Lagrangian, Hamiltonian, classical/quantum correspondence

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These notes can be seen as an introduction to the following excellent physics book [2]. A more mathematical and nice exposure is given in [1]. For interest readers by extension to infinite dimensional systems and partial differential equations describing physical systems governed by variational principles, we recommend the excellent book [3].

1 Lagrangian dynamics

1.1 Euler/Lagrange equations

Denote by $q = (q_1, \dots, q_n)$ a set of n real quantities corresponding to the so-called configuration variables or generalized coordinates. Take a trajectory $t \mapsto q(t)$, a smooth curve parameterized by the time-variable t, and consider the real value function $L(q, \dot{q}, t)$ called the Lagrangian : it depends smoothly on q, its velocity $\dot{q} = \frac{d}{dt}q$ and on time t. The action S from time t_a to time $t_b > t_a$ corresponds, for any smooth curve $[t_a, t_b] \ni t \mapsto q(t)$, to the following time integral

$$S = \int_{t_a}^{t_b} L(q(t), \dot{q}(t), t)dt. \tag{1}$$

We are looking for trajectories $q(t)$ minimizing the action. More precisely, we consider the following optimization problem :

$$\min_{\substack{[t_a, t_b] \ni t \mapsto q(t) \\ q(t_a) = a,\ q(t_b) = b}} \int_{t_1}^{t_2} L(q(t), \dot{q}(t), t)dt \tag{2}$$

where the initial and final configurations, a and b, are given.

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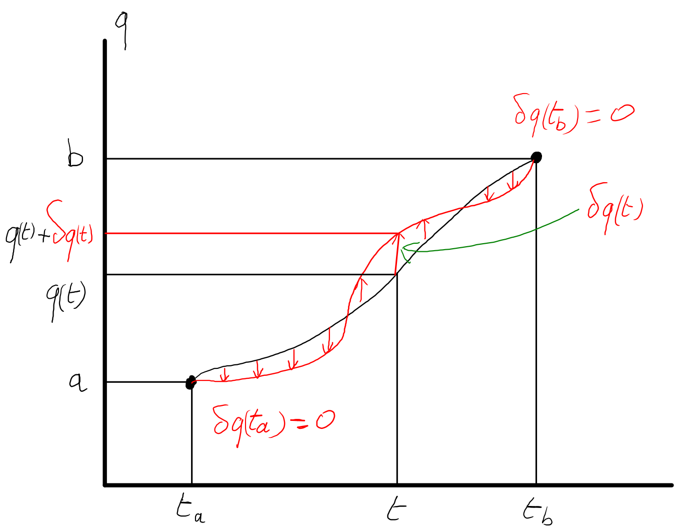

FIGURE 1 – The first variation of a trajectory $[t_a, t_b] \ni t \mapsto q(t)$ joining a and b, the prescribed values of q at t_a and t_b.

If $q(t)$ is a solution, then the first variation of S around q vanishes. This just means that for any very small deviation $\delta q(t)$ of $q(t)$ satisfying the constraints, i.e. $\delta q(t_a) = \delta q(t_b) = 0$, one has $\delta S = 0$. Trajectories $q(t)$ around which the first variation of S vanishes are said extremal trajectories. Standard conputations give

$$
\begin{aligned}
\delta S = \int_{t_a}^{t_b} \Big(L(q(t) + \delta q(t), \dot{q}(t) + \delta \dot{q}(t), t) - L(q(t), \dot{q}(t), t) \Big) dt \\
\approx \sum_{i=1}^{n} \int_{t_a}^{t_b} \left(\frac{\partial L}{\partial q_i} \delta q_i + \frac{\partial L}{\partial \dot{q}_i} \delta \dot{q}_i \right) dt \\
= \sum_{i=1}^{n} \int_{t_a}^{t_b} \left(\frac{\partial L}{\partial q_i} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_i} \right) \right) \delta q_i(t)\ dt = 0 \quad (3)
\end{aligned}
$$

where we neglect second-order terms in δq and $\delta \dot{q}$, use $\delta \dot{q}_i = \frac{d}{dt}(\delta q_i)$, and perfome an integration by part based on $\frac{\partial L}{\partial \dot{q}_i} \delta \dot{q}_i = \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_i} \delta q_i \right) - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_i} \right) \delta q_i$.

