Optimal Functions and Nanomechanics III

APP MTH 3022/7106

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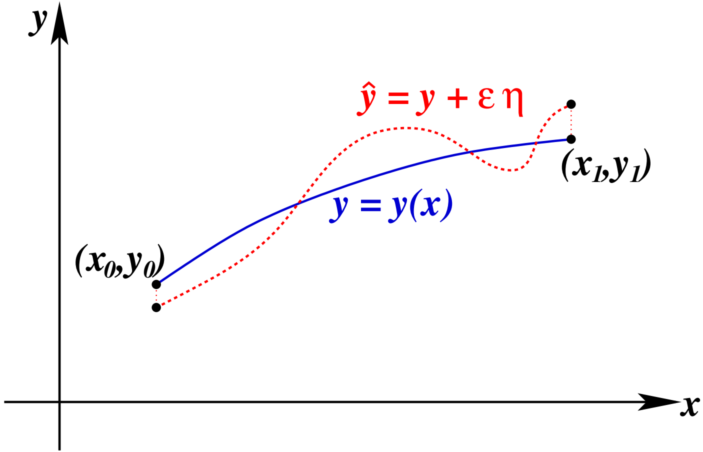
Lecture 25

Last lecture

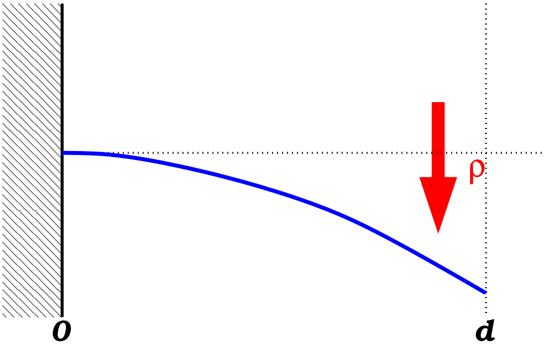
- Examined the problem of joining nanostructures
- Proposed a model based on minimising line curvature (the elastica)
- Solved the problem of joining a perpendicular nanotube to a graphene sheet

Free end points

In previous problem, we allow $y(x_0)$ and $y(x_1)$ to vary but kept x_0 and x_1 fixed.



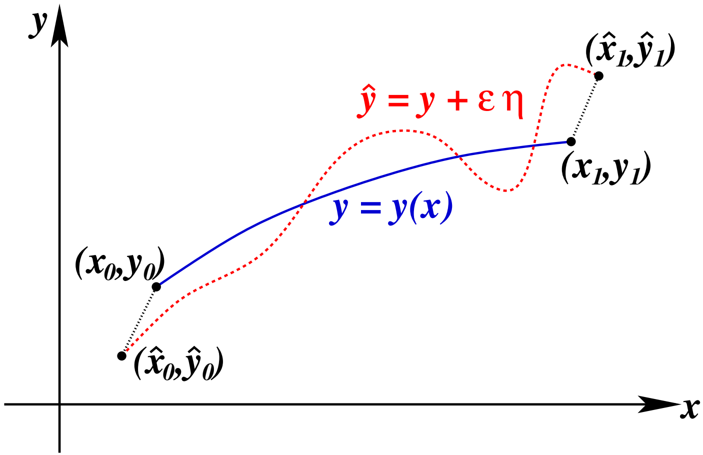
Example: Cantilever



But this can fail in some cases, for instance, if the left end of the cantilever isn't clamped (to have zero slope) then the right end can swing freely, and x_1 won't be fixed.

