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Mathematical Physics — *A Morse index invariant reduction of non-equilibrium thermodynamics*, by Franco Cardin and Leonardo Masci, communicated on March 10, 2017.

This paper is dedicated to the memory of Professor Giuseppe Grioli, master of mathematical physics.

Abstract. — We consider the finite dimensional reduction of the well known non-equilibrium thermodynamics theory developed through the last two decades by a team of researchers lead by Giovanni Jona-Lasinio, realized by considering a simplified version – a reaction-diffusion-like dynamics – of that theory. We begin with a clear axiomatic format of that framework, showing that the reaction-diffusion dynamics emerge in a direct way after a few assumptions. Our goal is to put focus on the relations between the reduced and the full theory and to underline some topological features of this theory, more precisely, by first showing that the Morse index distribution of the equilibria of the finite dimensional reduced system is exactly the same of the full original system, thus giving us eventually a good measure of the robustness of the reduction, and secondly, moving our framework to a Morse–Smale setting, by proposing an alternative way to compute the Morse index of the equilibria. In order to realize this last program, we propose a weak infinite-dimensional Maslov–Hörmander theorem.

Key words: Non-equilibrium thermodynamics, reaction-diffusion system, Lyapunov–Schmidt reduction, collective variables, Morse theory

Mathematics Subject Classification: 35Q82, 35B35, 35K57, 53D12, 58E05

Contents

1. Introduction

Most macroscopic systems that emerge in chemistry and biology are far from equilibrium. Classical thermodynamics though does not concern itself with this ubiquitous behaviour: it describes states of matter which do not change in time, or change so slowly that they can be described as a sequence of equilibria. In fact, out of equilibrium, there is no general agreement on the definition of most thermodynamic quantities like free energy or entropy.

In a series of papers [2, 3, 16, 1], G. Jona-Lasinio and coworkers have developed a theory, *Macroscopic Fluctuation Theory* (MFT), that describes macroscopic systems in a stationary non-equilibrium state, called *driven diffusive systems*. The ingredients of the theory are a finite number of fields that represent thermodynamical quantities like density of mass or charge, whose evolution is described by a continuity equation coupled with a constitutive equation that ties currents with the relative density fields. The theory has an axiomatic character, where the axioms derive from rigorous results in lattice gas theory in the hydrodynamic limit. Jona-Lasinio and coworkers then develop the macroscopic fluctuations of the system as a generalization of Friedlin–Wentzell theory to field variables. In this context, the infinite-dimensional analog of the quasi-potential can be interpreted as the *non-equilibrium free energy* of the system, with no assumption of small deviation from equilibrium.

The spirit of thermodynamics though is to describe the state of a macroscopical system via a *finite* number of variables, often called *collective variables*. The task of determining the adequate collective variables for a given system is absolutely nontrivial. The aim of this paper then is to consider a model of MFT given by a reaction-diffusion type equation, introduced in [5], and identify its collective variables using a Lyapunov–Schmidt-type finite-dimensional reduction, called Amann–Conley–Zehnder (ACZ) reduction. The resulting finite-dimensional system mimics two very important features of the system: its *gradient structure* and the stability properties of the equilibria, namely, the Morse index of the equilibria is preserved by the reduction. This is a novel feature: the Morse index of an equilibrium describes the number of unstable directions that stem from such equilibrium, and can be thought as a sort of *chemical affinity*. The reduced system can be used to calculate the number and the quality of the transitions emerging from equilibria.

In this paper we also develop the first steps towards a non-homogeneous Morse–Smale theory, setting the original theory in a symplectic environment. This extension is based on the construction of a path in the space of boundary data functions, whose formal cotangent bundle is equipped with a symplectic structure. The path is lifted on the Lagrangian submanifold that collects the whole set of solutions. Its description is through a generating function, in the

Tulczyjew–Weinstein sense [26, 25]. Such generating function is *precisely* the action functional of the system. This construction is allowed by a weak infinite-dimensional Maslov–Hörmander theorem, proposed in the Appendix. As far as we know, this result is original.

In our language, this Morse–Smale environment offers an alternative computation scheme for the Morse index, and shows how the Morse index is strictly linked to the intrinsic symplectic structure of the collection of the solutions of non-homogeneous Dirichlet problems.

