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E. B. Legrand

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DELFT UNIVERSITY OF TECHNOLOGY
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The undersigned hereby certify that they have read and recommend to the Faculty of
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by

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Abstract

This is an abstract.

Table of Contents

Preface	ix
Acknowledgements	xi
1 Introduction	1
1-0-1 About mathematical notation and sign conventions	2
2 Analytical economics	3
2-1 Symplectic formulation	3
2-2 The Liouville theorem	4
2-2-1 About divergence	4
2-3 Variational formulation	4
3 Dissipative Classical Mechanics	5
3-1 The Bateman approach	5
3-1-1 Towards the bicomplex Hamiltonian	6
4 Autonomous systems	9
4-1 Harmonic oscillator	9
4-1-1 Solution of the Liouville equation	10
4-1-2 Initial Gaussian distribution	14
4-1-3 Verification using a Monte-Carlo method	16
4-2 Damped harmonic oscillator	18
4-2-1 A quick tour of dissipative classical mechanics	18
4-2-2 Discounted state functions	19
4-2-3 Complex Hamiltonian	25
4-3 Nonlinear systems	25
4-3-1 Double pendulum	25
4-3-2 Van der Pol oscillator	25

Bibliography	27
Glossary	29
List of Acronyms	29
List of Symbols	29

List of Figures

- 4-1 The marginal distributions given by eq. (4-12). The solid line represents the evolution of the mean, while the shaded area is a 95% confidence interval, i.e. two standard deviations from the mean, given that the distribution is normal. 15
- 4-2 Numerical solution of the time-averaged distribution given by eq. (4-13), for $m = 1$, $k = 2$, $\Sigma = \begin{pmatrix} 0.2 & 0.10.1 & 0.2 \end{pmatrix}$ and $x_0 = (11)$. The marginalized distributions for p and q are shown as well. 17
- 4-3 Schematic of the damped harmonic oscillator. 18
- 4-4 Graphical illustration of the singularity of the Lagrangian. The fiber derivative provides a pointwise mapping between the cotangent space $T_x Q$, where $x = (q, t)$, and the cotangent bundle $T_x^* Q$, but this mapping is neither injective nor surjective. The mapping $\mathbb{F}\mathcal{L}$ acts injectively on the projectivization of the tangent space — in this case, \mathbb{R}^2 / \sim , where \sim denotes the equivalence relation $(v_q, v_t) \sim (\lambda v_q, \lambda v_t)$ — it takes the equivalence classes $[v_q : v_t]$ as an argument. Furthermore, the image of the entire tangent space is restricted to a parabolic subset of the cotangent space. 22

List of Tables

1-1	Caption	1
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Preface

Acknowledgements

I would like to thank my supervisor prof.dr.ir. M.Y. First Reader for his assistance during the writing of this thesis...

By the way, it might make sense to combine the Preface and the Acknowledgements. This is just a matter of taste, of course.

Delft, University of Technology
February 5, 2022

E. B. Legrand

“To doubt everything, or, to believe everything, are two equally convenient solutions; both dispense with the necessity of reflection.”

— *Henri Poincaré*

Chapter 1

Introduction

Original Liouville ideas:

- Showcase complex behaviour using the van der Pol oscillator
- (Optimal) control of the distributions using the Brockett approach
- (Stochastic) inputs, link with Langevin equations
- Liouville thing (in continuity form, not incompressibility) can be applied to any diff. eq.
- Bayesian inversion of chaotic systems; guess the initial state by sampling after a certain time
- Define as streamtube, continuity equation asserts that streamlines cannot cross; i.e. streamtubes are conserves. To reduce computational complexity, define level sets (curves in 2-D) and check how they deform through the evolution of the phase space fluid; should always contain the same amount of probability throughout the evolution of the system.

Notation check

Object	Roman lower	Roman upper	Greek lower	Greek upper
Standard	<i>abcde</i>	<i>ABCDE</i>	$\alpha\beta\gamma\delta\varepsilon$	$\Gamma\Delta\Upsilon\Omega\Theta$
Vector	<i>abcde</i>	<i>ABCDE</i>	$\alpha\beta\gamma\delta\varepsilon$	$\Gamma\Delta\Upsilon\Omega\Theta$
Tensor	<i>abcde</i>	<i>ABCDE</i>	$\alpha\beta\gamma\delta\varepsilon$	$\Gamma\Delta\Upsilon\Omega\Theta$

Table 1-1: Caption

Christoffel symbol: Γ

Math constants: $i\epsilon\pi$

Variation: δS

Musical isomorphism

Flat: X^\flat

Sharp: ω^\sharp

Lie derivative: $\mathcal{L}_X H$

Interior product: $X \lrcorner \omega$

Lowercase mathcal:

Kinematic momentum: $\mathfrak{p}p$

1-0-1 About mathematical notation and sign conventions

For symplectic geometry, the sign convention used by Abraham and Marsden [1] and Cannas da Silva [2] is observed — not the one used by Arnol'd in his *Mathematical methods of classical mechanics*, nonetheless often referred to in this text.

Analytical economics

2-1 Symplectic formulation

Lie derivatives & Max' question

The Lie derivative of the tautological form $\alpha = p dq$ with respect to the Hamiltonian vector field

$$X_H = \frac{\partial H}{\partial p} \frac{\partial}{\partial q} - \frac{\partial H}{\partial q} \frac{\partial}{\partial p}$$

is denoted by

$$\mathcal{L}_{X_H} \alpha.$$

Using Cartan's magic formula ($\mathcal{L}_V \theta = d(V \lrcorner \theta) + V \lrcorner d\theta$), this expression can be written as

$$\begin{aligned} \mathcal{L}_{X_H} p dq &= d(X_H \lrcorner p dq) + X_H \lrcorner d(p dq) \\ &= d(X_H \lrcorner p dq) - X_H \lrcorner \omega \\ &= d(X_H \lrcorner p dq) - dH \\ &= d\left(\frac{\partial H}{\partial p} p\right) - dH \\ &= d(\dot{q}p) - dH \\ &= d(\dot{q}p - H) \\ &= dL \end{aligned}$$

Explicitly in components:

$$\mathcal{L}_{X_H} \alpha = [X_H^\nu (\partial_\nu \alpha_\mu) + (\partial_\mu X_H^\nu) \alpha_\nu] dx^\mu$$

$$\begin{aligned}
\mathcal{L}_{X_H}\alpha &= \left[\frac{\partial H}{\partial p} \left(\frac{\partial}{\partial q} p \right) + \left(\frac{\partial}{\partial q} \frac{\partial H}{\partial p} \right) p - \frac{\partial H}{\partial q} \left(\frac{\partial}{\partial p} p \right) - \left(\frac{\partial}{\partial q} \frac{\partial H}{\partial q} \right) 0 \right] dq \\
&\quad + \left[\frac{\partial H}{\partial p} \left(\frac{\partial}{\partial q} 0 \right) + \left(\frac{\partial}{\partial p} \frac{\partial H}{\partial p} \right) p - \frac{\partial H}{\partial q} \left(\frac{\partial}{\partial q} 0 \right) - \left(\frac{\partial}{\partial p} \frac{\partial H}{\partial q} \right) 0 \right] dp \\
&= \left[\left(\frac{\partial}{\partial q} \frac{\partial H}{\partial p} \right) p - \frac{\partial H}{\partial q} \right] dq + \left[\left(\frac{\partial}{\partial p} \frac{\partial H}{\partial p} \right) p \right] dp
\end{aligned}$$

Compare this with the expression using the Cartan equation:

$$\begin{aligned}
d\left(\frac{\partial H}{\partial p} p - H\right) &= \frac{\partial}{\partial q} \left(\frac{\partial H}{\partial p} p \right) dq + \frac{\partial}{\partial p} \left(\frac{\partial H}{\partial p} p \right) dp - \frac{\partial H}{\partial q} dq - \frac{\partial H}{\partial p} dp \\
&= \left[p \frac{\partial}{\partial q} \left(\frac{\partial H}{\partial p} \right) + \frac{\partial H}{\partial p} \frac{\partial p}{\partial q} - \frac{\partial H}{\partial q} \right] dq + \left[p \frac{\partial}{\partial p} \left(\frac{\partial H}{\partial p} \right) + \frac{\partial H}{\partial p} \frac{\partial p}{\partial p} - \frac{\partial H}{\partial p} \right] dp
\end{aligned}$$

which coincides with the previous expression.