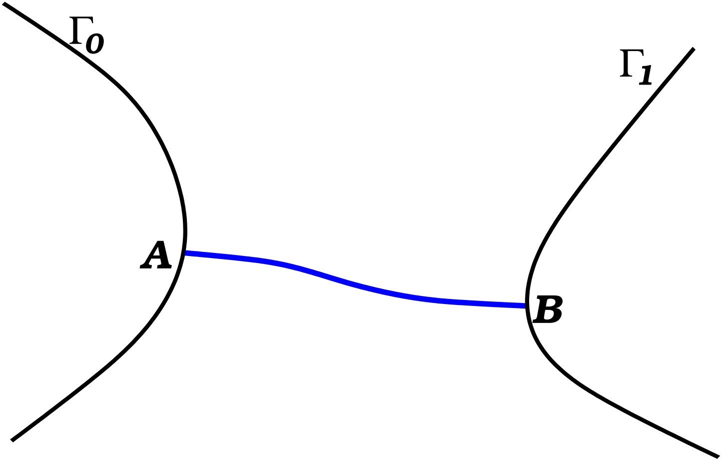
Free end points

In some problems we even want to allow x_0 and x_1 to vary.

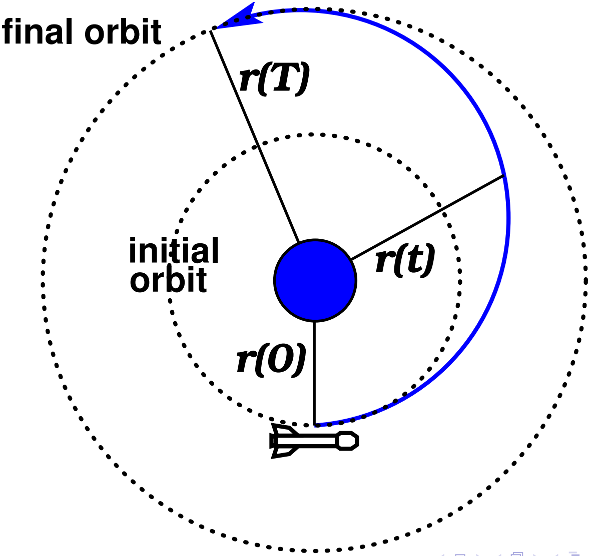


Example: shortest path

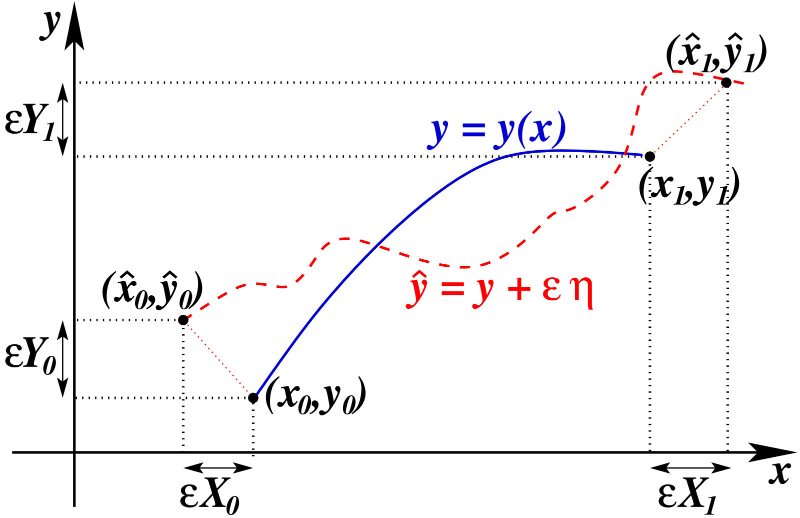
There may still be some constraints on the possible positions of end-points: e.g., shortest path between two curves



Example: Orbit Transfer Problem



Approach



y
x
εY_1
εY_0
εX_0
εX_1
$(\hat{x}_1, \hat{y}_1)$
(x_1, y_1)
$(\hat{x}_0, \hat{y}_0)$
(x_0, y_0)
$y = y(x)$
$\hat{y} = y + \varepsilon\,\eta$

Extension of y

Define $\tilde{x}_0 = \min(x_0, \hat{x}_0)$ and $\tilde{x}_1 = \max(x_1, \hat{x}_1)$
We can use Taylor's theorem to extend y onto the interval $[\tilde{x}_0, \tilde{x}_1]$, e.g.