This implies that for any t between t_a and t_b, the trajectory $q(t)$ satisfies n second-order differential scalar equations, called Euler-Lagrange equations :

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_i} \right) = \frac{\partial L}{\partial q_i}, \ i = 1, \ldots, n. \quad (4)$$

When $n = 1$, q is of dimension one and the Euler-Lagrange equation reads

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) = \frac{\partial L}{\partial q}. \tag{5}$$

1.2 Examples

1.2.1 Mass/spring system

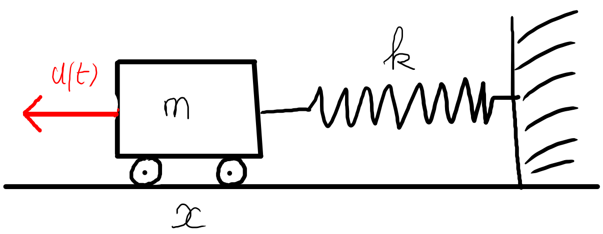

FIGURE 2 – A mass m submitted to a spring of stiffness k and an external time-varying force $u(t)$.

The Newton equation of a mass m moving along the line at position x, attached to a spring of stiffness k and submitted to a given external force $u(t)$ reads :

$$m\frac{d^2}{dt^2}x = -kx + u(t).$$

It corresponds to the Euler-Lagrange equation (5) with configuration variable $q = x$ and Lagrangian

$$L(x, \dot{x}, t) = \tfrac{m}{2}\dot{x}^2 - \tfrac{k}{2}x^2 + xu(t)$$

made of the difference between the kinetic energy $\frac{m}{2}\dot{x}^2$ and mechanical potential energy $\frac{k}{2}x^2 - xu(t)$.

1.2.2 LC circuit

The dynamics of a capacitor C connected in parallel to an inductor L with magnetic flux ϕ and to an external current source $I(t)$ reads

$$C\frac{d^2}{dt^2}\phi = -\frac{\phi}{L} + I(t).$$

It corresponds to the Euler-Lagrange equation (5) with configuration variable $q = \phi$ and Lagrangian

$$L(\phi, \dot{\phi}, t) = \tfrac{C}{2}\dot{\phi}^2 - \tfrac{1}{2L}\phi^2 + \phi I(t)$$

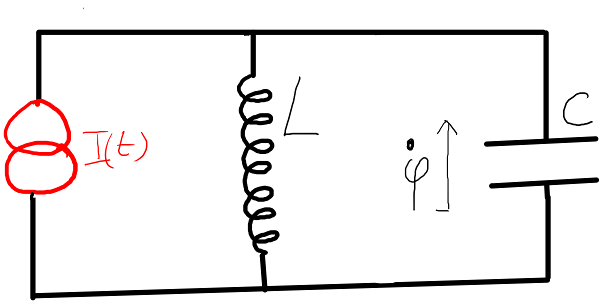

FIGURE 3 – A linear electrical LC circuit driven by a source of current $I(t)$.

made of the difference between the capacitor energy $\frac{m}{2}\dot\phi^2$ and magnetic energy $\frac{1}{2L}\phi^2 - \phi I(t)$.

1.2.3 1D pendulum dynamics

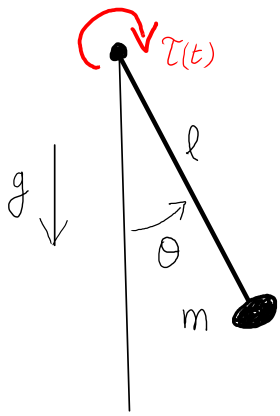

FIGURE 4 – A punctual pendulum of mass m, length ℓ in a vertical plane, submitted to gravity g and an external torque $\tau(t)$.

The conservation of momentum around the rotational horizontal axis of a punctual pendulum (mass m, length ℓ) in the vertical gravity field of acceleration g and submitted to an external torque $\tau(t)$ gives

$$m\ell^2 \frac{d^2}{dt^2}\theta = -mg\ell \sin\theta + \tau(t)$$

where θ is the angle between the pendulum and the vertical direction.

It corresponds to the Euler-Lagrange equation (5) with configuration variable $q = \theta$ defined modulo 2π, and Lagrangian

$$L(\theta, \dot{\theta}, t) = \tfrac{m\ell^2}{2}\dot{\theta}^2 + mg\ell\cos\theta + \theta\tau(t)$$

made of the difference between the rotational kinetic energy $\frac{m\ell^2}{2}\dot{\theta}^2$ and potential energy $-mg\ell\cos\theta - \theta\tau(t)$.