2-2 The Liouville theorem

This section explores the different forms in which the Liouville theorem appears, both in classical mechanics and the general study of differential equations.

2-2-1 About divergence

In this text, divergence appears in general levels of generalization, from the standard vector calculus definition to one in terms of differential forms that applies to curved spaces as well.

CHECK Foundations of mechanics p. 130 for a rigorous treatment of divergence on manifolds.

2-3 Variational formulation

Dissipative Classical Mechanics

3-1 The Bateman approach

The approach used by Bateman [3] starts from a simple linear scalar second-order differential equation:

$$\ddot{x} + 2c\dot{x} + kx = 0.$$

This equation can be written as the solution of a variational expression like so:

$$\delta \int \underbrace{y(\ddot{x} + c\dot{x} + kx)}_L dt = 0;$$

where the Lagrangian is the argument of the time integral. To account for the presence of \ddot{x} , Euler-Lagrange equation can be readily extended to higher derivatives. The most general expression is, for p functions of m independent variables up to the n th derivative:

$$\frac{\partial L}{\partial q_i} + \sum_{j=1}^n \sum_{\mu_1 \leq \dots \leq \mu_j} (-1)^j \frac{\partial^j}{\partial t_{\mu_1} \dots \partial t_{\mu_j}} \left(\frac{\partial L}{\partial q_{\mu_1 \dots \mu_j}} \right) = 0,$$

where $i = 1, \dots, p$ and $\mu_j = 1, \dots, m$. In this case however, there is only one independent variable, $m = 1$, and the highest derivative taken into account is $n = 2$. The variational problem then yields two equations: the original differential equation and a complementary equation in y :

$$\ddot{x} + 2c\dot{x} + kx = 0 \quad \ddot{y} - 2c\dot{y} + ky = 0$$

However, the presence of the second derivative in the Lagrangian is altogether undesirable, so one can effect the substitution

$$\ddot{x} y dt = d(\dot{x} y) - \dot{x} \dot{y} dt.$$

Because the solution of the Euler-Lagrange equation is independent from total differentials added to the Lagrangian, the first term can be neglected. As such, the Lagrangian becomes:

$$L = -\dot{x} \dot{y} + 2cy\dot{x} + kyx.$$

3-1-1 Towards the bicomplex Hamiltonian

From the two resulting differential equations, it is clear that x and y represent the state evolution in opposite directions of time (in case they are initialized properly); because first (odd) derivative carries the minus sign (that is canceled in the second derivative; which is invariant with respect to a time reversal). This symmetry may become more apparent from the Lagrangian by using integration by parts a second time, i.e.

$$d(xy) = \dot{x}y dt + y\dot{x} dt,$$

such that

$$L = -\dot{x}\dot{y} + c(y\dot{x} + d(xy) - \dot{y}x) + kyx,$$

where the total differential may again be neglected. This the negative of the Lagrangian considered by Dekker [4]; the latter is assumed in further calculations (of course, multiplying the Lagrangian by -1 does not alter the solutions of the variational problem). Using this Lagrangian, the two conjugate momenta are, by definition:

$$p_x \triangleq \frac{\partial L}{\partial \dot{x}} = \dot{y} - cy \quad p_y \triangleq \frac{\partial L}{\partial \dot{y}} = \dot{x} + cx.$$

A Legendre transform then leads to the associated Hamiltonian

$$H = p_x\dot{x} + p_y\dot{y} - L = p_xp_y - c(xp_x - yp_y) + (k - c^2)xy.$$

This expression already reflects the structure of the bicomplex Hamiltonian proposed by Hutters and Mendel [5]. However, it still contains the states of both the system and the antisystem, i.e. x , y , p_y , p_x . As shown by Bopp [6], a complexification of the states allows to rewrite the above Hamiltonian into two separate components corresponding to the system and the antisystem.

TODO write complex transformation from Bateman to Bopp

Complex state

Now consider the complexified state:

$$z = \frac{1}{\sqrt{2\omega_d}}(p + (\lambda - i\omega_d)q)$$

with $\omega_d = \sqrt{\omega - \lambda^2}$. The Bopp Hamiltonian then reads

$$\begin{aligned} H_{\text{Bopp}} &= (\omega_d - i\lambda)z\bar{z} \\ &= \frac{1}{2}\left(1 - i\frac{\lambda}{\omega_d}\right)((p + \lambda q)^2 + \omega_d^2 q^2) \\ &= \frac{1}{2}\left(1 - i\frac{\lambda}{\omega_d}\right)(p^2 + 2\lambda pq + \lambda^2 q^2 + \omega_d^2 q^2) \\ &= \frac{1}{2}\left(1 - i\frac{\lambda}{\omega_d}\right)(p^2 + 2\lambda pq + \omega^2 q^2) \end{aligned} \tag{3-1}$$

Then, choosing a new state $a = \frac{1}{\sqrt{2\omega}}(\omega q + ip)$ such that

$$\omega a \bar{a} = \frac{1}{2}(p^2 + \omega^2 q^2)$$

one can substitute

$$H_{\text{Bopp}} = \left(1 - i \frac{\lambda}{\omega_d}\right)(\omega a \bar{a} + \lambda pq) \quad (3-2)$$

Additionally,

$$a^2 = \frac{1}{2\omega}(\omega^2 q^2 - p^2 + 2i\omega pq)$$

such that $a^2 - \bar{a}^2 = 2ipq$, which can also be substituted in the Hamiltonian expression:

$$H_{\text{Bopp}} = \left(1 - i \frac{\lambda}{\omega_d}\right)\left(\omega a \bar{a} + i \frac{\lambda}{2}(a^2 - \bar{a}^2)\right) \quad (3-3)$$

Autonomous systems

4-1 Harmonic oscillator

Although the harmonic oscillator is a topic that has been studied in tremendous detail, also from a stochastic perspective because of its importance in quantum mechanics, it proves to be an instructive starting point for this research as well [7]. Several reasons apply, most importantly that the solutions may be obtained analytically and that the Hamiltonian phase space is two-dimensional, which allows for straightforward visualization of the result.

Although the Liouville theorem is usually expressed directly in terms of Poisson brackets (which, in turn, have a trivial form if expressed in Darboux coordinates), a slightly more insightful approach is taken here. More specifically, instead of applying the Poisson brackets directly, they are formulated like so:

$$\{f, g\} = X_g(f) = \mathcal{L}_{X_g}f$$

where X_g is the Hamiltonian vector field associated to g . The definition of Poisson brackets in terms of Hamiltonian vector fields makes it easy to draw connection between fluid mechanics and the classical mechanics.

For the undamped harmonic oscillator, the configuration manifold M is simply \mathbb{R} . As such, the cotangent bundle $T^*M = \mathbb{R}^2$. The Hamiltonian, being a smooth

$$H : T^*M \rightarrow \mathbb{R} : H(p, q) = \frac{m}{2}p^2 + \frac{k}{2}q^2. \quad (4-1)$$

To apply Liouville's theorem, the Hamiltonian vector field X_H associated with H must be found. By definition, one can do this by virtue of the canonical isomorphism induced by the symplectic 2-form:

$$dH(\cdot) = \omega(X_H, \cdot),$$

this isomorphism is sometimes denoted by ω^\sharp , colloquially called the ‘musical isomorphism’. In terms of the interior product, this pairing takes the form [8, 1]

$$X_H \lrcorner \omega = dH. \quad (4-2)$$

The differential 1-form dH is

$$dH = kq dq + \frac{p}{m} dp,$$

such that, by means of eq. (4-2), the Hamiltonian vector field becomes

$$X_H = \frac{p}{m} \frac{\partial}{\partial q} - kq \frac{\partial}{\partial p}.$$

Having found the Hamiltonian vector field, Liouville's theorem can be applied to an arbitrary distribution ρ over the phase space:

$$\frac{\partial \rho}{\partial t} = -\{\rho, H\} = -X_H(\rho) = -\frac{p}{m} \frac{\partial \rho}{\partial q} + kq \frac{\partial \rho}{\partial p}. \quad (4-3)$$

This is a simple transport equation without diffusion (that is, ρ is a *passive scalar*); hence, the initial probability distribution will simply 'drift' along the streamlines of the Hamiltonian flow. As such, this problem is analogous to a flow that is purely characterized by convection.