2. The reaction-diffusion system

We outline the premises of MFT and we propose a simplified model of the evolution equation for the fields given by a reaction-diffusion equation. Such reaction-diffusion system is studied in detail, showing that it can be formulated as an L^2-*gradient descent* equation.

2.1. Thermodynamic origin

As said before, the MFT is developed on axioms. The first axiom states the evolution equation and the constitutive equation of the theory. Let Ω be a bounded domain in $\mathbb{R}^n$, or an n-dimensional smooth manifold, define $\rho = \rho(t, x)$, $x \in \Omega$ as the macroscopic density field and $j = j(t, x)$ its density of current.

Axiom 1. *The macroscopic evolution of the field ρ is given by the continuity equation*

$$\frac{\partial \rho}{\partial t} + \nabla \cdot j = 0 \tag{2.1}$$

together with the constitutive equation

$$j(t, x) = J(t, \rho(t, x)) = -D(\rho(t, x))\nabla\rho(t, x) + \chi(\rho(t, x))E(t) \tag{2.2}$$

where D is the diffusion matrix, $E(t)$ an external field and χ the relative mobility matrix of the system with respect to the field.

Substituting the constitutive equation in the continuity equation, we obtain an equation in the variable ρ that describes its evolution in time:

$$\frac{\partial \rho}{\partial t} = \nabla \cdot (D(\rho)\nabla\rho) - \nabla \cdot (\chi(\rho)E(t)) \tag{2.3}$$

To put (2.3) in a reaction-diffusion form, the first thing we must do is approximate the ρ-dependent diffusion matrix $D = D(\rho)$ with a spatial one $D = D(x)$, and equip Ω with a Riemannian structure g such that its Laplace–Beltrami operator, $\triangle = \triangle_g = \mathrm{tr}\,\nabla^2$, mimics the first term:

$$\triangle(\bullet) = \nabla \cdot [D(x)\nabla(\bullet)] \quad x \in \Omega \tag{2.4}$$

If $\Omega \subseteq \mathbb{R}^n$, it is sufficient to define $g_{ij} = D\delta_{ij}$. This way, equation (2.3) reads

$$\frac{\partial \rho}{\partial t} = \triangle\rho - \nabla \cdot \chi E \tag{2.5}$$

Now, we simplify the source term $\nabla \cdot \chi E$ by representing the external field via a "potential function" $V : \mathbb{R} \to \mathbb{R}$. By doing this we obtain the desired form:

$$\frac{\partial \rho}{\partial t} = \triangle\rho - V'(\rho) \tag{2.6}$$

Note that the non-linearity of the source term is preserved by the introduction of V, while the elliptic term in the reaction-diffusion system is essentially tamer than the diffusion term.

In the MFT, the evolution equation (2.3) is supplied with a continuous distribution of chemical potential on the border, $\lambda = \lambda(t, x)$, $x \in \partial\Omega$, representing the presence of reservoirs in contact with the boundary of the system. In this way the complete evolution equation for MFT is

$$\begin{cases} \dfrac{\partial \rho}{\partial t} = \nabla \cdot (D(\rho)\nabla\rho) - \nabla \cdot (\chi(\rho)E(t)), \quad x \in \Omega \\ f'(\rho(t, x)) = \lambda(t, x), \quad x \in \partial\Omega \end{cases} \tag{2.7}$$

where f is the equilibrium free energy per unit volume. These constitute non-linear non-homogeneous Dirichlet boundary conditions, in the form $\varphi(\rho) = \lambda$, $x \in \partial\Omega$. To encompass the most general non-equilibrium situation in our simplified system while also maintaining a certain degree of tractability, we assume affine Dirichlet boundary conditions see $(2.8)_2$ below.