1.2.4 Propagation of light and Fermat principle

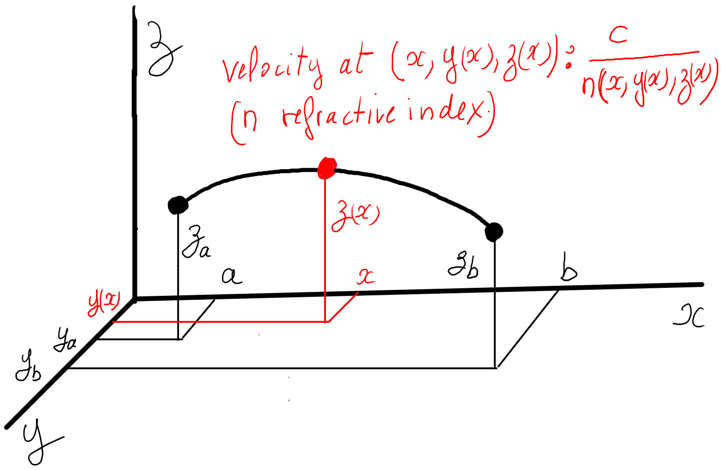

FIGURE 5 – According to Fermat principle, a classical light ray joining two points follows the path with the smallest travelling time. Here the refractive index is maximum along the axis x.

Consider a 3D transparent media with refractive index $n(x, y, z) \geq 1$ depending on the Cartesian coordinates (x, y, z). Consider classical light rays propagating around the direction x : it can be described by a 3D path $x \mapsto (x, y(x), z(x))$ parameterized by x. We are looking for the light ray connecting (a, y_a, z_a) and (b, y_b, z_b) with $a < b$. It obeys to Fermat principle : among all the possible paths between (a, y_a, z_a) and (b, y_b, z_b) , the light follows the path minimizing the travel time.

For any arbitrary path $x \mapsto (x, y(x), z(x))$, its arc length s is defined as

$$ds = \sqrt{dx^2 + dy^2 + dz^2} = \sqrt{1 + (dy/dx)^2 + (dz/dx)^2}\; dx.$$

Since the speed of light around $(x, y(x), z(x))$ is given by $c/n(x, y(x), z(x))$ where c is the speed of light in vacuum, the time to go from s to $s + ds$ is

$n(x, y(x), z(x))ds/c$. Thus the time to go from (a, y_a, z_a) to (b, y_b, z_b) following the path $(x, y(x), z(x))$ is thus given by the integral :

$$\int_a^b n(x, y(x), z(x)) \sqrt{1 + (dy/dx)^2 + (dz/dx)^2} \, \frac{dx}{c}. \tag{6}$$

With t replacing x, $(q_1, q_2) = (y, z)$ and $(\dot{q}_1, \dot{q}_2) = (dy/dx, dz/dx)$, the path follows by the light ray is solution of the Euler-Lagrange differential equations attached to the Lagrangian

$$L(y, z, y', z', x) = n(x, y, z)\sqrt{1 + (y')^2 + (z')^2}/c$$

where $'$ stand for d/dx.

Exercise. Explicit these Euler-Lagrange equations.

1.3 Change of configuration variables

Consider (2) and a time-varying change of configuration variables $q = \phi(\tilde{q}, t)$ of inverse $\tilde{q} = \psi(q, t)$ where ϕ and ψ are smooth mappings such that $\psi(\phi(\tilde{q}, t), t) \equiv \tilde{q}$ and $\phi(\psi(q, t), t) \equiv q$.

If around the trajectory $[t_a, t_b] \ni t \mapsto q(t)$ the first variation of S given by (1) vanishes, then the first variation of

$$\int_{t_a}^{t_b} L\left(\phi(\tilde{q}(t), t) \ , \ \frac{\partial \phi}{\partial \tilde{q}}(\tilde{q}(t), t)\dot{\tilde{q}}(t) + \frac{\partial \phi}{\partial t}(\tilde{q}(t), t) \ , \ t\right) dt$$

also vanishes. Thus the Euler-Lagrange equations derived from Lagrangian $L(q, \dot{q}, t)$ coincide with the Euler-Lagrange equations derived from Lagrangian $\tilde{L}(\tilde{q}, \dot{\tilde{q}}, t) = L\left(\phi(\tilde{q}, t) \ , \ \frac{\partial \phi}{\partial \tilde{q}}(\tilde{q}, t)\dot{\tilde{q}}(t) + \frac{\partial \phi}{\partial t}(\tilde{q}, t) \ , \ t\right)$.