4-1-1 Solution of the Liouville equation

The convection equation may be readily solved using the method of characteristics.

The method of characteristics

Equation (4-3) is part of a larger class of linear first-order PDE's of the form^a [9, p. 207].

$$\sum_{i=1}^n a_i(x_1, \dots, x_n, \rho) \frac{\partial \rho}{\partial x_i} = c(x_1, \dots, x_n, \rho), \quad (4-4)$$

which are traditionally solved using the *method of characteristics*. This method attempts to find characteristic lines along which the solution is constant, as to convert the PDE problem into an ODE problem. More specifically, one wishes to find a parameterization of x_i and ρ such that:

$$\begin{aligned} \frac{dx_i}{ds} &= a_i \\ \frac{d\rho}{ds} &= c. \end{aligned} \quad (4-5)$$

Given this parameterization, the PDE can be easily rewritten as follows: [9]

$$\frac{d\rho}{ds} = \sum_{i=1}^n \frac{\partial \rho}{\partial x_i} \frac{dx_i}{ds}.$$

The solution of the ODE problem then produces the trajectories for the characteristics. The reparameterization in terms of s must be accompanied by another reparameterization of the initial conditions in terms of the variable(s) r_i ; essentially, s provides the parameterization along the characteristic curves while r_i is the parameterization of the initial curves. The expressions for r_i are found by asserting that $x_i(0) = r_i$, and then solving for the integration constants that are still present in the found ODE solutions. Then, finally, one solves the ODE in terms of the characteristic parameterization

(s, r_1, \dots, r_n)

$$\frac{d\rho}{ds} + c(x_1(s, r), \dots, x_n(s, r))\rho = 0,$$

after which that solution can be written in terms of the old coordinates to obtain the solution of the PDE.

^aIf the functions a and c depend on ρ , the equation is called *semilinear*. This is, however, never the case for a PDE arising from the Liouville equation.

The former approach presents a ‘classical’ engineering perspective of the method of characteristics. However, the underlying mechanism may also be explained using the language of exterior calculus and contact geometry, which already plays a prominent role in this text. As outlined by Burke [10], the solution of a first-order PDE may be represented as an integral manifold of the *differential ideal* of two particular differential forms^a. The PDE given by eq. (4-4) is ‘encoded’ in two particular 1-forms that will constitute the differential ideal. The purpose is to find a general expression for the associated vector field that generates the integral manifold. The first 1-form, θ , contains the ‘total differential’ of ρ :

$$\theta = d\rho - \sum_{i=1}^n \underbrace{\frac{\partial \rho}{\partial x_i}}_{\xi_i} dx_i.$$

Secondly, the PDE itself (that is, the functions a_i, c) must be captured by another form, in this case the 0-form

$$\phi = \sum_{i=1}^n a_i \xi_i - c,$$

from which a 1-form can be constructed using the exterior derivative:

$$d\phi = \sum_{i=1}^n \left(a_i d\xi_i + \frac{\partial \phi}{\partial x_i} dx_i \right) + \frac{\partial \phi}{\partial \rho} d\rho.$$

The purpose is then to find characteristic vectors v, w , whose integral curves are the characteristics of the solution. The vectors v, w must satisfy the conditions: [10, p. 215]

$$v \lrcorner d\phi = 0 \quad w \lrcorner d\phi = 0 \quad (4-6)$$

to ensure that it satisfies the PDE equation (this means that v is tangent to the hypersurface given by ϕ);

$$v \lrcorner \theta = 0 \quad w \lrcorner \theta = 0, \quad (4-7)$$

to enforce that ξ are truly partial derivatives (they have no component pointing in the direction of the characteristics); and finally

$$w \lrcorner v \lrcorner d\theta = 0 \quad (4-8)$$

to form a integral ideal. The integral manifold of the characteristic vectors then constitutes the solution of the PDE.

^aFor an algebra A , an ideal is R is a subset of a A such that for all $a \in A$ and $x \in I$, it is true that $x \bullet a \in I$; i.e. it is closed under the multiplication operator \bullet of the algebra A [11]. In this case, the

vector space is the space of 1-forms on the contact space $(\mathbf{x}, \frac{\partial \rho}{\partial \mathbf{x}}, \rho)$. The \bullet operation of the algebra of forms is the exterior multiplication (or wedge product); the term *differential ideal* refers to the fact that the ideal is closed under the *derivation* on the algebra as well. Here, the derivation on the algebra of forms is the exterior derivative.

As it turns out, the method of characteristics takes a particularly simple form for the harmonic oscillator (and Hamiltonian systems in general). The reparameterization in terms of s is

$$\frac{dp}{ds} = -kq \quad \frac{dq}{ds} = \frac{p}{m} \quad \frac{dt}{ds} = 1. \quad (4-9)$$

which immediately yields $t = s + c_1$ (choose $c_1 = 0$ without loss of generalization), and the former two equations simply resort to a time-reversed solution of the Hamiltonian problem in terms of p and q . Solving the ODE to obtain the characteristic lines is therefore, rather unsurprisingly, equivalent to finding the phase trajectories of the Hamiltonian system. For the harmonic oscillator, these trajectories are

$$\begin{aligned} q(t) &= c_2 \cos(\omega t) + \frac{c_3}{m\omega} \sin(\omega t) \\ p(t) &= c_3 \cos(\omega t) - m\omega c_1 \sin(\omega t). \end{aligned} \quad (4-10)$$

Solving for $q(0) = r_1$ and $p(0) = r_2$, yields $r_1 = c_2$ and $r_2 = c_3$. Now, because the ‘forcing term’ $c(\cdot)$ is not present in the Liouville equation (for autonomous systems), the solution of the second ODE is trivial:

$$\rho(t) = \rho_0(r_1, \dots, r_2),$$

(... Jacobian? ...)

where ρ_0 is the initial distribution. It is an encouraging observation that the method of characteristics is easily extended towards non-autonomous systems, leaving the possibility for control action or external disturbances, which may well be of a stochastic nature themselves.

The solution to the Liouville equation is found by writing the initial distribution in terms of p , q and t . Since q and p depend linearly on r_1 and r_2 , this is a matter of taking the inverse of the associated matrix.

$$\begin{pmatrix} q \\ p \end{pmatrix} = \underbrace{\begin{pmatrix} \cos(\omega t) & \frac{1}{m\omega} \sin(\omega t) \\ -m\omega \sin(\omega t) & \cos(\omega t) \end{pmatrix}}_{\Phi(t)} \begin{pmatrix} r_1 \\ r_2 \end{pmatrix}.$$

This transformation matrix represents a symplectic transformation of the phase plane; symplectic matrices have a unit determinant¹. More specifically, the above matrix is a ‘squeezed’ rotation matrix. Inversion and resubstitution of t then yields:

$$\begin{pmatrix} r_1 \\ r_2 \end{pmatrix} = \begin{pmatrix} \cos(\omega t) & \frac{-1}{m\omega} \sin(\omega t) \\ m\omega \sin(\omega t) & \cos(\omega t) \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix},$$

this is the time-reversed flow of the Hamiltonian vector field; a counterclockwise rotation in the phase plane.

¹Due to the equivalence of $\text{Sp}(2, \mathbb{R})$ and $\text{SL}(2, \mathbb{R})$, having a unit determinant is a necessary and sufficient condition for a 2×2 matrix to be symplectic; this condition is only necessary for higher dimensional vector spaces [12].