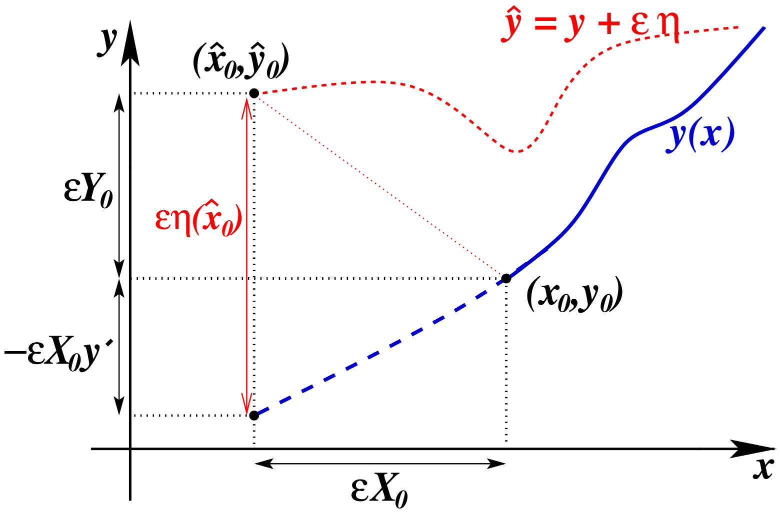
$$y(x) = \begin{cases} y(x_0) + (x_0 - x)y'(x_0) + \frac{(x_0-x)^2}{2}y''(x_0) + \cdots & x \in [\tilde{x}_0, x_0) \\ y(x) & x \in [x_0, x_1] \\ y(x_1) + (x - x_1)y'(x_1) + \frac{(x-x_1)^2}{2}y''(x_1) + \cdots & x \in (x_1, \tilde{x}_1] \end{cases}$$

For instance, if the perturbed end-point $\hat{x}_0 < x_0$, we get

$$y(\hat{x}_0) = y(x_0) - \epsilon X_0 y'(x_0) + \mathcal{O}(\epsilon^2)$$

We can likewise extend the perturbed curve $\hat{y}$.

Extension of y



Distance

However, we can no longer define distance as simply

- previous definition

$$d(y, \hat{y}) = \|y - \hat{y}\|$$

  where the norm could be defined in a number of ways, but an example might be

$$\|y - \hat{y}\| = \int_{x_0}^{x_1} |y(x) - \hat{y}(x)| \, dx$$

- x_0 and x_1 can vary now, so the range of integral is not well defined anymore
- if we just extend y to new interval, we don't take proper account of distortion from difference in x end-points

New distance

New distance metric

$$d(y, \hat{y}) = \|y - \hat{y}\| + |\boldsymbol{p}_0 - \hat{\boldsymbol{p}}_0| + |\boldsymbol{p}_1 - \hat{\boldsymbol{p}}_1|$$

where we define

$$|\boldsymbol{p}_k - \hat{\boldsymbol{p}}_k| = \sqrt{(x_k - \hat{x}_k)^2 + (y_k - \hat{y}_k)^2}$$

We want allowed perturbations to be close to y (according to the distance defined above), but don't specify the end-points except to require they be $\mathcal{O}(\epsilon)$ apart, e.g.

$$\hat{x}_k = x_k + \epsilon X_k, \quad \hat{y}_k = y_k + \epsilon Y_k$$

so that $|\boldsymbol{p}_k - \hat{\boldsymbol{p}}_k| = \epsilon\sqrt{X_k^2 + Y_k^2}$, for $k = 0, 1$