One can perform the change of variables $q = \phi(\tilde{q}, t)$ in the Euler-Lagrange equations with q. Usually, this is not the most efficient way to obtain these equations in the new set of configuration variables $\tilde{q}$. It is much more direct to perform the change of variables in the Lagrangian L and then to derive from $\tilde{L}$ the Euler-Lagrange equations in configuration variables $\tilde{q}$.

Exercise Derive the Euler-Lagrange equations of the Cartesian Lagrangian $\dot{q}_1^2 + \dot{q}_2^2 - q_1^2 - q_2^2$. What are these Euler-Lagrange equations in polar coordinates (r, θ) where $q_1 = r\cos\theta$ and $q_2 = r\sin\theta$?

1.4 Approximation around a steady-state

Assume that $(q, \dot{q}) = (\bar{q}, 0)$ is a critical point of the Lagrangian $L(q, \dot{q}, t)$, i.e. that, for all i, $\frac{\partial L}{\partial q_i}(\bar{q}, 0, t) = 0$ and $\frac{\partial L}{\partial \dot{q}_i}(\bar{q}, 0, t) = 0$. Then $t \mapsto q(t) = \bar{q}$ is a steady-state solution of (4). Up to second order terms in δq, the solution $t \mapsto q(t) = \bar{q} + \delta q(t)$ of (4) close to $\bar{q}$ ($\delta q(t)$ small) obey also to an Euler-Lagrange equation where the Lagrangian δL is obtained by the expansion up to second-order terms of L around $(\bar{q}, 0, t)$:

$$L(\bar{q} + \delta q, \delta\dot{q}, t) = L(\bar{q}, 0, t) + \delta L(\delta q, \delta\dot{q}, t) + O(\|\delta q\|^3 + \|\delta\dot{q}\|^3).$$

Then δL is a quadratic function of δq and $\delta\dot{q}$ given by

$$\delta L(\delta q, \dot{\delta q}, t) = \tfrac{1}{2} \sum_{i,j=1}^{n} \frac{\partial^2 L}{\partial \dot{q}_i \partial \dot{q}_j} \delta\dot{q}_i \delta\dot{q}_j + \frac{\partial^2 L}{\partial q_i \partial \dot{q}_j} \delta q_i \delta\dot{q}_j \dots \\ + \frac{\partial^2 L}{\partial \dot{q}_i \partial q_j} \delta\dot{q}_i \delta q_j + \frac{\partial^2 L}{\partial q_i \partial q_j} \delta q_i \delta q_j \quad (7)$$

Here the second-order partial derivatives are evaluated at $(\bar{q}, 0, t)$ and thus depend a priori on t. As for the change of configuration variables, usually it is simpler to approximate the Lagrangian up to second order terms and then to derived the linear differential equations satisfied by δq :

$$\sum_j \frac{d}{dt} \left(\frac{\partial^2 L}{\partial \dot{q}_i \partial \dot{q}_j} \delta\dot{q}_j + \frac{\partial^2 L}{\partial \dot{q}_i \partial q_j} \delta q_j \right) = \frac{\partial^2 L}{\partial q_i \partial \dot{q}_j} \delta\dot{q}_j + \frac{\partial^2 L}{\partial q_i \partial q_j} \delta q_j.$$

Exercise Derived the approximate dynamics around $\theta = 0$ and $\theta = \pi$ of the 1D pendulum of subsection 1.2.3 with $\tau(t) \equiv 0$.

Exercise For the Lagrangian of subsection 1.2.4, assume that, for y, z small, $n(x, y, z) = n_0 - \epsilon(y^2 + z^2)$ with $n_0 > 1$ and $0 < \epsilon \ll 1$. Derive then δL and the associated Euler-Lagrange equations for δy and δz. What is the shape of the solutions for the linearized Euler-Lagrange system when $\delta y(a) = \delta z(a) = 0$ and $\delta y'(a) = 1 = \delta z(a)$? Provide a simple physical interpretation ?