Motivation using exterior calculus In this section, the reasoning given by Burke [10] using exterior calculus is applied to the problem to motivate the validity of the solution given above. The solution is the integral manifold of tangent vectors to the contact space $(t, q, p, \xi_t, \xi_q, \xi_p, \rho)$, where $\xi_t = \frac{\partial \rho}{\partial t}$ etc. As such, the tangent vectors \mathbf{v} and \mathbf{w} can be associated with seven-tuples:²

$$\mathbf{v} = (v_t \quad v_q \quad v_p \quad v_{\xi_t} \quad v_{\xi_q} \quad v_{\xi_p} \quad v_\rho)$$

$$\mathbf{w} = (w_t \quad w_q \quad w_p \quad w_{\xi_t} \quad w_{\xi_q} \quad w_{\xi_p} \quad w_\rho).$$

Likewise, the one-forms θ and $d\phi$ can be written as seven-tuples, too:³

$$\theta = (-\xi_t \quad -\xi_q \quad -\xi_p \quad 0 \quad 0 \quad 0 \quad 1)$$

$$d\phi = \left(\frac{\partial \phi}{\partial t} \quad \frac{\partial \phi}{\partial q} \quad \frac{\partial \phi}{\partial p} \quad 1 \quad \frac{p}{m} \quad -kq \quad \frac{\partial \phi}{\partial \rho} \right).$$

Applying the conditions eq. (4-6) and eq. (4-7) to \mathbf{v} is simply equivalent to the application of a ‘dot product’ (i.e. a duality pairing);

$$\theta(\mathbf{v}) = 0 \iff v_\rho = v_t \xi_t + v_q \xi_q + v_p \xi_p.$$

$$d\phi(\mathbf{v}) = 0 \iff \frac{\partial \phi}{\partial t} v_t + \frac{\partial \phi}{\partial q} v_q + \frac{\partial \phi}{\partial p} v_p + v_{\xi_t} + \frac{p}{m} v_{\xi_q} - kq v_{\xi_p} + \frac{\partial \phi}{\partial \rho} v_\rho = 0.$$

Finally, all the conditions on \mathbf{w} can be combined into the following statement: since $\mathbf{w} \lrcorner \theta = 0$ and $\mathbf{w} \lrcorner d\phi = 0$, condition eq. (4-8) is equivalent to stating that the 1-form $\mathbf{v} \lrcorner d\theta$ is a linear combination of θ and $d\phi$ [10]. Using the Lagrange multipliers λ and μ , the condition reverts to

$$\mathbf{v} \lrcorner d\theta = \lambda \theta + \mu d\phi.$$

Using the properties of the interior product and the exterior derivative, one obtains

$$v_t d\xi_t - v_{\xi_t} dt + v_q d\xi_q - v_{\xi_q} dq + v_p d\xi_p - v_{\xi_p} dp = \lambda \theta + \mu d\phi.$$

A particular choice of the Lagrange multipliers can be made to cancel two of the seven components, in this case those in $d\xi_t$ and $d\rho$, respectively the fourth and last entry in the ordered tuple representation, $\lambda = -v_t \frac{\partial \phi}{\partial \rho}$ and $\mu = v_t$. This results in five additional equations:

$$v_{\xi_t} = -v_t \left(\xi_t \frac{\partial \phi}{\partial \rho} + \frac{\partial \phi}{\partial t} \right)$$

$$v_{\xi_q} = -v_t \left(\xi_q \frac{\partial \phi}{\partial \rho} + \frac{\partial \phi}{\partial q} \right)$$

$$v_{\xi_p} = -v_t \left(\xi_p \frac{\partial \phi}{\partial \rho} + \frac{\partial \phi}{\partial p} \right)$$

$$v_q = \frac{p}{m} v_t$$

$$v_p = -kq v_t$$

²With respect to the basis $\left(\frac{\partial}{\partial t} \quad \frac{\partial}{\partial q} \quad \frac{\partial}{\partial p} \quad \frac{\partial}{\partial \xi_t} \quad \frac{\partial}{\partial \xi_q} \quad \frac{\partial}{\partial \xi_p} \quad \frac{\partial}{\partial \rho} \right)$.

³With respect to the basis $(dt \quad dq \quad dp \quad d\xi_t \quad d\xi_q \quad d\xi_p \quad d\rho)$.

These equations, combined with the former two conditions can be used to determine \mathbf{v} up to a factor (choose $v_t = 1$):

$$\mathbf{v} = \begin{pmatrix} 1 & \frac{p}{m} & -kq & -\xi_t \frac{\partial \phi}{\partial \rho} - \frac{\partial \phi}{\partial t} & -\xi_q \frac{\partial \phi}{\partial \rho} - \frac{\partial \phi}{\partial q} & -\xi_p \frac{\partial \phi}{\partial \rho} - \frac{\partial \phi}{\partial p} & 0 \end{pmatrix}.$$

Now, observe that, because of the (semi-)linearity of the original equation, the vector \mathbf{v} can be projected to the (t, q, p) -space (the other components have no influence on the solution). As such, one must find the integral curves of the projected vector field

$$\frac{\partial}{\partial t} + \frac{p}{m} \frac{\partial}{\partial q} - kq \frac{\partial}{\partial p},$$

which is precisely the Hamiltonian vector field in the extended (contact) phase space, or to quote Arnol'd [12, p. 237], *the velocity vector of the phase flow in extended phase space*; the integral lines are the *vortex lines* of the integral invariant of Poincaré-Cartan $p dq - H dt$. Hence, to find a solution of the PDE problem, one strives to integrate the above vector field, where the initial conditions serve as parameters. The initial conditions can then be solved at the point $t = 0$ for the initial solution. This is precisely the methodology that is applied *ad hoc* in the previous section.

4-1-2 Initial Gaussian distribution

The solution of the Liouville equation to any initial distribution is simply found by substituting the (q, p) dependence with transformation stated above. This solution is simply obtained by effecting the substitution

$$\begin{pmatrix} q \\ p \end{pmatrix} \mapsto \Phi^{-1}(t) \begin{pmatrix} q \\ p \end{pmatrix}$$

in the original distribution ρ_0 . Alternatively, one can see this as an affine transformation of the original random variable in the other direction, that is,

$$\begin{pmatrix} q_0 \\ p_0 \end{pmatrix} \mapsto \Phi(t) \begin{pmatrix} q_0 \\ p_0 \end{pmatrix} = \begin{pmatrix} q \\ p \end{pmatrix}$$

For example, an initial bivariate Gaussian distribution centered at some initial point (q_0, p_0) with covariance matrix Σ subject to the linear transformation $\Phi = \Phi(t)$ yields again a Gaussian: [13]

$$\begin{pmatrix} q(t) \\ p(t) \end{pmatrix} \sim \mathcal{N}\left(\Phi \begin{pmatrix} q_0 \\ p_0 \end{pmatrix}, \Phi \Sigma \Phi^\top\right). \quad (4-11)$$

This result is, after all, not quite a surprise: the Gaussian distribution is transported by the convective stream of the phase space fluid; the mean drifts along its original phase space trajectory as if it were a single particle. The variance changes continuously by the transform given by Φ . Interestingly, because Φ has a unit determinant, $\det(\Phi \Sigma \Phi^\top) = \det(\Sigma)$; as such, the *entropy* of the Gaussian remains constant throughout, and equal to its initial value

$$\frac{1}{2} \log(\det(2\pi e \Sigma)).$$

Marginal distributions Equation (4-11) represents a specific bivariate Gaussian distribution at any point in time. Therefore, the marginal time-dependent distributions of p and q as a function of time may readily be obtained from the joint distribution: [13]

$$\begin{aligned} q(t) &\sim \mathcal{N}\left(\cos(\omega t)q_0 + \frac{1}{m\omega} \sin(\omega t)p_0, \sigma_q \cos^2(\omega t) + \frac{\sigma_{pq}}{m\omega} \sin(2\omega t) + \frac{\sigma_p}{m^2\omega^2} \sin^2(\omega t)\right), \\ p(t) &\sim \mathcal{N}(\cos(\omega t)p_0 - m\omega \sin(\omega t)q_0, \sigma_p \cos^2(\omega t) - \sigma_{pq}m\omega \sin(2\omega t) + \sigma_q m^2\omega^2 \sin^2(\omega t)) \end{aligned} \quad (4-12)$$

given that $\Sigma = \begin{pmatrix} \sigma_q & \sigma_{qp} \\ \sigma_{qp} & \sigma_p \end{pmatrix}$. Figure 4-1 shows the time-varying distribution of q and p in the form of the mean with a 2σ -confidence interval. Clearly, the uncertainty for p is largest