Forming the first variation

$$
\begin{aligned}
F\{\hat{y}\} - F\{y\} &= \int_{\hat{x}_0}^{\hat{x}_1} f(x, \hat{y}, \hat{y}')\, dx - \int_{x_0}^{x_1} f(x, y, y')\, dx \\
&= \int_{x_0+\epsilon X_0}^{x_1+\epsilon X_1} f(x, \hat{y}, \hat{y}')\, dx - \int_{x_0}^{x_1} f(x, y, y')\, dx \\
&= \int_{x_0}^{x_1} \left[f(x, \hat{y}, \hat{y}') - f(x, y, y') \right]\, dx \\
&\quad + \int_{x_1}^{x_1+\epsilon X_1} f(x, \hat{y}, \hat{y}')\, dx - \int_{x_0}^{x_0+\epsilon X_0} f(x, \hat{y}, \hat{y}')\, dx
\end{aligned}
$$

Forming the first variation

From earlier arguments

$$\int_{x_0}^{x_1} \left[f(x, \hat{y}, \hat{y}') - f(x, y, y') \right] dx =$$

$$\epsilon \left\{ \left[\eta \frac{\partial f}{\partial y'} \right]_{x_0}^{x_1} + \int_{x_0}^{x_1} \eta \left(\frac{\partial f}{\partial y} - \frac{d}{dx} \frac{\partial f}{\partial y'} \right) dx \right\} + \mathcal{O}(\epsilon^2)$$

and as ϵ is small

$$\int_{x_1}^{x_1 + \epsilon X_1} f(x, \hat{y}, \hat{y}')\, dx = \epsilon X_1 \left. f(x, y, y') \right|_{x_1} + \mathcal{O}(\epsilon^2)$$

$$\int_{x_0}^{x_0 + \epsilon X_0} f(x, \hat{y}, \hat{y}')\, dx = \epsilon X_0 \left. f(x, y, y') \right|_{x_0} + \mathcal{O}(\epsilon^2)$$

Forming the first variation

Therefore the first variation is

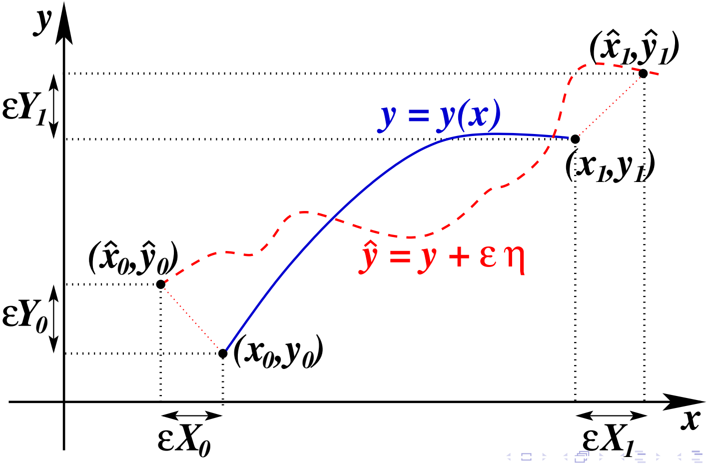
$$\begin{aligned} \delta F(\eta, y) &= \lim_{\epsilon \to 0} \frac{F\{\hat{y}\} - F\{y\}}{\epsilon} \\ &= \left[\eta \frac{\partial f}{\partial y'} \right]_{x_0}^{x_1} + \int_{x_0}^{x_1} \eta \left(\frac{\partial f}{\partial y} - \frac{d}{dx} \frac{\partial f}{\partial y'} \right) dx \\ &\qquad + X_1 \, f(x, y, y')\big|_{x_1} - X_0 \, f(x, y, y')\big|_{x_0} . \end{aligned}$$

But note that $\left[\eta \frac{\partial f}{\partial y'} \right]_{x_0}^{x_1}$ is no longer simple to calculate because we don't fix x_0 or x_1.

- how can we find x_0 and x_1?
- we need a new natural boundary condition that will give us this.