2.2. Properties of the reaction-diffusion system

Consider then the compact n-dimensional manifold (Ω, g) with $\mathscr{C}^1$ boundary $\partial\Omega$, and its Laplace–Beltrami operator $\triangle$. We will change notation, from a thermodynamical one to a more common one in the theory of PDEs, hoping no confusion will ensue: take a curve $\mathbb{R} \ni t \mapsto u(t, \cdot) \in \mathscr{H}$ where $\mathscr{H}$ is a suitable Hilbert space, to be selected later. The functions $u \in \mathscr{H}$ represent the *density* of a certain quantity, like mass. Take $V : \mathbb{R} \to \mathbb{R}$ a (possibly) nonlinear function. We will think of its derivative V' as the *mass production/consumption rate* function. The *reaction-diffusion equation* on Ω is

$$\begin{cases} \dfrac{\partial u}{\partial t} = \triangle u - V'(u), \quad x \in \Omega \\ u = q, \quad x \in \partial\Omega \end{cases} \tag{2.8}$$

where the function $q : \partial\Omega \to \mathbb{R}$ is the *stationary* boundary data that represents the external influence on the system. We take the various q in a Hilbert space $\mathscr{H}^{\partial\Omega}$.

REMARK 2.1. Since the reaction-diffusion equation requires the derivative of the t-parameter of the curve $t \mapsto u(t, \cdot)$, we are looking for curves in $H^1(\mathbb{R}; \mathscr{H})$.

2.2.1. Equilibria of the system and variational formulation. Note that the search for stationary solutions $\left(\frac{\partial u}{\partial t} = 0\right)$, the equilibria, of (2.8) is equivalent to solving the nonlinear Poisson equation

$$\begin{cases} \triangle u = V'(u) \\ u|_{\partial\Omega} = q \end{cases} \tag{2.9}$$

This equation can be split into a Laplace equation with non-homogeneous boundary conditions, and a Poisson equation with homogeneous boundary conditions:

$$\begin{cases} \triangle Q = 0, & x \in \Omega \\ Q|_{\partial\Omega} = q, \end{cases} \quad \text{and} \quad \begin{cases} \triangle u^0 = F_Q(u^0) := V'(Q + u^0), & x \in \Omega \\ u^0|_{\partial\Omega} = 0 \end{cases} \tag{2.10}$$

It is clear that $u = u^0 + Q \in \mathscr{H}$ proposes all the solutions of (2.9).

REMARK 2.2. The splitting clarifies certain properties of the system that we are studying:

- Note that equation $(2.10)_1$ has existence and uniqueness for suitable prescribed boundary data $q \in \mathscr{H}^{\partial\Omega}$, hence we must explicit the functional spaces $\mathscr{H}$, $\mathscr{H}^{\partial\Omega}$. Since the equation involves the Laplacian, we take $\mathscr{H} = H^2(\Omega; \mathbb{R})$. Then the *trace* $Q|_{\partial\Omega}$ of Q on $\partial\Omega$ must be in $H^{2-\frac{1}{2}}(\Omega; \mathbb{R}) = H^{\frac{3}{2}}(\Omega; \mathbb{R})$ [4, chapter 9, pg. 315]. The natural choice for the boundary data functions is thus $\mathscr{H}^{\partial\Omega} = H^{\frac{3}{2}}(\Omega; \mathbb{R})$.
- Proceeding with observations on functional spaces, the boundary conditions of $(2.10)_2$ can be restated by taking the u^0 in the subspace

$$\mathscr{H}^0 := \{u \in \mathscr{H} : u|_{\partial\Omega} = 0\} \equiv H_0^2(\Omega; \mathbb{R}) \tag{2.11}$$

  where $u|_{\partial\Omega}$ is intended always in the trace sense.
- The preceding observation also prompts that the solution of $(2.10)_1$ proposes a map

$$\begin{aligned} \mathscr{H}^{\partial\Omega} &\to \mathscr{H} \\ q &\mapsto Q(q) \end{aligned} \tag{2.12}$$

  which is at least injective. This means that the Laplace part $(2.10)_1$ carries *all* of the boundary information of the original problem.

Now, once a solution of $(2.10)_1$ has been found, we can formulate $(2.10)_2$ with a variational principle: define the functional

$$
\begin{aligned}
&J : \mathscr{H}^0 \times \mathscr{H}^{\partial\Omega} \to \mathbb{R} \\
&(u^0, q) \mapsto J[u^0, q] = \int_\Omega \frac{\|\nabla(u^0)\|^2}{2} + V(u^0 + Q(q))\,\mathrm{d}x
\end{aligned}
\tag{2.13}
$$

The stationary points of J in the $\mathscr{H}^0$-component are the solutions of $(2.10)_2$.