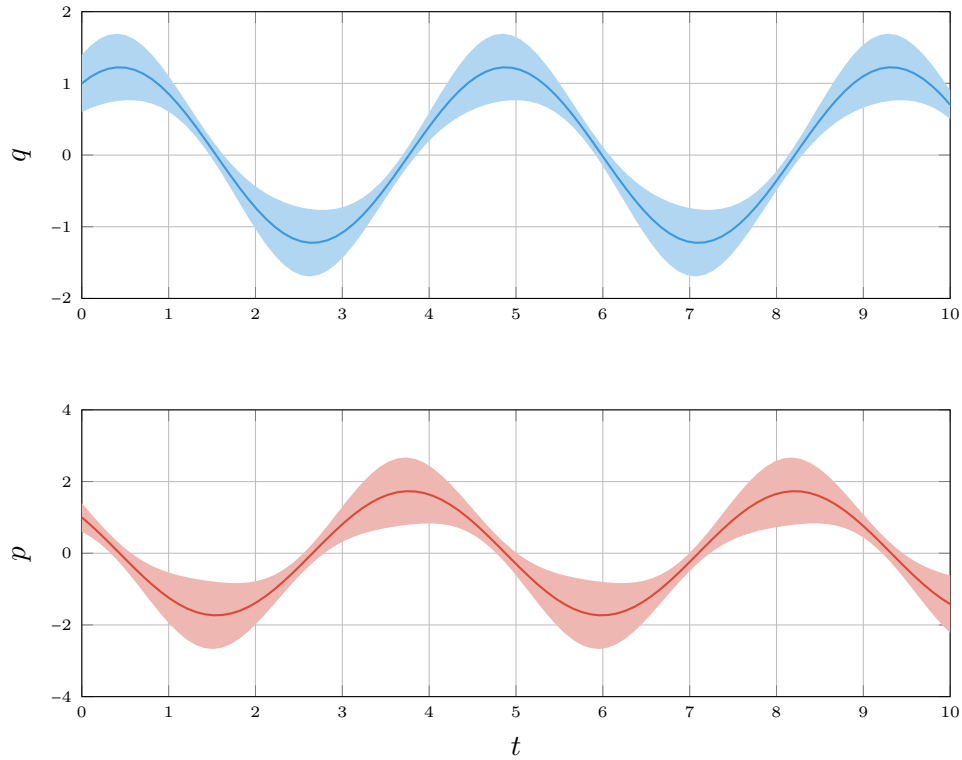


Figure 4-1: The marginal distributions given by eq. (4-12). The solid line represents the evolution of the mean, while the shaded area is a 95% confidence interval, i.e. two standard deviations from the mean, given that the distribution is normal.

when it's change is minimal; at the troughs and peaks of the sine wave; the same is true for q . Because both are a quarter cycle out of phase, their uncertainties 'exchange'. This is a compelling substantiation of Heisenberg's uncertainty principle, which states that canonical variables such as p and q cannot be measured simultaneously to arbitrary precision. [discuss with Max]

Fourier duality and the Heisenberg uncertainty principle

Bla bla bla

Averages in time The motion of the harmonic oscillator is periodic. As such, the ‘average distribution over time’ may be given a compact support over a single period. The distribution given by eq. (4-11) may be considered to be a distribution *conditioned* on time. To find the averaged distribution, the joint distribution $\Pr(p, q, t) = \Pr(p, q | t) \Pr(t)$ may be marginalized with respect to t :

$$\rho(p, q) = \int \rho(p, q | t) \rho(t) dt.$$

Assuming that time is uniformly distributed over the period of the oscillations, the former expression is equivalent to:

$$\begin{aligned} \rho(\mathbf{x}) &= \int_0^\infty \rho_{\text{normal}}(\mathbf{x}; \Phi(t)\mathbf{x}_0, \Phi(t)\Sigma\Phi(t)^\top) \rho_{\text{uni}}(t; 0, T) dt \\ &= \int_0^\infty \frac{1}{T\sqrt{4\pi^2 \det(\Sigma)}} e^{-\frac{1}{2}(\mathbf{x}-\Phi(t)\mathbf{x}_0)^\top (\Phi\Sigma\Phi^\top)^{-1}(\mathbf{x}-\Phi(t)\mathbf{x}_0)} (u_0(t) - u_T(t)) dt, \\ &= \int_0^T \frac{1}{T\sqrt{4\pi^2 \det(\Sigma)}} e^{-\frac{1}{2}(\mathbf{x}-\Phi(t)\mathbf{x}_0)^\top (\Phi(t)\Sigma\Phi(t)^\top)^{-1}(\mathbf{x}-\Phi(t)\mathbf{x}_0)} dt, \end{aligned} \quad (4-13)$$

where u_c refers to the Heaviside step delayed by c , and $\mathbf{x} = (p \ q)$. Furthermore, probability density functions are unconventionally denoted by $\rho(\cdot; \cdot)$ to maintain the analogy with fluid dynamics, where the arguments and parameters are separated by a semicolon. In this case $\rho_{\text{normal}}(\mathbf{x}; \boldsymbol{\mu}, \Sigma)$ refers to a multivariate normal distribution with mean vector $\boldsymbol{\mu}$ and covariance matrix Σ , and $\rho_{\text{uni}}(t; a, b)$ refers to a scalar uniform distribution with bounds a and b . Figure 4-2 visualizes a numerical solution for this integral for some particular parameter values. Equation (4-13) may be solved analytically for a simple case (normalized units and diagonal covariance), where the final solution is expressed in terms of the modified Bessel functions.⁴

Energy distribution The energy distribution is a generalized chi-squared distribution, because it is a general quadratic form of a normally distributed vector with nonzero mean [15].

4-1-3 Verification using a Monte-Carlo method

⁴In this case Φ becomes an orthogonal matrix, which considerably simplifies the evaluation of the integral; the time-dependent argument of the exponential then reverts to a simple rotation, which can then be solved using the integral identity:

$$\int_0^{2\pi} e^{A \cos(\varphi) + B \sin(\varphi)} d\varphi = 2\pi I_0(\sqrt{A^2 + B^2}),$$

I_0 being the modified Bessel function of the first kind [14].

