

Lecture 2

Examples and applications of variational principles:

Power dissipation in a passive resistive network.

Energy eigenvalues in quantum mechanics.

Fulvio Zonca

<https://www.afs.enea.it/zonca/>

Center for Nonlinear Plasma Science and ENEA C.R. Frascati, 00044 Frascati, Italy.

Institute for Fusion Theory and Simulation, Zhejiang University, Hangzhou 310027, P.R.C.

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A general methodology for constructing variational principles (...continued).

- Continuing from Lecture 1: An important class of variational principles is constructed for systems, whose governing equations can be derived from a Lagrangian. But what if the corresponding field equations cannot be formulated as Euler's equations?
- Here, we follow the general methodology for constructing a variational principle for a given (arbitrary) functional $\mathcal{F}[\varphi]$, adopting the approach by [Gerjuoy, Rau and Spruch 1983].
- The functional $\mathcal{F}[\varphi]$ can be complex valued, and φ can be multi component complex field, subject to field equations in the form $\mathcal{B}[\varphi] = 0$. Here, $\mathcal{B}[\varphi] = 0$ can also be multi component.

- By analogy of what was done in [Lecture 1](#) for the isoperimetric problem (pp. 26-28), the [existence of constraints](#) in the form of [field equations](#) is taken into account by the introduction of proper [Lagrange multipliers](#), $\mathcal{L}$, which in general are field themselves.
- The quantities $\mathcal{L}$ are called [auxiliary functions](#) by [Gerjuoy 1983] and are needed to construct the variational principle for the functional $\mathcal{F}[\varphi]$, which, introducing the [trial estimates](#) φ_t and $\mathcal{L}_t$, we choose in the form

$$\mathcal{F}_v[\varphi_t, \mathcal{L}_t] = \mathcal{F}[\varphi_t] + \mathcal{L}_{at}^\dagger \mathcal{B}[\varphi_t] + \mathcal{B}^\dagger[\varphi_t] \mathcal{L}_{bt} , \quad \delta\varphi = \varphi_t - \varphi , \quad \delta\mathcal{L} = \mathcal{L}_t - \mathcal{L} .$$

- Here, the [dagger](#) notation indicates, as usual, the transpose of the complex conjugate. We also assume that a proper inner product has been introduced (cf. [Lecture 1](#) p. 13), which, in a simple case, can be

$$\mathcal{L}_{at}^\dagger \mathcal{B}[\varphi_t] = \int \mathcal{L}_{at}^\dagger(\mathbf{r}) \{ \mathcal{B}[\varphi_t] \} (\mathbf{r}) d\mathbf{r} .$$

- Note that, since the functional $\mathcal{F}[\varphi]$ and the fields φ can be complex valued, we can assume – as it is common practice – that φ and $\varphi^\dagger$ are varied independently. Thus the multi component auxiliary functions $\mathcal{L}$ must consist of $\mathcal{L}_a$ components, needed to construct the inner product with $\mathcal{B}[\varphi]$, and $\mathcal{L}_b$ components, to construct the inner product with $\mathcal{B}^\dagger[\varphi]$. Formally, we may think of $\mathcal{L} = (\mathcal{L}_a, \mathcal{L}_b)$.
- Now let us introduce the general definition of variational principle for the functional $\mathcal{F}[\varphi]$.
- The functional $\mathcal{F}_v[\varphi_t, \mathcal{L}_t]$ is a variational principle for the considered $\mathcal{F}[\varphi]$ if the following two conditions hold:
 - $\mathcal{F}_v[\varphi_t, \mathcal{L}_t]$ coincides with $\mathcal{F}[\varphi]$ if the trial estimate φ_t coincides with the exact φ , whether or not the trial estimate $\mathcal{L}_t$ coincides with the exact $\mathcal{L}$.

- In the error

$$\delta\mathcal{F}_v = \mathcal{F}_v[\varphi_t, \mathcal{L}_t] - \mathcal{F}[\varphi] ,$$

the total first-order error, composed of terms of order $\|\delta\varphi\|$ and $\|\delta\mathcal{L}\|$, vanishes.