2.2.2. Gradient-descent weak formulation for the complete system. The reaction-diffusion equation does not have a variational formulation, but the search for weak solutions can be put in a *gradient descent* form through a restatement of the equation that is based on the variational formulation of the equilibria.

Observe that the splitting introduced in (2.10) induces a splitting for the reaction-diffusion equation (2.8). These two equations are a heat equation with affine Dirichlet boundary conditions, and a reaction-diffusion equation, with *homogeneous* boundary conditions.

$$
\begin{cases}
\dfrac{\partial Q}{\partial t} = \triangle Q \\
Q|_{\partial\Omega} = q \in \mathscr{H}^{\partial\Omega}
\end{cases}
\tag{2.14}
$$

This is a very well known heat equation. Once a solution $Q : \Omega \to \mathbb{R}$ for (2.14) is found, consider the equation

$$
\begin{cases}
\dfrac{\partial u^0}{\partial t} = \triangle u^0 - F_Q(u^0) \\
u^0 \in \mathscr{H}^0
\end{cases}
\tag{2.15}
$$

We have split the flow $t \mapsto u(t, \cdot)$ into two separate flows $t \mapsto Q(t, \cdot) \in \mathscr{H}$ and $t \mapsto u^0(t, \cdot) \in \mathscr{H}^0$, both of regularity class H^1.

When a solution of (2.15) has been found, we have solved (2.8), simply by posing $u = u^0 + Q$:

$$
\begin{cases}
\dfrac{\partial(u^0 + Q)}{\partial t} = \triangle u^0 + \triangle Q - F_Q(u^0) = \triangle u - V'(u) \\
(u^0 + Q)|_{\partial\Omega} = Q|_{\partial\Omega} = q
\end{cases}
\tag{2.16}
$$

This splitting shows that again we may encode the affine boundary conditions into the function Q that solves a better known, linear equation.

Consider now equation (2.15), and look for its weak solutions, by taking $h \in \mathscr{C}_0^\infty$:

$$
\int_\Omega \frac{\partial u^0}{\partial t} h\,\mathrm{d}x = \int_\Omega (\triangle u^0 - F_Q(u^0)) h\,\mathrm{d}x \Leftrightarrow \left\langle \frac{\partial u^0}{\partial t}, h \right\rangle = -\partial_{u^0} J[u^0, q] h
\tag{2.17}
$$

Via Riesz representation theorem we can find a $\nabla J[u^0, q] \in \mathscr{H}^0$, $\forall u^0$, q such that $\partial_{u^0} J[u^0, q]h = \langle \nabla J[u^0, q], h \rangle_{L^2}$. In this way we can relax the distributional form into

$$\frac{\partial u^0}{\partial t} = -\nabla J[u^0, q] \tag{2.18}$$

which is manifestly a gradient system, which is called L^2-*gradient descent* form. Coupled with the heat equation, this equation reproduces all the solutions of the original system.

3. Finite reduction

In this section we reduce the search of the equilibria (2.9) with a Lyapunov–Schmidt type global reduction, called Amann–Conley–Zehnder (ACZ) exact finite reduction, that reduces a variational problem to an ODE and the search of a fixed point of a map on an infinite-dimensional Banach space. Heuristically, the reduction works by decomposing the functions in an orthonormal basis of eigenfunctions for $\triangle$, then keeping the first N components. On these first N components, the equation is a finite system of equations, while to recover the remaining components of the solution a fixed-point problem must be solved, after a suitable choice of N has been made (see equation (3.11) below).

Such reduction is then extended to the reaction-diffusion equation, near the equilibria. We show that the reduction preserves (2.8)'s gradient-like structure, through the identification of a "reduced action".