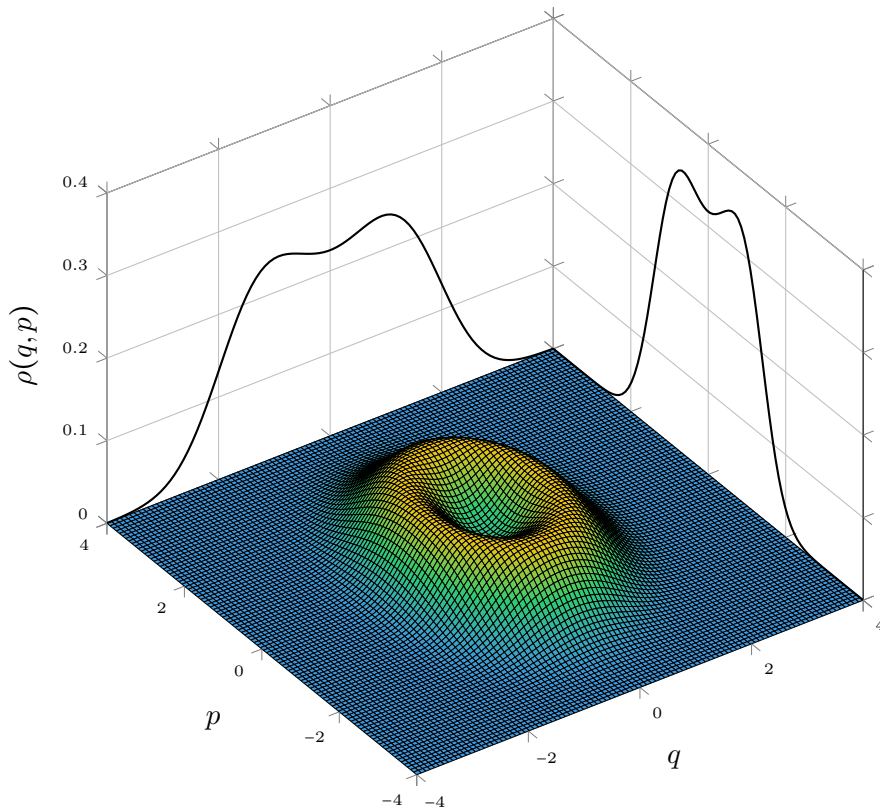


Figure 4-2: Numerical solution of the time-averaged distribution given by eq. (4-13), for $m = 1$, $k = 2$, $\Sigma = \begin{pmatrix} 0.2 & 0.1 \\ 0.1 & 0.2 \end{pmatrix}$ and $x_0 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$. The marginalized distributions for p and q are shown as well.

4-2 Damped harmonic oscillator

In their most traditional fashion, the Hamiltonian and Lagrangian treatments of mechanical systems do not incorporate energy dissipation; that is, they assume the conservation of (mechanical) energy in the system. The classical theory does allow for an optional explicit time-dependence of the Hamiltonian and Lagrangian, but although this may allow one to incorporate dissipation, it is no direct solution for the dissipation problem. Although this may seem odd from the perspective of the engineering field, where dissipation really is the rule rather than the exception, dissipation is arguably not of primary concern for physicists. This is because dissipation is considered to be a *macro-phenomenon*; that is, it arises because one chooses not to model certain degrees of freedom in the system, while physicists are often concerned with ideal system descriptions on the macro-scale. Nonetheless, the celebrated report by Dekker [4] provides an overview of the (often fruitful) attempts that have been made to include dissipation in the Hamiltonian and Lagrangian description; the former may allow one to consider dissipation on the quantum level as well — this is beyond the scope of this text. In addition to these methods, recent developments in the economic engineering group have proposed two new methods to deal with linear damping in mechanical systems, see Hutters [16] and Mendel [17]. In the following section, these methods are placed in a slightly more rigorous (read: geometric) context, after which they serve as the apparatus for the Liouville equation on the damped harmonic oscillator.

4-2-1 A quick tour of dissipative classical mechanics

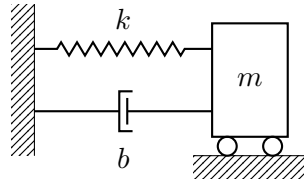


Figure 4-3: Schematic of the damped harmonic oscillator.

The damped harmonic oscillator considered in this text is the one that features a damper ‘in parallel’ with the spring, as shown in fig. 4-3. The corresponding second-order differential equations are:⁵

$$\frac{d}{dt} \begin{pmatrix} q \\ \dot{q} \end{pmatrix} = \begin{pmatrix} 0 & 1/m \\ -k/m & -b/m \end{pmatrix} \begin{pmatrix} q \\ \dot{q} \end{pmatrix} \quad \text{or} \quad m\ddot{q} + b\dot{q} + kq = 0. \quad (4-14)$$

The state-transition matrix has eigenvalues

$$\lambda = \frac{1}{2} \left(-\frac{b}{m} \pm \sqrt{\left(\frac{b}{m}\right)^2 - 4\frac{k}{m}} \right)$$

which is often expressed in ‘polar coordinates’, using the *damping ratio* ζ and the *undamped natural frequency* Ω :

$$\lambda = -\Omega \left(\zeta \pm i\sqrt{1 - \zeta^2} \right)$$

⁵Although a linear potential force is assumed here, this treatment generalizes to any potential function $U = U(q, t)$ that does not involve the generalized velocity in a straightforward manner.

Moreover, the system is assumed to be underdamped, or equivalentl $\zeta < 1$. Solutions are then of the form

4-2-2 Discounted state functions

The method proposed by Mendel [17] is closely related to the time-dependent Caldirola-Kanai Hamiltonian (as mentioned, the corresponding Lagrangian was already devised by Bateman in 1931 [3, 4]). However, there are some important differences: the time-dependent method takes the dissipation into account simply wrapping the Lagrangian with an exponential discount function so as to include the real part of the eigenvalues into the solution. In contrast, the Mendel method makes use of the ‘homogenization trick’ in combination with a rheonomic constraint, which allow to describe the system in an extended configuration space that includes the time t . The Lagrangian method is discussed first, after which the Dirac method is used to make the passage from the Lagrangian to the Hamiltonian description.

(... discuss contribution ...)

Lagrangian function

The starting point of Mendel’s method is a Lagrangian over the extended configuration space X^6 , which includes both the regular position coordinate q as well as the time t . The tangent bundle TX then has two additional coordinates for the respective generalized velocities, a position velocity v_q and a ‘time velocity’ v_t ; they are the components of the tangent vector to a generalized position $\mathbf{x} = (q, t)$ in the chart-induced basis. The role of the path indexation variable that is normally reserved for time is now played by τ , appropriately named ‘proper time’ by Mendel [17]. The Lagrangian is then a function over the contact bundle $TX \times \mathbb{R}$.

In general, the Lagrangian function $\mathcal{L} : TX \times \mathbb{R} \rightarrow \mathbb{R}$ is given as the homogenization of the traditional Lagrangian L , which is the difference between the kinetic and potential energy in the system. This is a common approach in classical mechanics literature as a trick to ‘fake’ a time-dependence in the Lagrangian, e.g. to show the conservation of energy as a consequence of the Noether theorem (see Arnol’d [12, p. 90]). In the remainder of this section, the general derivation will be given on par with the specific case for the damped harmonic oscillator. The ‘proper’ Lagrangian is then defined as:

GENERAL

$$\mathcal{L}\left(q, t, \underbrace{\frac{dq}{d\tau}}_{v_q}, \underbrace{\frac{dt}{d\tau}}_{v_t}\right) = L\left(q, \underbrace{\frac{dq/d\tau}{dt/d\tau}}_{\dot{q}}, \underbrace{\frac{dt}{d\tau}}_{v_t}\right)$$

PARAMETERIZED

$$\mathcal{L} = v_t \left(\frac{1}{2} m \left(\frac{v_q}{v_t} \right)^2 - \frac{1}{2} k q^2 \right).$$

⁶In this section, X refers to the extended configuration space, with the corresponding coordinate vector referred to as $\mathbf{x} = (q, t)$. Proper time derivatives are either denoted explicitly or by a prime. In case of the generalized velocities, the notation v_q, v_t is used instead, to highlight the fact that they are indeed independent coordinates of the tangent bundle.

Please note that the old generalized velocity \dot{q} is not an independent variable anymore but rather expressed as v_q/v_t as a consequence of the chain rule.

Now, the homogenization trick does not cause any special properties of the Lagrangian in and of its own. The second ingredient of the method is the following holonomic constraint

$$\frac{d^2\tau/dt^2}{d\tau/dt} = -\gamma \quad \text{such that} \quad \tau = C_2 - \frac{C_1}{\gamma} e^{-\gamma t}, \quad (4-15)$$

where C_1 and C_2 are arbitrary integration constants — the proper time is therefore only defined up to affine transformations. In the case of the damped harmonic oscillator, $\gamma = b/m$ denotes the decay rate of the system. This constraint can be rewritten in the form $\phi(t, \tau) = 0$, and is *rheonomic*, for it is (proper) time-dependent. It could be used to reduce the number of degrees of freedom directly, but the Lagrangian would then immediately reduce to time-dependent Caldirola-Kanai form. This would defeat the purpose of the Lagrangian formulation in the extended configuration space. Rather, one wishes not to ‘spend’ the constraint, but keep it in implicit form using Lagrange multipliers to explicitly determine the constraint forces that keep the system on the submanifold that would otherwise be assumed a priori. The reason to do so is twofold: (i) the constraint forces have a compelling physical interpretation and (ii) it can be used in more general damping cases where the constraint eq. (4-15) cannot be integrated explicitly.