- Because of the explicit form of $\mathcal{F}_v[\varphi_t, \mathcal{L}_t]$ introduced above, the first condition is verified by definition.
- Thus, $\mathcal{F}_v[\varphi_t, \mathcal{L}_t]$ will be a variational principle for the considered $\mathcal{F}[\varphi]$ if the first order variation in $\delta\mathcal{F}_v$ can be made to vanish.
- Since $\mathcal{F}_v[\varphi_t, \mathcal{L}_t]$ is formally linear in $\mathcal{L}_t$ by construction, the second order variation in $\delta\mathcal{F}_v$ will contain terms of order $(\delta\varphi)^2$ and $\delta\mathcal{L}\delta\varphi$, but not $(\delta\mathcal{L})^2$.
- Let us now introduce

$$\delta\mathcal{F}[\varphi] = \mathcal{F}[\varphi_t] - \mathcal{F}[\varphi] , \quad \delta\mathcal{B}[\varphi] = \mathcal{B}[\varphi_t] - \mathcal{B}[\varphi] , \quad \delta\mathcal{B}^\dagger[\varphi] = \mathcal{B}^\dagger[\varphi_t] - \mathcal{B}^\dagger[\varphi] ,$$

and compute $\delta\mathcal{F}_v$ from its definition.

- By substitution, we have

$$\begin{aligned}
 \delta\mathcal{F}_v &= \delta\mathcal{F}[\varphi] + (\mathcal{L}_a^\dagger + \delta\mathcal{L}_a^\dagger) (\mathcal{B}[\varphi] + \delta\mathcal{B}[\varphi]) \\
 &\quad + (\mathcal{B}^\dagger[\varphi] + \delta\mathcal{B}^\dagger[\varphi]) (\mathcal{L}_b + \delta\mathcal{L}_b) , \\
 &= \delta\mathcal{F}[\varphi] + \mathcal{L}_a^\dagger \delta\mathcal{B}[\varphi] + \delta\mathcal{B}^\dagger[\varphi] \mathcal{L}_b \\
 &\quad + \delta\mathcal{L}_a^\dagger \delta\mathcal{B}[\varphi] + \delta\mathcal{B}^\dagger[\varphi] \delta\mathcal{L}_b .
 \end{aligned}$$

- Here, by using the **explicit form of the field equations**, $\mathcal{B}[\varphi] = 0$, the second equality shows that, in general, the linear dependence of $\delta\mathcal{F}_v$ on $\delta\mathcal{L}$ vanishes [Gerjuoy 1983], and **$\delta\mathcal{L}$ will enter only at the second order**.
- The condition that the linear contribution to $\delta\mathcal{F}_v$ vanishes is therefore

$$\delta\mathcal{F}_v = \delta\mathcal{F}[\varphi] + \mathcal{L}_a^\dagger \delta\mathcal{B}[\varphi] + \delta\mathcal{B}^\dagger[\varphi] \mathcal{L}_b = 0 .$$

E: Repeat the derivation step by step and demonstrate that the equation above is what you need for constructing the variational principle. Could you solve it in general introducing a proper functional derivative?

- Noting that φ and $\varphi^\dagger$ are varied independently, the above equations can be formally written and determine the auxiliary fields $\mathcal{L}$, once the boundary conditions on φ and $\varphi^\dagger$ are specified, thus imposing homogeneous boundary conditions on $\delta\varphi$ and $\delta\varphi^\dagger$.
- This means that, in general, $\mathcal{L}$ and the corresponding variational principle can be at least written for about any functional of interest, $\mathcal{F}[\varphi]$. This, of course, does not mean that the equations for $\mathcal{L}$ will be simple to solve and/or that analytic expressions for $\mathcal{L}$ can be provided in general.
- This approach will be applied in Lecture 3 to the problem of shear Alfvén waves in tokamaks, and used for the corresponding variational formulation and variational principle, yielding the integral form of the dispersion relation: the general fishbone like dispersion relation (GFLDR) [Z&C 2014].
- In the remaining part of Lecture 2, the general approach will be illustrated further by means of two academic examples: (i) Power dissipation in a passive resistive network; and (II) Energy eigenvalues in quantum mechanics [Gerjuoy 1983].

Power dissipation in a passive resistive network

[Gerjuoy 1983]

- Consider the problem of estimating the power loss P of a two-terminal passive resistive network, knowing the input current I and the various resistances R_i .
- A well-known theorem states that if we approximate the branch currents I_i by trial estimates I_{it} , such that current conservation is satisfied at each junction, the expression $\sum_i R_i I_{it}^2$ is a variational principle for P . In fact, the expression represents an extremum of P .
- Here, we analyze the problem for two resistances R_1 and R_2 , adopting the general methodology illustrated above.
- In this case, the functional is

$$P = R_1 I_1^2 + R_2 I_2^2 ,$$

where I_1 and I_2 play the role of the fields φ . This is indeed a simpler case, where the functional is algebraic and does not involve integration.

