (9) and the exact slope is  $(\delta\phi_{21}^\dagger, H\phi_1 - S)$  where  $\delta\phi_{21}^\dagger = \phi_2^\dagger - \phi_1^\dagger$ .

Variational interpolation using the Schwinger functional comes closer to preserving the slope. Using eqn. (11) with  $\phi_1$  and  $\phi_2^\dagger$  as input functions, the approximate slope is

$$\left. \frac{\partial I_S}{\partial \alpha} \right|_{\alpha_1} = (s^\dagger, \phi_1) - \frac{(S^\dagger(\alpha_1), \phi_1)}{(\phi_2^\dagger, S)} [(\phi_2^\dagger, H\phi_1) - (\phi_2^\dagger, S)] \quad (31)$$

Let  $\Delta(\frac{\partial R}{\partial \alpha})$  be the difference in slope from the exact value. One then finds that

$$\Delta(\frac{\partial R}{\partial \alpha}) = ((\delta\phi_{21}^\dagger - \frac{(\delta\phi_{21}^\dagger, S)}{(\phi_1^\dagger, S)} \phi_1^\dagger), (H\phi_1 - S)) \quad (32)$$

neglecting second order terms. Compared with  $(\delta\phi_{21}^\dagger, H\phi_1)$ , we see now the additional term  $\frac{(\delta\phi_{21}^\dagger, S)}{(\phi_1^\dagger, S)} \phi_1^\dagger$  in the inner product on the right hand side of eqn. (32). This term is independent of the amplitude of  $\phi_1^\dagger$  but does depend on the difference,  $\delta\phi_{21}^\dagger$ . This added term attempts to correct for first order differences in the adjoint functions. This, if the shape of the adjoint function tends to be preserved, the slope will tend to be preserved to second order. Further, interpolation between  $\alpha_1$  and  $\alpha_2$  based on eqn. (11) will not be linear in  $\alpha$ . This is an important distinction between the Roussopoulos and Schwinger functionals which will be clearly illustrated in the

numerical examples. For higher order interpolation, the method used to derive the combining coefficients,  $\{a_i\}$  and  $\{b_i\}$ , is the same as that applied to derive the Schwinger principal from the Roussopoulos functional.<sup>(10)</sup> The interpolation will therefore be nonlinear and should have the same renormalized character as the Schwinger principal.<sup>(9)</sup> Moreover, if one chooses  $\phi_i$  and  $\phi_i^\dagger$  at the same reference point in eqns. (17) and (18), i.e.

$$\phi_T(\alpha) = \phi_1 + \sum_{i=2}^N a_i(\alpha)(\phi_i - \phi_1) \quad (17-a)$$

$$\phi_T^\dagger(\alpha) = \phi_1^\dagger + \sum_{i=2}^N b_i(\alpha)(\phi_i^\dagger - \phi_1^\dagger) \quad (18-a)$$

the general procedure is equivalent to the variational synthesis method discussed by Kaplan.<sup>(11)</sup>

Now consider the exact form of the error term in two point variational interpolation when  $\phi_1$  and  $\phi_1^\dagger$ , evaluated at  $\alpha = \alpha_1$ , are used as trial functions in the Roussopoulos principle, eqn. (4), to estimate  $(S^\dagger(\alpha), \phi)$ ,  $\alpha \neq \alpha_1$ . The error is

$$\epsilon_R = -(\delta\phi_1^\dagger, L(\alpha)\delta\phi_1) \quad (33)$$

Here,  $\delta S = S - S_1$ ,  $\delta\phi_1 = \phi - \phi_1$ ,  $\delta\phi_1^\dagger = \phi^\dagger - \phi_1^\dagger$  and  $\phi$  and  $\phi^\dagger$  are the exact solutions in system  $\alpha$ . When  $\phi_1$  and  $\phi_2^\dagger$  are used in the variational interpolation method, the error is

$$\epsilon_{VI} = -(\delta\phi_2^\dagger, L(\alpha)\delta\phi_1) + (\delta\phi_2^\dagger, \delta S) \quad (34)$$

(This is another way of proving eqn. (9) is exact at  $\alpha = \alpha_1$  and  $\alpha = \alpha_2$ .) By comparing eqns. (33) and (34), it becomes clear that variational interpolation relies on cancellation of error for  $\alpha$  between  $\alpha_1$  and  $\alpha_2$ . That is, e.g., as  $\alpha$  approaches  $\alpha_1$  from  $\alpha_2$ ,  $\delta\phi_2^\dagger$  is increasing while  $\delta\phi_1$  and  $\delta S$  are tending to zero. Thus, one should not expect great accuracy if  $\alpha$  does not lie between the two reference parameters. Similar error terms can be derived for higher order interpolation formulas and they all show the same basic characteristic of cancellation of error.