Given the Lagrangian function, the equations of motion can be obtained using the Euler-Lagrange equations:

$$\frac{d}{d\tau} \left(\frac{\partial \mathcal{L}}{\partial v^\mu} \right) - \frac{\partial \mathcal{L}}{\partial x^\mu} = \lambda \frac{\partial \phi}{\partial x^\mu} \quad \mu = 1, 2. \quad (4-16)$$

It is worthwhile to dwell briefly on the conjugate momenta $\partial \mathcal{L} / \partial v^\mu$ and their proper time derivatives. Evaluating the partial derivatives yields:

GENERAL

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial v_q} &= v_t \frac{\partial L}{\partial \dot{q}} \frac{\partial \dot{q}}{\partial v_q} = \frac{\partial L}{\partial \dot{q}} \equiv p \\ \frac{\partial \mathcal{L}}{\partial v_t} &= L - v_t \frac{\partial L}{\partial \dot{q}} \frac{\partial \dot{q}}{\partial v_t} = L - p\dot{q} \equiv D \end{aligned}$$

PARAMETERIZED

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial v_q} &= m \left(\frac{v_q}{v_t} \right) = m\dot{q} \\ \frac{\partial \mathcal{L}}{\partial v_t} &= - \left(\frac{1}{2} m \dot{q}^2 + \frac{1}{2} k q^2 \right) \end{aligned}$$

Hence, the following observations are made:

- (i) The momentum the position velocity coincides with the ‘traditional’ notion of momentum.
- (ii) The momentum conjugate to time is the negative of the mechanical energy in the system. Given an appropriate initial constant for the initial energy, this represents exactly the energy dissipated by the damper.

Furthermore, the corresponding derivatives with respect to proper time are

GENERAL

$$\begin{aligned} \frac{d}{d\tau} \left(\frac{\partial \mathcal{L}}{\partial v_q} \right) &= \\ \frac{d}{d\tau} \left(\frac{\partial \mathcal{L}}{\partial v_t} \right) &= \end{aligned}$$

PARAMETERIZED

$$\begin{aligned} \frac{d}{d\tau} \left(\frac{\partial \mathcal{L}}{\partial v_q} \right) &= \frac{m}{v_t^2} \left(\frac{dv_q}{d\tau} v_t - v_q \frac{dv_t}{d\tau} \right) \\ \frac{d}{d\tau} \left(\frac{\partial \mathcal{L}}{\partial v_t} \right) &= \end{aligned}$$

Legendre transform

The usual story in classical mechanics professes that the Lagrangian representation is equivalent to the Hamiltonian representation, which are connected through the so-called Legendre transform. From a geometric perspective, the Legendre transform switches the Lagrangian function on the tangent bundle in favour of the Hamiltonian function on the cotangent bundle, or vice versa. Along with the transformed function, the associated *variational problem* in the Lagrangian setting converts to the integration of the Hamiltonian vector field generated by the Hamiltonian function. In physics, the deeper significance of the Legendre transform is often discarded in favour of the expression $\dot{q}^i p_i - L$, which only holds when the Lagrangian is strictly convex, or hyperregular, and assuming on-the-fly that $p_i \equiv \partial L / \partial \dot{q}^i$. In this text a more geometric approach is taken in accordance with Abraham and Marsden [1], where the concept of the ‘fiber derivative’ is favoured over the Legendre transform. For well-behaved Lagrangians the traditional notion of the fiber derivative and the Legendre transform coincide; but if not, there are some subtle complications that are relevant for this discussion.

As mentioned, the Legendre transform (or fiber derivative) ‘preserves information’ — that is, it is involutive and unique — if the the function at issue is strictly convex. The Hessian of \mathcal{L} with respect to the generalized velocities is

$$\begin{pmatrix} \frac{\partial^2 L}{\partial \dot{q} \partial v_q} & \frac{\partial^2 L}{\partial \dot{q} \partial v_t} \\ \frac{\partial^2 L}{\partial \dot{q} \partial v_t} & \frac{\partial}{\partial v_t} \left(L - \frac{\partial L}{\partial \dot{q}} \dot{q} \right) \end{pmatrix} = \begin{pmatrix} \frac{\partial^2 L}{\partial \dot{q} \partial v_q} & \frac{\partial^2 L}{\partial \dot{q} \partial v_t} \\ \frac{\partial^2 L}{\partial \dot{q} \partial v_t} & -\frac{\partial^2 L}{\partial \dot{q} \partial v_t} \dot{q} \end{pmatrix} = \begin{pmatrix} \frac{\partial p}{\partial v_q} & \frac{\partial p}{\partial v_t} \\ \frac{\partial p}{\partial v_t} & -\frac{\partial p}{\partial v_t} \dot{q} \end{pmatrix}$$

such that the determinant of this Hessian is

$$\frac{\partial p}{\partial v_q} \dot{q} \frac{\partial p}{\partial v_t} - \left(\frac{\partial p}{\partial v_t} \right)^2 \stackrel{7}{=} \left(\frac{\partial p}{\partial v_t} \right)^2 - \left(\frac{\partial p}{\partial v_t} \right)^2 = 0,$$

i.e. the Hessian is singular and has one vanishing eigenvalue; because the other eigenvalue is positive (the trace of the Hessian can be shown to be positive if v_t is), the Hessian is positive semidefinite. This prevents one to easily effect the Legendre transform of \mathcal{L} , for this Hessian is the Jacobian of the fiber derivative $\mathbb{F}\mathcal{L}$, which means that the fiber derivative does not provide a bijective mapping between the tangent and cotangent bundles (cf. the implicit function theorem). For the damped harmonic oscillator, the fiber derivative results in

$$\begin{aligned} p &\equiv \frac{\partial \mathcal{L}}{\partial v_q} = m \frac{v_q}{v_t} \\ W &\equiv \frac{\partial \mathcal{L}}{\partial v_t} = -\frac{1}{2} \left(m \left(\frac{v_q}{v_t} \right)^2 + k q^2 \right). \end{aligned} \tag{4-17}$$

Equation (4-17) shows that there is no unique way to assign the velocity pair (v_q, v_t) to a conjugate momentum pair (p, W) through the fiber derivative. Indeed, as discussed by Cannas da Silva [2, p. 122], *strict convexity* of a function \mathcal{L} , that is, the Hessian of \mathcal{L} be positive definite, is required for the Legendre transform to be a diffeomorphism between TQ and T^*Q . The root of this issue can be found in the fact that p, W only depend on \dot{q} , which fixes only the relative proportion between v_q and v_t — roughly speaking, it acts on the *projectivization* of the cotangent space, as shown in section 4-2-2.

⁷Because $\frac{\partial p}{\partial v_q} \dot{q} = \frac{\partial p}{\partial v_t} \frac{\partial v_t}{\partial \dot{q}} \frac{\partial \dot{q}}{\partial v_q} \dot{q} = \frac{\partial q}{\partial v_t} \frac{-v_q}{\dot{q}^2} \frac{1}{v_t} \dot{q} = -\frac{\partial p}{\partial v_t}$.

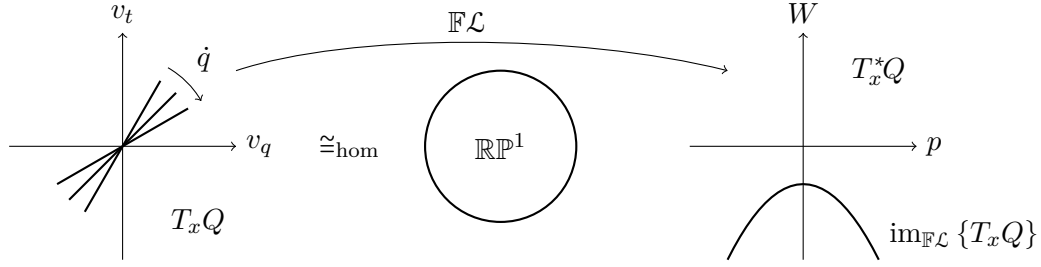


Figure 4-4: Graphical illustration of the singularity of the Lagrangian. The fiber derivative provides a pointwise mapping between the cotangent space $T_x Q$, where $x = (q, t)$, and the cotangent bundle $T_x^* Q$, but this mapping is neither injective nor surjective. The mapping \mathbb{FL} acts injectively on the projectivization of the tangent space — in this case, \mathbb{R}^2 / \sim , where \sim denotes the equivalence relation $(v_q, v_t) \sim (\lambda v_q, \lambda v_t)$ — it takes the equivalence classes $[v_q : v_t]$ as an argument. Furthermore, the image of the entire tangent space is restricted to a parabolic subset of the cotangent space.

