Virtual Limitation of Variational Principle

If $\psi(x)$ and $\psi^*(x)$ are the solutions of the inhomogeneous equations

$$H\psi(x) = S(x) \tag{1}$$

and

$$H^*\psi^*(x) = S^*(x) \ , \tag{2}$$

then it is well known that the error E in the estimation of (ψ, S^*) by the variational principle

$$L[\phi, \phi^*] = (\phi, S^*) + (\phi^*, S - H\phi)$$

is of second order and is given by

$$E = -(\delta\phi^*, H\delta\phi) \ .$$

Here, $\phi(x)$ and $\phi^*(x)$ are the trial functions and $\delta\phi$ and $\delta\phi^*$ are the departures from the exact solution given by the following equations:

$$\phi(x) = \psi(x) - \delta\phi$$

$$\phi^*(x) = \psi^*(x) - \delta\phi^* \ .$$

The notation (f, g) above denotes the inner product defined as

$$(f,g) = (g,f) = \int f(x)\, g(x)\, dx \ .$$

Pomraning[1] has pointed out that for the class of trial functions satisfying the condition

$$(\phi^*, S - H\phi) = 0 \ , \tag{3}$$

the error E is of first order given by

$$E = -(\delta\phi^*, H\delta\phi) = (\delta\phi, S^*) \ .$$

This is an equality between second-order and first-order terms. This contradiction can easily be explained, if we expand $\psi(x)$ and $\psi^*(x)$ in terms of a parameter ϵ, such that zeroth, first, second, etc., powers of ϵ correspond to zeroth-, first-, second-, etc., order correction to $\psi(x)$ and $\psi^*(x)$.

$$\psi(x) = \phi(x) + \epsilon\eta_1(\kappa) + \epsilon^2\eta_2(\kappa) + \ldots \tag{4}$$

$$\psi^*(x) = \phi^*(x) + \epsilon\eta_1^*(x) + \epsilon^2\eta_2^*(x) + \ldots \tag{5}$$

Substituting the values of $\phi(x)$ and $\phi^*(x)$ from Eqs. (4) and (5) in Eq. (3), we have

$$(\psi^* - \epsilon\eta_1^* - \epsilon^2\eta_2^* - \ldots, S - H\psi + H\epsilon\eta_1 + H\epsilon^2\eta_2 + \ldots) = 0 \ .$$

Using Eqs. (1) and (2) and the adjoint property of H and H^*, we have

$$\epsilon(S^*, \eta_1) + \epsilon^2(S^*, \eta_2) - \epsilon^2(\eta_1^*, H\eta_2)$$
$$- \epsilon^3(\eta_1^*, H\eta_2) - \epsilon^3(\eta_2^*, H\eta_1) - \ldots = 0 \ .$$

Equating the coefficients of various powers of ϵ to zero, we have

$$(S^*, \eta_1) = 0 \tag{6}$$

$$(S^*, \eta_2) = (\eta_1^*, H\eta_1) \ . \tag{7}$$

Equation (6) clearly indicates that the first-order error (S^*, η_1) in the estimation of (S^*, ψ) vanishes. Equation (7) states that $(\eta_1^*, H\eta_1)$ acts as a second-order quantity, and this clarifies the objections raised by Pomraning.[1]

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[1] G. C. POMRANING, *Nucl. Sci. Eng.*, **28**, 150 (1967).