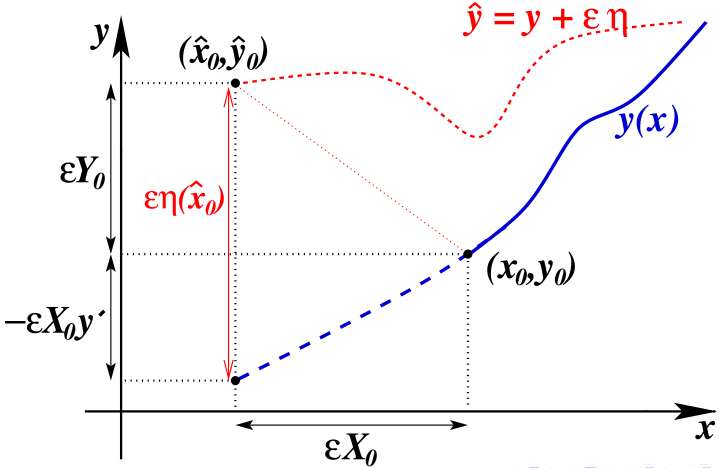
End-point compatibility

The perturbed end-points, and perturbation function η must satisfy certain conditions to be compatible.



End-point compatibility

The perturbed end-points, and perturbation function η must satisfy certain conditions to be compatible.



End-point compatibility

Remember that

$$\hat{x}_0 = x_0 + \epsilon X_0, \quad \hat{y}_0 = y_0 + \epsilon Y_0.$$

Notice that

$$\hat{y}_0 = \hat{y}(\hat{x}_0) = \hat{y}(x_0 + \epsilon X_0) = y(x_0 + \epsilon X_0) + \epsilon\eta(x_0 + \epsilon X_0)$$

From Taylor's theorem, for small ϵ

$$\begin{aligned} y(x_0 + \epsilon X_0) &= y(x_0) + \epsilon X_0 y'(x_0) + \mathcal{O}(\epsilon^2) \\ &= y_0 + \epsilon X_0 y'(x_0) + \mathcal{O}(\epsilon^2) \end{aligned}$$

$$\epsilon\eta(x_0 + \epsilon X_0) = \epsilon\eta(x_0) + \mathcal{O}(\epsilon^2)$$

End-point compatibility

So

$$
\begin{aligned}
y_0 + \epsilon Y_0 &= y_0 + \epsilon X_0 y'(x_0) + \epsilon \eta(x_0) + \mathcal{O}(\epsilon^2) \\
\epsilon Y_0 &= \epsilon X_0 y'(x_0) + \epsilon \eta(x_0) + \mathcal{O}(\epsilon^2) \\
\eta(x_0) &= Y_0 - X_0 y'(x_0) + \mathcal{O}(\epsilon)
\end{aligned}
$$

Similarly

$$\eta(x_1) = Y_1 - X_1 y'(x_1) + \mathcal{O}(\epsilon)$$

The First Variation

Substituting the end-point compatibility constraints into the first variation we get

$$
\begin{aligned}
\delta F(\eta, y) &= \left[\eta \frac{\partial f}{\partial y'}\right]_{x_0}^{x_1} + \int_{x_0}^{x_1} \eta \left(\frac{\partial f}{\partial y} - \frac{d}{dx}\frac{\partial f}{\partial y'} \right) dx \\
&\quad + X_1 \, f(x, y, y')\big|_{x_1} - X_0 \, f(x, y, y')\big|_{x_0} \\
&= \int_{x_0}^{x_1} \eta \left(\frac{\partial f}{\partial y} - \frac{d}{dx}\frac{\partial f}{\partial y'} \right) dx \\
&\quad + Y_1 \left.\frac{\partial f}{\partial y'}\right|_{x_1} - Y_0 \left.\frac{\partial f}{\partial y'}\right|_{x_0} \\
&\quad + X_1 \left.\left(f - y' \frac{\partial f}{\partial y'} \right)\right|_{x_1} - X_0 \left.\left(f - y' \frac{\partial f}{\partial y'} \right)\right|_{x_0}
\end{aligned}
$$