1.5 Conservation of energy

Consider a solution $q(t)$ of the Euler-Lagrange equations (4) and

$$E(q, \dot{q}, t) = \sum_{i=1}^{n} \frac{\partial L}{\partial \dot{q}_i} \dot{q}_i - L \quad (8)$$

corresponding to its energy. Standard computations give

$$\frac{d}{dt}E = \sum_{i=1}^{n} \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\dot{q}_i\right) - \frac{d}{dt}L$$
$$= \sum_{i=1}^{n} \frac{\partial L}{\partial \dot{q}_i}\ddot{q}_i + \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right)\dot{q}_i - \frac{\partial L}{\partial q_i}\dot{q}_i - \frac{\partial L}{\partial \dot{q}_i}\ddot{q}_i - \frac{\partial L}{\partial t}$$
$$= -\frac{\partial L}{\partial t}.$$

Thus, if L is independent of t and thus only a function of q and $\dot{q}$, E is constant along any solution of (4). It is a constant of motion also called a first integral.

Exercise Compute E for the 1D pendulum of subsection 1.2.3 with $\tau(t) \equiv 0$.

Exercise Compute E for the Lagrangian of subsection 1.2.4.

1.6 System with a single configuration variable

For a single configuration variable with a time-invariant Lagrangian $L(q, \dot{q})$ the conservation of energy E provides a direct way to solve almost explicitly (up to inversion and quadrature of scalar nonlinear functions).One can obtained $\dot{q}$ as a function of q by solving the equation $E(q, x) = E(q(0), \dot{q}(0))$ where x is the unknown. Denote by $h(q, q_0, \dot{q}_0)$ this function :

$$E(q, h(q, q(0), \dot{q}(0))) \equiv E(q(0), \dot{q}(0))$$

for all q, $q(0)$ and $\dot{q}(0)$. Then $\frac{d}{dt}q = h(q, q(0), \dot{q}(0))$ implies that

$$dt = \frac{dq}{h(q, q(0), \dot{q}(0))}.$$

An integration between 0 and t gives

$$t = \int_0^t dt = \int_{q(0)}^{q(t)} \frac{dq}{h(q, q(0), \dot{q}(0))}$$

, i.e. a nonlinear equation providing $q(t)$ versus t by solving

$$t = f(q, q(0), \dot{q}(0))$$

where f is the primitive of $q \mapsto 1/h(q, q(0), \dot{q}(0))$ vanishing at $q = q(0)$.

Exercise Apply this method for the 1D pendulum of subsection 1.2.3 with $\tau(t) \equiv 0$.

2 Hamiltonian dynamics

2.1 From Lagrangian to Hamiltonian formulation

The Euler-Lagrange equations (4) is a set of n second-order differential equations versus $q = (q_1, \ldots, q_n)$. With $\dot{q}_i = v_i$, it yields a set of $2n$ first-order differential equations versus (q, v) where $v = (v_1, \ldots, v_n)$:

$$\frac{d}{dt} q_i = v_i, \quad \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}(q, v, t)\right) = \frac{\partial L}{\partial q_i}(q, v, t), \quad i = 1, \ldots, n$$

This system is implicit since one has to express $\frac{d}{dt} v$ as function of (q, v, t) by inverting the $n \times n$ matrix $J_{ij}(q, v, t) = \frac{\partial^2 L}{\partial \dot{q}_i \partial \dot{q}_j}$ assumed to be invertible :

$$\frac{d}{dt} v_i = \sum_j \left(J^{-1}\right)_{ij} \left(\frac{\partial L}{\partial q_j} - \frac{\partial^2 L}{\partial \dot{q}_j \partial t} - \sum_k \frac{\partial^2 L}{\partial \dot{q}_j \partial q_k} v_k\right).$$

If instead of $v = \dot{q}$ one takes $p_i = \frac{\partial L}{\partial \dot{q}_i}$, one get another following implicit system in (q, p) where $p = (p_1, \ldots, p_n)$ is the conjugate momentum associated to q :

$$\frac{\partial L}{\partial \dot{q}_i}\left(q, \frac{d}{dt} q, t\right) = p_i, \quad \frac{d}{dt} p_i = \frac{\partial L}{\partial q_i}\left(q, \frac{d}{dt} q, t\right), \quad i = 1, \ldots, n.$$

Here $\frac{d}{dt} q = \dot{q}$ is implicitly defined as a function of (q, p, t) by solving a system with n equations

$$p_i = \frac{\partial L}{\partial \dot{q}_i}(q, \dot{q}, t), \quad i = 1, \ldots, n. \tag{9}$$