#### b. Two Point Variational Interpolation and Homogeneous Equations

The Rayleigh quotient<sup>(4)</sup> is a homogeneous functional which is widely used to estimate eigenvalues. In general, because an eigenvalue equation is homogeneous, only homogeneous functional can be of interest. As such, these functionals are nonlinear and we have not succeeded in constructing N point

variational interpolation procedures in this case. Indeed, because the functionals of interest here are nonlinear, it may not be possible to do so. It is possible, however, to construct the simplest case, two point variational interpolation, and this can sometimes be useful. For example, it is often of interest to determine the sensitivity of an energy level to the interaction potential in quantum mechanics. If the potential is characterized by one or more parameters which can vary over a specified range, interpolation can be used to determine the change in the eigenvalue as the parameters change.

Consider, therefore, the general eigenvalue equation

$$L(\alpha)\phi_i = \lambda_i F(\alpha)\phi_i \quad (35)$$

and the adjoint equation

$$L^\dagger(\alpha)\phi_i^\dagger = \lambda_i F^\dagger(\alpha)\phi_i^\dagger \quad (36)$$

It is assumed that  $L(\alpha)$  and  $F(\alpha)$  are real, though not necessarily self adjoint, and that the eigenvalues  $\lambda_i$  are discrete and nondegenerate.  $\phi_i$  and  $\phi_i^\dagger$  are biorthogonal with respect to  $F(\alpha)$ , i.e.,

$$(\phi_j^\dagger, F\phi_i) = (F^\dagger\phi_j^\dagger, \phi_i) = \delta_{ij} \quad (37)$$

A variational expression for the  $k^{\text{th}}$  eigenvalue is the Rayleigh quotient

$$E_\lambda[\phi_K^\dagger, \phi_K; \alpha] = \frac{(\phi_K^\dagger, L(\alpha)\phi_K)}{(\phi_K^\dagger, F(\alpha)\phi_K)} \quad (38)$$

Consider two systems characterized by  $\alpha_1$  and  $\alpha_2$ . Ordinarily, one evaluates the effect of changes in  $\alpha$  from, e.g.,  $\alpha_1$  by using  $\phi_{1K}$  and  $\phi_{1K}^\dagger$  as trial functions. These functions are solutions of

$$L(\alpha_1)\phi_{1K} = \lambda_K(\alpha_1)\phi_{1K} F(\alpha_1)\phi_{1K} \quad (39)$$

and

$$L^\dagger(\alpha_1)\phi_{1K}^\dagger = \lambda_K(\alpha_1)F^\dagger(\alpha_1)\phi_{1K}^\dagger, \quad (40)$$

respectively. With these trial functions, one proceeds to use  $L(\alpha)$  and  $F(\alpha)$  to evaluate the Rayleigh quotient.

The expression for  $E_\lambda[\phi_{1K}^\dagger, \phi_{1K}; \alpha]$  can be written as

$$E_\lambda[\phi_{1K}^\dagger, \phi_{1K}; \alpha] = \lambda_K(\alpha) \left[ 1 + \frac{(\delta\phi_{1K}^\dagger, L(\alpha)\delta\phi_{1K}) - (\delta\phi_{1K}^\dagger, F(\alpha)\delta\phi_{1K})}{(\phi_{1K}^\dagger, F(\alpha)\phi_{1K})} \right] \quad (41)$$

where  $\delta\phi_{1K} = \phi_K - \phi_{1K}$ ,  $\delta\phi_K^\dagger = \phi_K^\dagger - \phi_{1K}^\dagger$ , and higher order terms have been neglected.

Now consider choosing  $\phi_{1K}$  and  $\phi_{2K}^\dagger$  as trial functions, where  $\phi_{1K}$  satisfies eqn. (39) and  $\phi_{2K}^\dagger$  satisfies

$$L^\dagger(\alpha_2)\phi_{2K}^\dagger = \lambda_K(\alpha_2)F^\dagger(\alpha_2)\phi_{2K}^\dagger. \quad (42)$$