Deriving Euler-Lagrange equations

The end-points are free, but this includes the case where they sit on the extremal, i.e. we can always *choose* the end-points so that $X_k = Y_k = 0$, for $k = 0, 1$. For instance, when $X_0 = X_1 = Y_0 = Y_1 = 0$, then the first variation collapses to

$$\delta F(\eta, y) = \int_{x_0}^{x_1} \eta \left(\frac{\partial f}{\partial y} - \frac{d}{dx} \frac{\partial f}{\partial y'} \right) dx,$$

and so the Euler-Lagrange equations hold here.
Likewise, when $X_1 = Y_0 = Y_1 = 0$, but $X_0 \neq 0$ we can see that this creates one of the natural boundary conditions

$$X_0 \left(f - y' \frac{\partial f}{\partial y'} \right) \bigg|_{x_0} = 0.$$

Notation

Some notation

- Hamiltonian

$$H = y' \frac{\partial f}{\partial y'} - f$$

  we saw the Hamiltonian H earlier.

- p is often identified with momentum of a particle, but we can use it for other systems as well.

$$p = \frac{\partial f}{\partial y'}$$

- we'll replace the notations X_k and Y_k for $k = 0, 1$ with

$$\delta x(x_k) = X_k, \quad \text{and} \quad \delta y(y_k) = Y_k.$$

The Euler-Lagrange equations

As before, we can always choose the end-points so that $X_k = Y_k = 0$, for $k = 0, 1$, so that the Euler-Lagrange equation

$$\frac{\partial f}{\partial y} - \frac{d}{dx}\frac{\partial f}{\partial y'} = 0,$$

must be satisfied plus the additional constraints:

$$\Big[p\,\delta y - H\,\delta x\Big]_{x_0}^{x_1} = 0.$$

Including constraints

Typically the end-points satisfy some set of constraints, in the most general form $g(x_0, y_0, x_1, y_1) = 0$, but often these constraints separate to constraint a single end-point, e.g. we have constraints

$$g_k(x_j, y_j) = 0$$

for $j = 0, 1$, and some number of constraints, typically $k < 4$.

For example, the fixed end-point problem has constraints that specify the values of (x_0, y_0) and (x_1, y_1) precisely.

Separable constraints

Where the constraints for one end point are not linked to those of the other, we may separate the conditions to get

$$\Big[p\,\delta y - H\,\delta x\Big]_{x_0} = 0$$
$$\Big[p\,\delta y - H\,\delta x\Big]_{x_1} = 0$$

Note not all possible end constraints make sense!

Simple example: fixed x

We have already considered this condition:

- $\delta x = 0$ and $\delta y \neq 0$
- conditions

$$\Big[p\,\delta y - H\,\delta x\Big]_{x_i} = 0,$$

  reduce down to

$$p(x_i) = \left.\frac{\partial f}{\partial y'}\right|_{x_i} = 0,$$

  at the relevant end points.
- and that is just the natural boundary conditions we derived earlier.

Simple example: fixed y

Imagine a problem where we have to get to a fixed state y, but the point at which that happens is variable, so that

- $\delta y = 0$ and $\delta x \neq 0$
- conditions

$$\Big[p\,\delta y - H\,\delta x \Big]_{x_i} = 0,$$

  reduce down to

$$H(x_i) = 0,$$

  at the relevant end points.

Simple example: fixed y

Minimise

$$F\{y\} = \int_0^{x_1} (1 + y'^2)\, dx,$$

subject to $y(0) = 1$ and $y(x_1) = L > 1$, but with x_1 unspecified.