The total differential of L versus q and $\dot{q}$ reads

$$dL = \frac{\partial L}{\partial t} dt + \sum_i \frac{\partial L}{\partial q_i} dq_i + \frac{\partial L}{\partial \dot{q}_i} d\dot{q}_i = \frac{\partial L}{\partial t} dt + \sum_i \frac{\partial L}{\partial q_i} dq_i + p_i d\dot{q}_i.$$

Since

$$d\left(\sum_i p_i \dot{q}_i\right) = \sum_i p_i d\dot{q}_i + \dot{q}_i dp_i$$

We have, with $H=\sum_i p_i \dot{q}_i - L$ corresponding to the energy,

$$dH = -\frac{\partial L}{\partial t}dt + \sum_i \dot{q}_i dp_i - \frac{\partial L}{\partial q_i}dq_i.$$

H is a priori a function of $(q, \dot{q}, t)$ but since p is a function of $(q, \dot{q}, t)$ via (9), we can also consider H as a function of (q, p, t). The above calculations based on total derivatives prove that

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad -\frac{\partial L}{\partial q_i} = \frac{\partial H}{\partial q_i}, \quad -\frac{\partial L}{\partial t} = \frac{\partial H}{\partial t}.$$

This means that the Euler-Lagrange equations (4) become with the Hamilton variables (q, p) a set of $2n$ first-order equations :

$$\frac{d}{dt}q_i = \frac{\partial H}{\partial p_i}, \quad \frac{d}{dt}p_i = -\frac{\partial H}{\partial q_i}, \quad i = 1, \ldots, n \tag{10}$$

where the expression of the Hamiltonian $H(q, p, t)$ is derived from $L(q, \dot{q}, t)$ by eliminating $\dot{q}$ from the following relationships

$$H = \sum_i \frac{\partial L}{\partial \dot{q}_i}(q, \dot{q}, t)\dot{q}_i - L(q, \dot{q}, t) \text{ and } p_j = \frac{\partial L}{\partial \dot{q}_j}(q, \dot{q}, t) \text{ for } j = 1, \ldots, n.$$

2.2 Lagrangian quadratic versus velocities

When the dependence of $L(q, \dot{q}, t)$ in $\dot{q}$ is quadratic, the passage from the Lagrangian to the Hamiltonian relies on the inversion of an $n \times n$ matrix those entries could depends on q and t. More precisely, with

$$L(q, \dot{q}, t) = \tfrac{1}{2}\sum_{i,j} J_{ij}(q, t)\dot{q}_i\dot{q}_j - U(q, t)$$

where $\frac{1}{2}\sum_{i,j} J_{ij}(q, t)\dot{q}_i\dot{q}_j$ is the kinetic energy and $U(q, t)$ the potential energy, one gets

$$p_i = \sum_j J^{-1}_{ij}(q, t)\dot{q}_j, \quad H(q, p, t) = \tfrac{1}{2}\sum_{i,j} J^{-1}_{ij}(q, t)p_i p_j + U(q, t).$$

Here $J^{-1}_{ij}(q, t)$ are the entries of $J^{-1}(q, t)$ the inverse of the $n \times n$ matrix $J(q, t)$ of entries $J_{ij}(q, t)$.

Exercise Compute $H(\theta, p_\theta, t)$ for the 1D pendulum of subsection 1.2.3.

Exercise Compute $H(y, z, p_y, p_z, x)$ from the Lagrangian of subsection 1.2.4.

2.3 First integral and Poisson bracket

When the Lagrangian and thus the Hamiltonian are independent t, $H(q, p)$ is constant along any solution of (10), i.e. H is a first integral.

It is interesting to note that a scalar function $f(q, p)$ is a first integral if, and only if, for all q and p, we have

$$0 = \frac{d}{dt} f = \sum_i \frac{\partial f}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial H}{\partial q_i} = \{f, H\}$$

where the Poisson bracket between two functions f and g of (q, p) is defined by

$$\{f, g\} = \sum_i \frac{\partial f}{\partial q_i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q_i} \tag{11}$$

The Poisson bracket admits nice properties. In particular for any functions f,g and h of (q, p), one has

$$\{f, gh\} = \{f, g\}h + g\{f, h\} \text{ (Leibnitz rule)}$$

and

$$\{f, \{g, h\}\} + \{g, \{h, f\}\} + \{h, \{f, g\}\} = 0 \text{ (Jacobi identity).}$$

Thus, if f and g are two first integrals, i.e., $\{f, H\} = \{g, H\} = 0$ then $\{f, g\}$ is also a first integral (use Jacobi identity with $h = H$).