The functional

$$E_\lambda[\phi_{2K}^\dagger, \phi_{1K}; \alpha] = \frac{(\phi_{2K}^\dagger, L(\alpha)\phi_{1K})}{(\phi_{2K}^\dagger, F(\alpha)\phi_{1K})} \quad (43)$$

is exact when  $\alpha$  equals either  $\alpha_1$  or  $\alpha_2$  and can therefore be used to interpolate for  $\lambda_K(\alpha)$  when  $\alpha$  differs from  $\alpha_1$  or  $\alpha_2$ . Further, this functional can be expressed, using  $\delta\phi_{2K}^\dagger = \phi_K^\dagger - \phi_{2K}^\dagger$ , as

$$E_\lambda[\phi_{2K}^\dagger, \phi_{1K}; \alpha] = \lambda_K(\alpha) \left[ 1 + \frac{(\delta\phi_{2K}^\dagger, L(\alpha)\delta\phi_{1K}) - (\delta\phi_{2K}^\dagger, F(\alpha)\delta\phi_{1K})}{(\phi_{2K}^\dagger, F(\alpha)\phi_{1K})} \right] \quad (44)$$

neglecting higher order terms. The cancellation of error characteristic is again clear on examination of the interpolation formula. As  $\alpha$  approaches  $\alpha_1$ ,

$\delta\phi_{2K}^\dagger$  remains finite as  $\delta\phi_{1K}$  tends to zero while the reverse is true as  $\alpha$  tends to  $\alpha_2$ . This is analogous to the result found previously for linear functionals of the solution to an inhomogeneous equation.

### III. Illustrative Numerical Application

To illustrate the application of variational interpolation, we have examined a relevant problem of current interest in the neutron transport analysis of conceptual fusion reactor blanket systems. A quantity of primary interest for a reactor based on fusions of deuterium and tritium is the tritium breeding ratio, i.e., the number of tritons produced in the blanket per triton consumed. The sample blanket is shown in Fig. 1. Tritium is produced by neutron reactions in lithium, particularly the  ${}^6\text{Li}(n,\alpha)t$  and  ${}^7\text{Li}(n,n'\alpha)t$  reactions. We study here the breeding ratio from reactions in  ${}^6\text{Li}$ , labeled  $T_6$ , from  ${}^7\text{Li}$ , labeled  $T_7$ , and the total breeding ratio, labeled BR.  $T_6$ ,  $T_7$  and BR are defined as

$$T_6 = (\Sigma_6(n,\alpha), \phi),$$

$$T_7 = (\Sigma_7(n,n'\alpha), \phi),$$

and

$$\text{BR} = ((\Sigma_6(n,\alpha) + \Sigma_7(n,n'\alpha)), \phi) .$$

$\phi$  is normalized to one incident 14.1 MeV neutron, and  $\Sigma_6(n,\alpha)$  and  $\Sigma_7(n,n'\alpha)$  are the macroscopic, energy and space dependent cross sections for the two pertinent nuclear reactions. This, for  $T_6$ ,  $S^\dagger = \Sigma_6(n,\alpha)$  while for BR,  $S^\dagger = \Sigma_6(n,\alpha) + \Sigma_7(n,n'\alpha)$ .

The numerical evaluation of the inner products required for variational interpolation were carried out using the program, SWANLAKE, <sup>(12)</sup> developed to apply conventional variational procedures. The computational method to solve the neutron transport equation in multigroup form and the nuclear data employed are the same as described previously. <sup>(8)</sup>



The illustrative examples are based on asking the question, "How does the breeding ratio change as a function of the percentage of structural material in the tritium breeding zones?" (zones (2) and (4))

We have chosen 5% structure as reference system  $\alpha_1$  and 25% structure as reference system  $\alpha_2$ . Two point variational interpolation is used in the analysis.  $\phi_1$  and  $\phi_1^\dagger$  have also been used as trial functions in eqns. (4) and (11) to provide a comparison with the more conventional application of variational techniques. The parameters  $\alpha$  used in the theory are the appropriate atomic densities of the materials in zones (2) and (4).

Fig. 2 shows  $T_7$  as a function of the percent structure based on several calculational procedures. The open circles are taken as exact from direct numerical calculation. Zeroth order perturbation theory is simply the evaluation of  $(\Sigma_7, \phi_1)$  where  $\Sigma_7$  changes as the percentage of lithium changes in the breeding zones. The value of  $T_7$  is preserved at the reference point but not the slope. Two point variational interpolation based on the Roussopoulos functional also does not preserve slope but gives correct values at the two reference points. The Roussopoulos functional using  $\phi_1$  and  $\phi_1^\dagger$  as the trial functions preserves both the value of  $T_7$  and the slope at reference point  $\alpha_1$  but is quite inaccurate at  $\alpha = \alpha_2$ . Finally, two point variational interpolation based on the Schwinger functional, eqn. (11), is exact when  $\alpha$  equals  $\alpha_1$  or  $\alpha_2$  and yields a nonlinear interpolation that is quite close to the exact values for  $\alpha$  between  $\alpha_1$  and  $\alpha_2$ .