- The constraints $\mathcal{B}[\varphi]$ in the present case are given by the two conditions

$$B_1(I_1, I_2) \equiv I_1 + I_2 - I = 0 ,$$

$$B_2(I_1, I_2) \equiv R_1 I_1 - R_2 I_2 = 0 .$$

The first condition represents conservation of current, while the second states that the voltage drop in each resistance is the same.

- Using the general definition (p. 3), we have

$$P_v = R_1 I_{1t}^2 + R_2 I_{2t}^2 + \lambda_{1t}(I_{1t} + I_{2t} - I) + \lambda_{2t}(R_1 I_{1t} - R_2 I_{2t}) .$$

- The values of $\lambda_{1t}, \lambda_{2t}$ are generally functions of I_{1t}, I_{2t} and must be determined from the condition that the expression above is a true **variational principle**. $\Rightarrow \delta P_v = \delta P[I_1, I_2] + \lambda_1 \delta(I_1 + I_2 - I) + \lambda_2 \delta(R_1 I_1 - R_2 I_2) = 0$.

E: Show that the condition above is what you obtain from the general condition on p.6. Why variations w.r.t. λ_1 and λ_2 do not enter?

E: Derive the expression of δP_v from its definition, including first and second order variations. Show that the first order variations with respect to λ_1 and λ_2 vanish identically. Why?

E: Show that the condition for P_v to be a variational principle, given on p. 9, consists of two independent equations that determine λ_1 and λ_2 as functions of I_1 and I_2 .

□ Isolating independent variations w.r.t. I_1 and I_2 , respectively, the general condition on p. 9 yields

$$2R_1I_1 + \lambda_1 + \lambda_2R_1 = 0 ,$$

$$2R_2I_2 + \lambda_1 - \lambda_2R_2 = 0 .$$

□ The solution of this system yields

$$\lambda_1 = -R_1I_1 - R_2I_2 + \frac{R_1 - R_2}{R_1 + R_2}(R_1I_1 - R_2I_2) = -R_1I_1 - R_2I_2 , \quad \lambda_2 = -\frac{2(R_1I_1 - R_2I_2)}{R_1 + R_2} = 0 .$$

E: Derive the expressions above for λ_1 and λ_2 . Do you find different functional forms? Why?

□ Given the results above, we can choose,

$$\lambda_{1t} = -R_1 I_{1t} - R_2 I_{2t} , \quad \text{and} \quad \lambda_{2t} = 0 .$$

□ Once substituted into the variational principle, these values give

$$P_v = (R_1 I_{1t} + R_2 I_{2t}) I - (R_1 + R_2) I_{1t} I_{2t} .$$

E: Show that this expression is a variational principle. What happens if $I_{1t} + I_{2t} = I$? Can you explain the physical meaning of this?

Energy eigenvalues in quantum mechanics

[Gerjuoy 1983]

- Another instructive example is the determination of bound-state energy eigenvalues in quantum mechanics.
- In this case, the field φ (the eigenfunction), obeys the Schrödinger equation

$$H\varphi = E\varphi ,$$

where H is Hermitian and E is the energy eigenvalue.

- The normalization condition of the bound state

$$\varphi^\dagger \varphi - 1 = 0$$

is the additional constraint.

- Proceeding by the general approach, we can write the variational expression of the energy E as

$$E_v = E_t + \mathcal{L}_{at}^\dagger [(H - E_t)\varphi_t] + [(H - E_t)\varphi_t]^\dagger \mathcal{L}_{bt} + \lambda_t(\varphi_t^\dagger \varphi_t - 1) .$$

- Again, the first order variation of δE_v will not depend on $\delta \mathcal{L}$ and $\delta \lambda$.

E: Show that the first order variation of δE_v does indeed not depend on $\delta \mathcal{L}$ and $\delta \lambda$. Can you explain why?

E: Derive the general expression for δE_v and show it reduces to the form that is readily constructed from the general condition for E_v to be a variational principle (cf. p. 6).

- The condition for E_v to be variational reads

$$\delta E_v = \delta E + \mathcal{L}_a^\dagger \delta [(H - E)\varphi] + \delta [(H - E)\varphi]^\dagger \mathcal{L}_b + \lambda \delta (\varphi^\dagger \varphi - 1) = 0 .$$

E: Show that the conditions obtained by independently varying E , φ and $\varphi^\dagger$, are sufficient for determining the auxiliary fields $\mathcal{L} = (\mathcal{L}_a, \mathcal{L}_b)$ and the Lagrange multiplier λ .