3.1. *Exact finite reduction of equilibria*

To reduce the complete equation (2.9) we must pass through the splitting proposed in Section 2.2.2. Let $\{u_j\}_{j\in\mathbb{N}} \in \mathscr{H}^0$ be the set of eigenfunctions of $\triangle$. Since $\triangle$ is an elliptic operator, the following identities hold:

$$\begin{cases} \triangle u_j = -\lambda_j u_j \\ u_j|_{\partial\Omega} = 0 \end{cases} \Rightarrow \langle u_i, u_j \rangle = \int_\Omega u_i u_j \, \mathrm{d}x = \delta_{ij}, \quad \lambda_0 = 0 \leq \lambda_1 \leq \lambda_2 \leq \cdots \tag{3.1}$$

and also $\{u_j\}_{j\in\mathbb{N}}$ is a basis of $\mathscr{H}^0$ (orthonormal). Via the spectral representation of $\triangle$ we can define an *inverse Laplacian operator* that acts on $\mathscr{H}^0$: for any $f \in \mathscr{H}^0$

$$g(f) := -\sum_{j>0} \frac{\langle f, u_j \rangle}{\lambda_j} u_j \Rightarrow \triangle g(f) = -\sum_{j>0} \frac{\langle f, u_j \rangle}{\lambda_j} \triangle u_j = \sum_{j>0} \langle f, u_j \rangle u_j = f \tag{3.2}$$

which means that $\triangle \circ g = g \circ \triangle = id_{\mathscr{H}^0}$.

Since $\{u_j\}_{j\in\mathbb{N}}$ is an orthonormal basis of $\mathscr{H}^0$, we can decompose any function $f \in \mathscr{H}^0$ a finite-dimensional "head" and an infinite-dimensional "tail" by considering the projectors

$$
\begin{aligned}
&\mathbb{P}_N : \mathscr{H}^0 \to \mathscr{U}_N = \mathbb{P}_N \mathscr{H}^0 \\
&\qquad f \mapsto \mathbb{P}_N f = \mu = \sum_{j=1}^{N} \langle f, u_j \rangle u_j \\
&\mathbb{Q}_N : \mathscr{H}^0 \to \mathscr{V}_N = \mathbb{Q}_N \mathscr{H}^0 \\
&\qquad f \mapsto \mathbb{Q}_N f = \eta = \sum_{j=N+1}^{\infty} \langle f, u_j \rangle u_j
\end{aligned}
\tag{3.3}
$$

Note that $\mathscr{U}_N$ is a finite-dimensional subspace of $\mathscr{H}^0$ while $\mathscr{V}_N$ is infinite-dimensional. Moreover, $\mathscr{H}^0 = \mathscr{U}_N \oplus \mathscr{V}_N$.

Through the inverse Laplacian g we may translate equation (2.9) to the search of a fixed point of a map on $\mathscr{H}$. To do this, we must first assume that F_Q actually is in $\mathscr{H}^0$, which is equivalent to asking that

$$
V'(Q(x) + u^0(x))|_{\partial\Omega} = V'(q(x)) = 0 \tag{3.4}
$$

REMARK 3.1. This condition has a justification in the simple physical interpretation that we are considering, where V' is the mass production/consumption rate and u is the mass density. What we are asking is that the mass production rate must be zero on the boundary, a condition that is compatible with the request of the assignment of a *stationary* mass distribution q on the boundary.

Moreover, consider the case of q continuous. Then its image must be compact in $\mathbb{R}$. Since we are prescribing the value of V' on the image of q, we observe that the condition (3.4) is not too restrictive, for example, if V' is with compact support, disjoint from the support of q. In this case, the subsequent condition (3.8) is automatically satisfied. A compactly supported V' is also synergic with the physical justification given above: the mass production/consumption is creative only inside our Ω.

REMARK 3.2. Solving (2.9) is equivalent to solving the following equation:

$$
u = g(F_Q(u^0)) + Q \Leftrightarrow u^0 = g(F_Q(u^0)) \tag{3.5}
$$

As above, we suppose the function Q is known. The statement of (3.5) is easily verifiable:

$$
\begin{cases}
\triangle u = \triangle[g(F_Q(u^0)) + Q] = F_Q(u^0) = V'(u) \\
u|_{\partial\Omega} = -\displaystyle\sum_j \frac{\langle F_Q(u^0(\cdot)), u_j \rangle}{\lambda_j} u_j|_{\partial\Omega} + Q|_{\partial\Omega} = q
\end{cases}
\tag{3.6}
$$