3 Classical/quantum correspondence

Throughout this section we assume here that the classical Hamiltonian $H(q, p)$ admits the following structure :

$$H(q, p) = \tfrac{1}{2} \sum_j A_{jj'} p_j p_{j'} + U(q) \tag{12}$$

where the $n \times n$ real matrix $A = (A_{jj'})$ is symetric, positive definite and constant. The classical Hamilton equations read :

$$\frac{d}{dt} q_j = \sum_{j'} A_{jj'} p_{j'}, \quad \frac{d}{dt} p_j = -\frac{\partial U}{\partial q_j} \text{ for } j = 1, \ldots, n$$

3.1 Correspondence rules

The quantum dynamics associated to such H are obtained by the following correspondence rules.

To the classical Hamiltonian variables q_j and p_j correspond the Hermitian operators $\widehat{q}_j$ and $\widehat{p}_j$ defined on a suitable Hilbert space (defined below) satisfying the commutation rules

$$[\widehat{q}_j, \widehat{p}_j] = i\hbar, \qquad [\widehat{q}_j, \widehat{q}_{j'}] = [\widehat{q}_j, \widehat{p}_{j'}] = [\widehat{p}_j, \widehat{p}_{j'}] = 0 \text{ for } j \neq j'$$

where $i = \sqrt{-1}$ here.

To $H(q,p)$ defined by (12) corresponds the operator $\widehat{H}$ given by

$$\frac{\widehat{H}}{\hbar} = \tfrac{1}{2} \sum_j A_{jj'} \widehat{p}_j \widehat{p}_{j'} + U(\widehat{q}).$$

Notice that since $[\widehat{p}_j, \widehat{p}_{j'}] = 0 = [\widehat{q}_j, \widehat{q}_{j'}]$ there is no ambiguity here. This is not the case if, for example, the Hamiltonian contains terms like $q_j^2 p_j = q_j p_j q_j = p_j q_j^2$ and thus yielding to different possible corresponding Hermitian operators such as

$$(\widehat{q}_j^2 \widehat{p}_j + \widehat{p}_j \widehat{q}_j^2)/2 \text{ or } \widehat{q}_j \widehat{p}_j \widehat{q}_j.$$

The time derivative along classical trajectories $t \mapsto (q(t), p(t))$ of any function $f(q,p)$ is given by the Poisson bracket with the Hamiltonian :

$$\frac{d}{dt} f = \{f, H\}$$

Similarly the time derivative of any operator $\widehat{f}$ is then given by

$$\frac{d}{dt} \widehat{f} = [\widehat{f}, \widehat{H}]/(i\hbar).$$

Thus Poisson brackets correspond to commutators divided by $i\hbar$.

This results simply from the following computations for the averaged value of operator (observable) $\widehat{f}$ attached to the time-varying wave function $|\psi\rangle$, solution of the Schrödinger dynamics, $i\hbar \frac{d}{dt} |\psi\rangle = \widehat{H} |\psi\rangle$:

$$\frac{d}{dt} \big(\langle\psi| \widehat{f} |\psi\rangle \big) = \langle\psi| [\widehat{f}, \widehat{H}] |\psi\rangle / (i\hbar) \triangleq \langle\psi| \frac{d}{dt} \widehat{f} |\psi\rangle .$$

Any operator $\widehat{f}$ commuting with $\widehat{H}$ yields thus to a first integral of the dynamics, i.e., its averaged value is an invariant, i.e. independent of time.

3.2 Two examples

3.2.1 Mass/spring system

Consider the mass/sping system of subsection 1.2.1. Its Hamiltonian reads

$$H(x,p,t) = \frac{p^2}{2m} + \frac{kx^2}{2} - xu(t).$$

The corresponding quantum Hamiltonian is thus

$$\widehat{H} = \frac{\widehat{p}^2}{2m} + \frac{k\widehat{x}^2}{2} - \widehat{x}u(t)$$

with $[\widehat{x},\widehat{p}] = i\hbar$.

The annihilation operator $\widehat{a}$ is then defined by

$$\widehat{a} = \frac{\widehat{x}}{\sqrt{2\hbar/\sqrt{mk}}} + i\frac{\widehat{p}}{\sqrt{2\hbar\sqrt{mk}}}$$

Then

$$\widehat{H} = \hbar\omega\left(\widehat{a}^\dagger\widehat{a} + \tfrac{1}{2}\right) - \sqrt{\tfrac{\hbar}{2\sqrt{mk}}}u(t)(\widehat{a} + \widehat{a}^\dagger)$$

where $\omega = \sqrt{k/m}$ is the pulsation of the harmonic oscillator (either classical or quantum).