□ Condition from δE variation:

$$1 - \mathcal{L}_a^\dagger \varphi - \varphi^\dagger \mathcal{L}_b = 0 .$$

E: Derive the condition above.

□ Condition from $\delta \varphi^\dagger$ variation (note, without using Hermiticity of H):

$$(H - E)^\dagger \mathcal{L}_b + \lambda \varphi = 0 .$$

E: Derive the condition above.

□ By taking the inner product with $\varphi^\dagger$ from the left of the above equation and using the Schrödinger equation, one readily derives $\lambda = 0$.

E: Show this explicitly!

- Condition from $\delta\varphi$ variation:

$$\mathcal{L}_a^\dagger(H - E) + \lambda\varphi^\dagger = 0 .$$

- By taking the inner product with φ from the right of the above equation and using the Schrödinger equation, one readily derives $\lambda = 0$.

E: Show this explicitly!

- Summarizing, and explicitly using the Hermiticity of H (and E being real, E: Show this!), we consistently derive

$$\lambda = 0 \quad \Rightarrow \quad \lambda_t = 0 .$$

The other conditions for E_v to be a proper variational principle are

$$1 - \mathcal{L}_a^\dagger\varphi - \varphi^\dagger\mathcal{L}_b = 0 ,$$

$$(H - E)\mathcal{L}_a = 0 ,$$

$$(H - E)\mathcal{L}_b = 0 .$$

- These conditions mean that the normalization condition **does not explicitly enter in the variational principle through λ_t , which vanishes.**
- Further to this, the auxiliary fields $\mathcal{L}_a$ and $\mathcal{L}_b$ are the solution of the same Schrödinger equation of the considered bound-state. In other words

$$\mathcal{L}_a = a\varphi , \quad \text{and} \quad \mathcal{L}_b = b\varphi ,$$

with a and b complex numbers that must satisfy the normalization condition

$$1 - \mathcal{L}_a^\dagger \varphi - \varphi^\dagger \mathcal{L}_b = 0 \quad \Rightarrow \quad a^* + b = 1 .$$

- Substituting back these results into the expression for E_v , with $\mathcal{L}_{at} = a\varphi_t$ and $\mathcal{L}_{bt} = b\varphi_t$, we have

$$E_v = E_t(1 - \varphi_t^\dagger \varphi_t) + \varphi_t^\dagger H \varphi_t .$$

E: Show that this expression is variational. Discuss similarities and differences with your recollection of your quantum mechanics course. Where does the difference enter? Why?

- Note that the normalization condition has not been assumed for the trial eigenfunction of the bound-state.
- If we assume $\varphi_t^\dagger \varphi_t = 1$, the above variational estimate reduces to

$$E_v = \varphi_t^\dagger H \varphi_t ,$$

which is the well-known and expected result from quantum mechanics.

E: Repeat the procedure above, but without assuming that the normalization constraint applies. Show that all equations derived above are reproduced, except for the normalization condition that is replaced by $a^* + b = (\varphi^\dagger \varphi)^{-1}$. What is the obtained variational expression for E_v ? How does it relate to the previous result?

- If we do not impose the normalization constraint $\varphi^\dagger \varphi = 1$ and follow the same general approach, the variational principle becomes

$$E_v = \frac{\varphi_t^\dagger H \varphi_t}{\varphi_t^\dagger \varphi_t} .$$

- Noting that, if φ_t is a good guess for the normalized φ bound-state

$$\frac{1}{\varphi_t^\dagger \varphi_t} = \frac{1}{1 - (1 - \varphi_t^\dagger \varphi_t)} \simeq 1 + (1 - \varphi_t^\dagger \varphi_t) + \dots ,$$

the variational principle becomes

$$E_v = \frac{\varphi_t^\dagger H \varphi_t}{\varphi_t^\dagger \varphi_t} \simeq \varphi_t^\dagger H \varphi_t + (1 - \varphi_t^\dagger \varphi_t) \varphi_t^\dagger H \varphi_t .$$

E: Note similarities and differences of this result with the variational principle on p. 16. What can you conclude?

- The present analysis shows that the general methodology for constructing variational principles [Gerjuoy 1983] is solid and straightforward, and can be applied to nearly any functional of interest, although it may sometimes seem somewhat clumsy.
- This approach, in [Lecture 3](#), will be applied to shear Alfvén waves in tokamaks.

References and reading material

I. M. Gelfand and S. V. Fomin, *Calculus of Variations*, Prentice-Hall, Inc. (Englewood Cliffs, NJ, 1963).

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