We must impose some conditions on V' to guarantee that the problem (3.5) admits a solution. To find these conditions, consider the decomposition of $(3.5)_2$

on the finite- and infinite-dimensional subspaces $\mathscr{U}_N$, $\mathscr{V}_N$:

$$\begin{cases} \mu = \mathbb{P}_N g(F_Q(\mu+\eta)) \\ \eta = \mathbb{Q}_N g(F_Q(\mu+\eta)) \end{cases} \tag{3.7}$$

Equation $(3.7)_1$ is a finite-dimensional equation and poses no convergence problem, while for $(3.7)_2$ we need to find conditions for which the r.h.s is a contraction. Suppose that V' is globally Lipschitz, that is,

$$\mathrm{Lip}(V') = C < \infty \tag{3.8}$$

Then the question is reduced to finding the appropriate N such that for any fixed $\bar{\mu} \in \mathscr{U}_N$ the map

$$\begin{aligned} \mathscr{V}_N &\to \mathscr{V}_N \\ \eta &\mapsto \mathbb{Q}_N g(F_Q(\bar{\mu}+\eta)) \end{aligned} \tag{3.9}$$

is a contraction. This is possible for the properties of the spectral decomposition of $\triangle$: let $\eta_1, \eta_2 \in \mathscr{V}_N$, then

$$\|\mathbb{Q}_N g(F_Q(\mu+\eta_2)) - \mathbb{Q}_N g(F_Q(\mu+\eta_1))\| \leq \frac{C}{\lambda_N}\|\eta_2 - \eta_1\| \tag{3.10}$$

so we can choose N such that

$$\frac{C}{\lambda_N} < 1 \tag{3.11}$$

since the sequence of eigenvalues is growing and unbounded. Note that this does not depend on the choice of $\bar{\mu}$: with the appropriate N the problem $(3.7)_2$ admits a solution for any μ.

Proceeding with the reduction, suppose we have chosen N satisfying (3.11). Then there is an unique solution to the fixed-point problem $(3.7)_2$, which we will call $\tilde{\eta}_Q$. Such solution depends on the choice of a $\mu \in \mathscr{U}_N$, so we will write

$$\tilde{\eta}_Q(\mu) = \mathbb{Q}_N g(F_Q(\mu + \tilde{\eta}_Q(\mu))) \tag{3.12}$$

Once this solution has been found, equation (2.9) is equivalent to solving the finite-dimensional equation

$$\mu = \mathbb{P}_N g(F_Q(\mu + \tilde{\eta}_Q(\mu))) \tag{3.13}$$

3.1.1. Variational character of the reduced equation (3.13). The reduced equation (3.13) can still be obtained by a variational problem. To see this, consider the functional J defined above. As a first step, note that the reduced equation (3.13) can be restated introducing the action functional's "gradient" (in the sense of Riesz representation), ∇J:

$$\mu = \mathbb{P}_N g(F_Q(\mu + \tilde{\eta}_Q(\mu))) \Leftrightarrow \mathbb{P}_N \nabla J[\mu + \tilde{\eta}_Q(\mu), q] = 0 \tag{3.14}$$

this can be easily seen by taking the Laplacian of both sides of (3.13) and noting that $\mathbb{P}_N$ and $\triangle$ commute; moreover, we can see in the same way (taking the Laplacian) that equation (3.12) is an identity once J is introduced, that is,

$$\tilde{\eta}_Q(\mu) = \mathbb{Q}_N g(F_Q(\mu + \tilde{\eta}_Q(\mu))) \Leftrightarrow \mathbb{Q}_N \nabla J[\mu + \tilde{\eta}_Q(\mu), q] = 0 \tag{3.15}$$

This will be an important fact in the rest of the section.