3.2.2 A Josephson electrical circuit

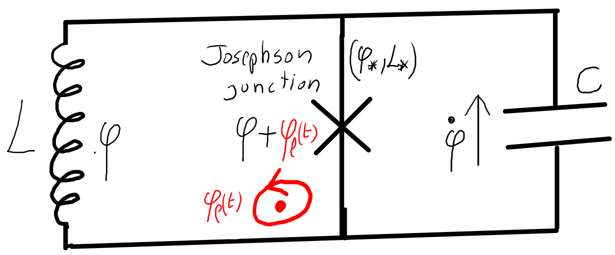

FIGURE 6 – An electrical circuit with a non linear inductance corresponding to a Josephson junctionand submitted to an external flux $\phi_e(t)$.

The Lagrangian of the squid circuit of figure 6 is as follows :

$$L(\phi, \dot{\phi}, \phi_e(t)) = \tfrac{C}{2}\dot{\phi}^2 - \tfrac{1}{2L}\phi^2 + \tfrac{\phi_*^2}{L_*}\cos\left(\frac{\phi + \phi_e(t)}{\phi_*}\right)$$

where $C > 0$ and $L > 0$ are the linear capacitor and indutance, $\phi_* > 0$ and $L_* > 0$ are parameters describing the Josephson junction and $\phi_e(t)$ is the external magnetic flux through the loop made of the linear inductor and Josephson junction.

The conjugate variable of ϕ, $\frac{\partial L}{\partial \dot{\phi}}$ corresponds to the capacitor charge $Q = C\dot{\phi}$, and the resulting Hamiltonian is :

$$H(\phi, Q, \phi_e(t)) = \tfrac{1}{2C}Q^2 + \tfrac{1}{2L}\phi^2 - \tfrac{\phi_*^2}{L_*}\cos\left(\frac{\phi + \phi_e(t)}{\phi_*}\right).$$

The quantum Hamiltonian is then

$$H(\widehat{\phi}, \widehat{Q}, \phi_e(t)) = \tfrac{1}{2C}\widehat{Q}^2 + \tfrac{1}{2L}\widehat{\phi}^2 - \tfrac{\phi_*^2}{L_*}\cos\left(\frac{\widehat{\phi} + \phi_e(t)}{\phi_*}\right)$$

where $[\widehat{\phi}, \widehat{Q}] = i\hbar$ and $\phi_e(t)$ is a scalar drive, the control input used to manipulate this system in super-conducting quantum circuit.

When the Josephson energy $\frac{\phi_*^2}{2L_*}\cos\left(\frac{\widehat{\phi}+\phi_e(t)}{\phi_*}\right)$ is small compared to the LC energy $\frac{1}{2C}\widehat{Q}^2 + \frac{1}{2L}\widehat{\phi}^2$, an adapted scaling is the following. With

$$\omega = \sqrt{1/LC}$$

denoting the pulsation of the linear circuit, consider the normalized phase-space operators

$$\widehat{q} = \frac{\widehat{\phi}}{\sqrt{\hbar\omega L}} \text{ and } \widehat{p} = \frac{\widehat{Q}}{\sqrt{\hbar\omega C}}$$

satifying $[\widehat{q}, \widehat{p}] = i$ and the annihilation operator $\widehat{a}$ as

$$\widehat{a} = \frac{\widehat{q} + i\widehat{p}}{\sqrt{2}} \text{with } [\widehat{a}, \widehat{a}^\dagger] = 1.$$

Then the Hamiltonian operator becomes

$$\frac{\widehat{H}}{\hbar} = \omega\left(\widehat{a}^\dagger\widehat{a} + \tfrac{1}{2}\right) + \omega\tfrac{Lq_*}{L_*}\cos\left(\frac{\widehat{q} + q_e(t)}{q_*}\right)$$

where $q_e(t) = \frac{\phi_e(t)}{\sqrt{\hbar\omega L}}$ and $q_* = \frac{\phi_*}{\sqrt{\hbar\omega L}}$. A Josephson energy relatively small means $\frac{Lq_*}{L_*} \ll 1$.

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