

APPLICATION OF COMPLEMENTARY BIVARIATIONAL PRINCIPLES TO PERTURBATION THEORY

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Abstract

A complementary bivariational formulation of Hamiltonian boundary value Problem is given. Results in perturbation theory are obtained using complementary bivariational principles.

Introduction

Complementary bivariational bounds play an important part in mathematical physics for following reasons; they (i) unify many diverse fields (ii) lead to new theoretical results, and (iii) provide powerful methods of calculation.

Energy principles of Dirichlet in the theory of electrostatics, Thomson principle, and Ritz and Temple bounds for eigenvalues constitute the earliest examples of bivariational bounds.

There are many methods to obtain Complementary bivariational bounds like involutory transformation [1] and the hypercircle method [2]. However, the canonical form of Euler Lagrange variational theory provides one of the most straightforward method to obtain complementary bivariational bounds. This method was introduced by Noble [3] in 1964.

The paper is in continuation of an earlier one by the author [4], recommending suggestions so as to obtain similar results for anisotropic plates. In this paper, we use Euler Lagrange bivariational theory to obtain complementary bivariational bounds for the class of problems pertaining to the perturbation theory. A numerical is also included.

1. Abstract Formalism

Hamiltonian boundary value problems are described by equation of the form,

$$T = W_u \text{ in } R \quad \sigma_\varphi = M_u \text{ on } \partial R_1 \longrightarrow \quad (1)$$

$$T^* u = f - Q\varphi = W_\varphi \text{ in } R, \quad \delta^* u = N_\varphi \text{ on } \partial R_2 \quad (2)$$

Here Q is the symmetric positive operator and u are elements of the real linear vector spaces V_1 and V_2 of function defined in bounded region R with boundary $\partial R = \partial R_1 + \partial R_2$. These spaces are formed into real inner product spaces H_1 and H_2 . $T: H_2 \longrightarrow H_1$ is a linear operator with formal adjoint $T^*: H_1 \longrightarrow H_2$ defined by

$$(u, T\varphi) = \langle T^* u, \varphi \rangle + (u, \sigma\varphi), \quad u \in H_1, \quad \varphi \in H_2 \longrightarrow \quad (3)$$

Where $(u, \sigma\varphi)$ corresponds to boundary term, σ being an operator mapping H_2 into H_1 , σ^* adjoint σ^* defined by

$$(u, \sigma\varphi)_{\partial R} = \langle \sigma^* u, \varphi \rangle_{\partial R}$$

and f is a given function in H_2 .

Arthur [5] showed that the following conditions ensure the uniqueness of the solution $I(u, \varphi)$

- W is convex in, u concave in
- M and N both concave
- at least one of these is definite

In this paper we consider the application of complementary bivariational aspects to perturbation theory.

2. Application of Bivariational Principles to perturbation theory

In this section we will obtain some results in perturbation theory using bivariational methods.

The boundary value problem arising in the theory of quantum mechanics is given by

$$(S_1 - P) \Psi_0 = (h - \eta_0) \varphi \text{ (IN ALL SPACE)} \quad (5)$$

$$\text{With } \varphi = 0 \text{ at } \infty \text{ and first-order correction } \varphi \text{ to } \Psi_0 \quad (6)$$

Where S_1 is the first-order correction to the unperturbed ground state Ψ energy η_0 and a perturbation ρ is applied, and h is the Hamiltonian operator, then

$$S_1 = \langle \Psi_0, \rho \Psi_0 \rangle \quad (7)$$

the second order correction is given by

$$S_2 = \langle \varphi, (P - S_1) \Psi_0 \rangle \quad (8)$$

Where Ψ_0 is normalized.

Since $(h - \eta_0)$ is positive for all function $\varphi \in D_h$ and using the theory developed in section 1 and the results of Arthurs and Reaves [5], the above, B.V.P can be rewritten as,

$$T^* T = h - \eta_0 \quad (9)$$

$$f = (S_1 - P) \Psi_0 \text{ and boundary } \varphi = 0 \text{ on } \partial R$$

2.(a) Reduction to bivariational bounds

Consider the following functional

$$J_1(\Phi) = 1/2 \langle \Phi, h - \eta_0 \rangle - \langle (S_1 - P) \Psi, \Phi \rangle \quad (10)$$

$$\text{and } I(\Psi) = J(\varphi) = 1/2 \langle (P - S_1) \Psi_0 \rangle = 1/2 S_2 \quad (11)$$

By minimum Principle [5], we get $I(\varphi) \leq J(\Phi)$, $\Phi = 0$ at ∞ using this and (11),

$$\text{We obtain } S_2 \leq 2J(\Phi)$$

This result is known in the literature as Hylleraas upper bound. To get complementary lower bound for S_2 , the B.V.P. (5) is written in the form

$$(S_1 - P) \Psi_0 = \{(h - \eta_1) + (\eta_1 - \eta_0)\} \varphi \quad (12)$$

Where η_1 is the unperturbed first excited — state energy.

2.(b) Introduce the functional

$$G(T\Psi) = -1/2 \langle \Psi, (h - \eta_1) \Psi \rangle - \frac{1}{2(\eta_1 - \eta_0)} \langle (S_1 - P) \Psi_0, (h - \eta_1) \Psi \rangle - \langle (S_1 - P) \Psi_0, (h - \eta_1) \Psi \rangle \quad (13)$$

By a principle due to Arthur and Reeves [5], we get

$$G(T\Psi) \leq I(\varphi), \quad (14)$$

Using (11) in (14) we get

$$2G(T\Psi) \leq S_2 \quad (15)$$

This result provides the lower bound and appears to be new.

2.(c) Examples

Following is a simple example to illustrate the complementary bivariational bounds presented in the foregoing section.

$$\text{Let } \Psi_0 = \pi^{-1/2} e^{-r}, P = -z, \eta_0 = -1/2, S_1 = 0 \quad (16)$$

Take trial function

$$\Phi = A \pi^{-1/2} z e^{-\alpha r}, \Psi = B \pi^{-1/2} z e^{-\beta r} \quad (17)$$

On application of the above theory, we obtain the bounds.

$$-2.27 \leq S_2 \leq -2.24$$

With $B = 1.45, \beta = 0.66, A = 1.31, \alpha = 0.80$, The exact result is

$$S_2 = -2.25, \varphi = \pi^{-1/2} (1 + 1/2 r) z e^{-r}$$

Conclusion

In principle, the results of section 1 could be applied to a class of nonlinear problems; non linear integral equations, non linear networks and certain integro-differential equations form few such examples.

References

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