As a second example, the change in BR,  $T_6$ , and  $T_7$  as a function of the fraction of  ${}^6\text{Li}$  making up the lithium in zones (2) and (4) has been evaluated. (Natural lithium is 7.42%  ${}^6\text{Li}$  and 92.58%  ${}^7\text{Li}$ .) Two point interpolation has been used with  $\alpha_1$  at 7.42%  ${}^6\text{Li}$  and  $\alpha_2$  at 30%  ${}^6\text{Li}$ . The results are given in Fig. 3 with the open circles indicating exact values. Again, formula (11) yields a nonlinear interpolation between the reference values.

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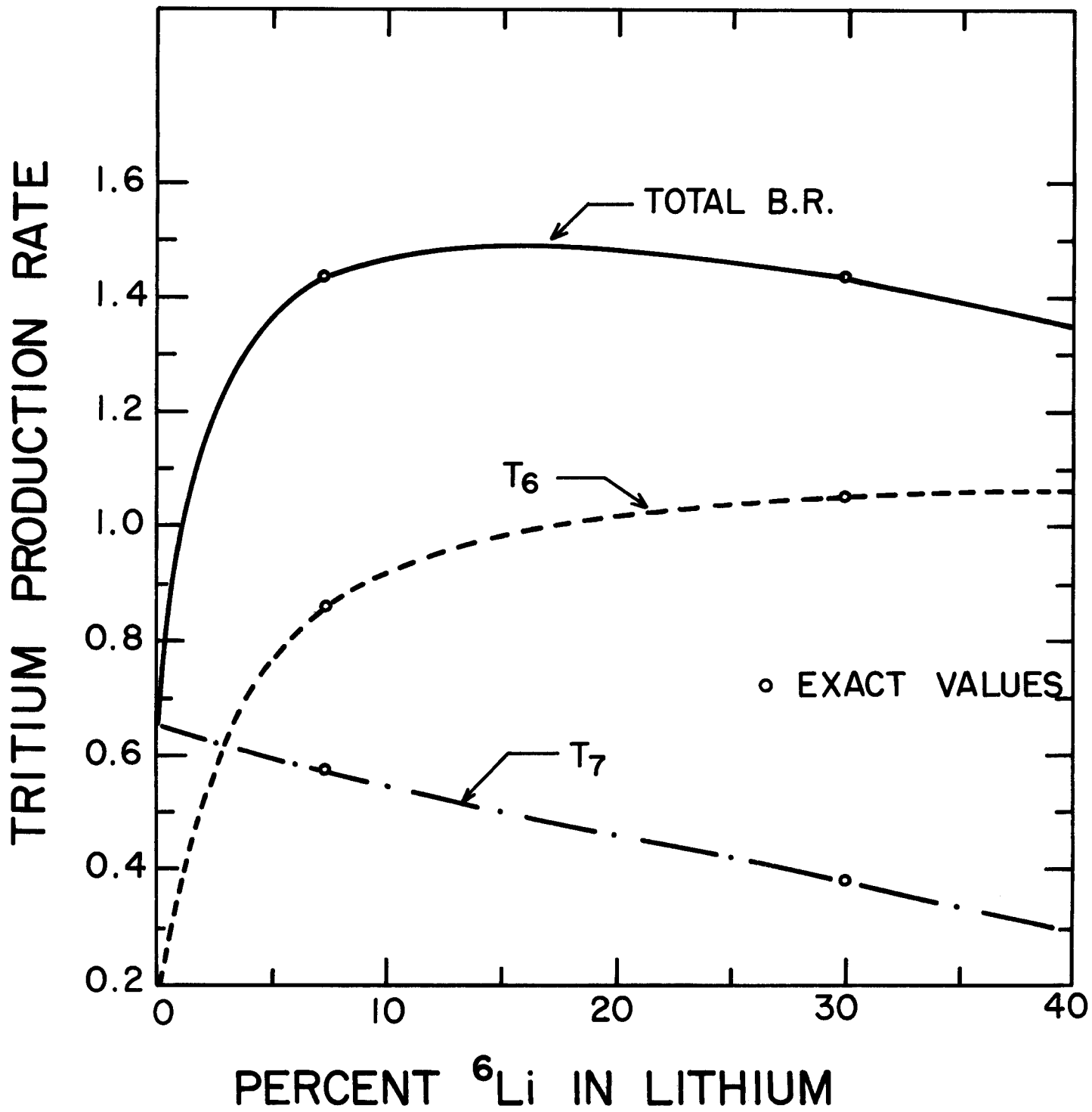


FIGURE 3