All of this boils down to the fact that the fiber derivative/Legendre transform is unable to express the transformed Lagrangian function completely in terms of the coordinates of the cotangent bundle. In this case, the Lagrangian function is called *degenerate* or *singular*; Lagrangians for which the fiber derivative produces a global diffeomorphism are called *hyperregular* [1, p. 236].

An additional observation is that the Lagrangian \mathcal{L} is *homogeneous of the first degree* in the generalized velocities v_q and v_t ; i.e. multiplication of all velocities by a factor λ is equal to multiplying the Lagrangian itself by that factor (to the ‘first power’, hence the first degree). This is, as discussed by Abraham and Marsden [1] and Dirac [18], a classical example of a singular Lagrangian. This makes the homogeneous Lagrangian function subject to the Euler theorem (on homogeneous functions); which means that the Lagrangian is a linear combination of its partial derivatives with respect to the generalized velocities [18]. Given that the Lagrangian is homogeneous, the Euler theorem asserts that

$$\mathcal{L} = v_q \frac{\partial \mathcal{L}}{\partial v_q} + v_t \frac{\partial \mathcal{L}}{\partial v_t} = v_q p + v_t W.$$

Substitution by the found expressions for p and W indeed recovers the original definition of the discounted Lagrangian. The point is though, that the above is *precisely* equal to the duality pairing that is used for the Legendre transform; as such, a ‘naive’ Legendre transform $v_q p + W v_t - \mathcal{L}$ will simply vanish in the strong fashion. Hence, according to the Dirac method,

$$H = v \phi$$

where ϕ is the first-order constraint

$$W + \frac{1}{2m} p^2 + \frac{1}{2} k q^2 = 0$$

Singular Lagrangians and the Dirac method

As mentioned, singular Lagrangians are Lagrangians for which the mass matrix

$$\left[\frac{\partial^2 \mathcal{L}}{\partial \dot{q}_i \partial \dot{q}_j} \right]$$

is rank-deficient. With slight abuse of notation, L denotes a general Lagrangian and \dot{q} the corresponding generalized velocities. This prevents one from finding the corresponding Hamiltonian representation in the traditional fashion using the Legendre transform, since this entire process hinges on the above Hessian to provide a bijective mapping between the tangent and cotangent spaces (pointwise), that is, to find a mapping between velocities and momenta. Paul Dirac developed a method to overcome this problem, as discussed by Dirac [18], Künzle [19], and Cisneros-Parra [20]. It is interesting to note that the last author considers degeneracy to be a property reserved for ‘artificial’ Lagrangians; by which he means those which do not correspond to real mechanical systems. This claim is, of course, refuted by the Mendel approach given in this text.

Because of the singularity of the Hessian, there must be a number of conditions on the conjugate momenta such that there remains an additional dependence between the conjugate momenta:

$$\phi_k(\mathbf{p}, \mathbf{q}, t) = 0.$$

Using Dirac’s method, the resulting Hamiltonian is of the form: [20]

$$H = H_0 + \sum_k v_k \phi_k,$$

where H_0 denotes the ‘naive’ Hamiltonian found by taking a straightforward Legendre transform, and v_k new independent variables (i.e, additional coordinates of the cotangent space as to span its entirety). Aside from the *primary restrictions* ϕ_k , the Dirac method also imposes a consistency condition of the form

$$\dot{\phi}_k = 0,$$

from which the *secondary restrictions* are obtained.

Make sure to read https://en.wikipedia.org/wiki/First_class_constraint#Geometric_theory for a geometric interpretation.

NOTE: Max uses ‘vanish identically’, is the same as strong/weak equality by Dirac

The Lagrangian 1-form is the pullback of the tautological 1-form under the fiber derivative. Lagrangian 1-form and 2-form, economic interpretation: market elasticities. Lagrange 2-form contains the market elasticities, quite literally the geometric encoding of the corresponding bond graph.

Time-dependent Hamiltonian

In this section, the method proposed by Mendel [17] is used to deal with the problem of dissipative systems in the framework of Hamiltonian mechanics. The prototypical example

that is the harmonic oscillator with a linear (parallel) damping element. As noted, using a time-dependent Hamiltonian to include dissipative mechanics is not quite a new idea (cf. Dekker [4]), but the salient point here is the *symplectization* of the contact structure that normally underlies such a system. That is to say, there is an additional dimension on top of p, q, t to allow the manifold to be symplectic in the first place. For the damped harmonic oscillator, this boils down to a 2-dimensional configuration manifold Q with coordinates (q, t) , with at each point attached a cotangent space which contains elements of the form $\alpha dq + \beta dt$. To turn the cotangent bundle into a symplectic manifold by virtue of the bundle structure, define the tautological 1-form

$$\alpha = p dq + W dt \quad \alpha \in T^*(T^*Q),$$

from which the symplectic 2-form is obtained:

$$\omega = -d\alpha = dq \wedge dp + dt \wedge dW.$$

This results in a four-dimensional symplectic manifold (M, ω) .

Multi-degree of freedom systems As noted by Udwadia and Cho [21], the general solution of the ‘inverse problem’ in Lagrangian mechanics becomes quickly intractable if the number of degrees of freedom in the grows (although the Helmholtz equations theoretically guarantee a solution). For linear systems, this can be easily understood from simple ideas in linear systems theory (which is not mentioned in the work of Udwadia and Cho [21]). The differential equation of the matrix solution for a general mechanical system has the form:

$$\begin{pmatrix} \dot{q} \\ \dot{p} \end{pmatrix} = \begin{pmatrix} 0 & I \\ -M^{-1}K & -M^{-1}B \end{pmatrix}$$

where M , K and B are the mass matrix, stiffness matrix and damping matrix respectively. Now, finding the ‘exponential envelope’ that is used in the Caldirola-Kanai style Lagrangians or Hamiltonians becomes a complicated matter in the general case: one needs to decouple the system into individual solutions, each with its discount factor. Naturally, this coincides precisely with an eigenvalue decomposition of the system, i.e.

$$\begin{pmatrix} q \\ p \end{pmatrix} = T \exp(J) T^{-1} \begin{pmatrix} q_0 \\ p_0 \end{pmatrix}.$$

If one assumes that all the system dynamics are underdamped and the matrix A is simple, then the J is diagonal with complex entries (each of which is paired with its complex conjugate). This is equivalent to a linear combinations of solutions $e^{\gamma t}(c_1 \cos(\Omega t) + c_2 \sin(\Omega t))$. Theoretically, one can find a Lagrangian for all the decoupled parts, each with their own discount ‘envelope’ to formulate the Lagrangian of the overall problem. Unfortunately, this is not possible in a closed-form fashion (only up to two degrees of freedom in general, for which it is the maximal polynomial order to which a closed form solution exist for the roots). One could however construct a ‘numerical Lagrangian’, by computing the eigenvalues given the parameters. Of course, this does not make the solution of the ODE’s easier, but it the Lagrangian itself can help to offer insights in the nature of the system.

4-2-3 Complex Hamiltonian

Coen's method

4-3 Nonlinear systems

SYMPLECTIC INTEGRATORS!!!

4-3-1 Double pendulum

use a wrapped normal distribution / von Mises distribution for the circular dimensions

4-3-2 Van der Pol oscillator

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Glossary

List of Acronyms