- We could derive the E-L equations, but note that this problem is autonomous (no x dependence) so

$$H = \text{const.}$$

- The free end point at x_1 means that

$$H(x_1) = 0$$

- Hence for all $x \in [0, x_1]$ we have $H = 0$.

Simple example: fixed y

Minimise

$$F\{y\} = \int_0^{x_1} (1 + y'^2)\,dx.$$

So

$$H = y'\frac{\partial f}{\partial y'} - f = 2y'^2 - y'^2 - 1 = y'^2 - 1 = 0$$

Hence

$$y' = \pm 1,$$

subject to $y(0) = 1$ and $y(x_1) = L > 1$ so we take $y' = 1$ and therefore

$$y = x + 1.$$

Extension to several dependant variables

$$F\{\boldsymbol{q}\} = \int_{t_0}^{t_1} L(t, \boldsymbol{q}, \dot{\boldsymbol{q}})\, dt$$

If F is stationary at $\boldsymbol{q}$ then it can be shown that the Euler-Lagrange equations are given by

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_k} - \frac{\partial L}{\partial q_k} = 0$$

for $k = 1, \ldots, n$ and that at the end points t_0 and t_1

$$\sum_{k=1}^{n} p_k\, \delta q_k - H\, \delta t = 0,$$

where

$$p_k = \frac{\partial L}{\partial \dot{q}_k}, \quad \text{and} \quad H = \sum_{k=1}^{n} \dot{q}_k p_k - L.$$

Simple Example

Find extremals of

$$F\{\boldsymbol{q}\} = \int_0^1 \left[\dot{q}_1^2 + (\dot{q}_2 - 1)^2 + q_1^2 + q_1 q_2\right] dt,$$

for $\boldsymbol{q}(0) = \boldsymbol{q}_0$ and $\boldsymbol{q}(1)$ free, i.e., we can finish anywhere on the plane $t = 1$.

The Euler-Lagrange equations are

$$\begin{aligned} 2\ddot{q}_1 - 2q_1 - q_2 &= 0, \\ 2\ddot{q}_2 - q_1 &= 0. \end{aligned}$$

Simple example

As earlier we can combine the E-L equations to get

$$4q_2^{(4)} - 4\ddot{q}_2 - q_2 = 0$$

which has solutions in the form

$$q_2(t) = c_1 \cosh(At) + c_2 \sinh(At) + c_3 \cos(Bt) + c_4 \sin(Bt)$$

where

$$A = \left(\frac{\sqrt{2}+1}{2}\right)^{1/2}, \quad B = \left(\frac{\sqrt{2}-1}{2}\right)^{1/2}.$$

Now we need to determine the arbitrary constants c_i from the natural boundary conditions.

Simple example

Natural boundary conditions

$$\left[\sum_{k=1}^{n} p_k \, \delta q_k - H \, \delta t \right]_{t=1} = 0.$$

But $t = 1$ is fixed at the RHS, so $\delta t = 0$, and we can vary q_k independently, so we can take any combination of $\delta q_k = 0$, and hence all of the $p_k = 0$ at $t = 1$, i.e.,

$$p_k(1) = \left. \frac{\partial L}{\partial \dot{q}_k} \right|_{t=1} = 0.$$

Simple example

$$p_k(1) = \left.\frac{\partial L}{\partial \dot{q}_k}\right|_{t=1} = 0.$$

So

$$\begin{aligned} p_1(1) &= 2\dot{q}_1(1) = 0, \\ qp_2(1) &= 2(\dot{q}_2(1) - 1) = 0. \end{aligned}$$

The natural boundary conditions reduce to

$$\dot{q}_1(1) = 0, \quad \dot{q}_2(1) = 1, \quad \Rightarrow \quad \dot{\boldsymbol{q}}(1) = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \dot{\boldsymbol{q}}_1$$

Combine these with the conditions at the start point ($\boldsymbol{q}(0) = \boldsymbol{q}_0$) we have enough constraints to find the constants of integration, c_i.