Define the real valued function

$$\begin{aligned} W : \mathscr{U}_N \cong \mathbb{R}^N &\to \mathbb{R} \\ \mu &\mapsto W(\mu) := J[\mu + \tilde{\eta}_Q(\mu), q] \end{aligned} \tag{3.16}$$

Now calculate its gradient:

$$\begin{aligned} \nabla W(\mu) &= \nabla J[u^0, q]|_{u^0 = \mu + \tilde{\eta}_Q} \left(\mathbb{P}_N + \mathbb{Q}_N \frac{\mathrm{d}\tilde{\eta}_Q}{\mathrm{d}\mu} \right) \\ &= \mathbb{P}_N \nabla J[u^0, q]|_{u^0 = \mu + \tilde{\eta}_Q} + \mathbb{Q}_N \nabla J[u^0]|_{u^0 = \mu + \tilde{\eta}_Q} \frac{\mathrm{d}\tilde{\eta}_Q}{\mathrm{d}\mu} \\ &\overset{(3.12)}{=} \mathbb{P}_N \nabla J[u^0, q]|_{u^0 = \mu + \tilde{\eta}_Q} \end{aligned} \tag{3.17}$$

This shows that μ stationarizes W if and only if $u = \mu + \tilde{\eta}_Q(\mu) + Q$ stationarizes J. We have thus identified a *finite dimensional representation* of the action functional, which we will call *reduced action function*.

3.2. *Reduction out of equilibrium and gradient structure*

We can use the fact that the equilibria admit an exact reduction to construct a reduction of the reaction-diffusion equation. Consider the same decomposition of $\mathscr{H}^0$, and project equation (2.15) on the subspaces $\mathscr{U}_N$ and $\mathscr{V}_N$:

$$\begin{cases} \dfrac{\partial \mu}{\partial t} = \triangle \mu - \mathbb{P}_N F_Q(\mu + \eta) \\ \dfrac{\partial \eta}{\partial t} = \triangle \eta - \mathbb{Q}_N F_Q(\mu + \eta) \end{cases} \tag{3.18}$$

As a reduction, we propose to substitute any occurrence of η with the "stationary tail" $\tilde{\eta}_Q(\mu)$. Thus the projected equation becomes

$$\begin{cases} \dfrac{\mathrm{d}\mu}{\mathrm{d}t} = \triangle \mu - \mathbb{P}_N F_Q(\mu + \tilde{\eta}_Q(\mu)) \\ 0 = \triangle \tilde{\eta}_Q(\mu) - \mathbb{Q}_N F_Q(\mu + \tilde{v}(\mu)) \end{cases} \tag{3.19}$$

While $(3.19)_2$ is an identity, completely equivalent to the definition of $\tilde{\eta}_Q$, equation $(3.19)_1$ is the reduced equation we were looking for:

$$\begin{aligned}\triangle\mu - \mathbb{P}_N F_Q(\mu + \tilde{\eta}_Q(\mu)) &= \mathbb{P}_N[\triangle(\mu + \tilde{\eta}_Q(\mu)) - F_Q(\mu + \tilde{\eta}_Q(\mu))] \\ &= -\mathbb{P}_N \nabla J[\mu + \tilde{\eta}_Q(\mu), q] \equiv -\nabla W(\mu)\end{aligned} \tag{3.20}$$

thus we have obtained a finite-dimensional gradient-like ODE:

$$\frac{\mathrm{d}\mu}{\mathrm{d}t} = -\nabla W(\mu) \tag{3.21}$$

Although this reduction is not exact anymore – an error estimate is worked out in [5] – it preserves the gradient structure of the original PDE, found in equation (2.18) Note that due to the form of equation (3.21), W has the right to be called *potential energy* of the system.

3.3. Thermodynamic features of the reduction

The heart of the reduction of the complete system around its equilibria is the substitution of the stationary tail $\tilde{\eta}_Q(\mu)$ to the non-stationary one. This procedure must be justified. To do this we can find estimates of the "error" committed in the substitution. Moreover, such substitution carries a strong thermodynamical interpretation. Both such discussions can be found in [5], and in this section we present the major results stated there without their development.

The first clue pointing to the adequacy of this type of reduction can be found in a well-known phenomenology in chemistry: the eigenvalues of the elliptic operator that describes the system present a *large gap* [17, 20, 21]. Such large gap is a flag of the emergence of a finite-dimensional description of the system, obtained through the leading eigenvalues. We can indeed identify a large gap for the reaction-diffusion equation: the "head" μ, on sufficiently long periods of time, is larger, in a precise sense, of the non-stationary head η, once the cutoff N has been chosen large enough. This means that substituting the stationary tail to the non-stationary one does not perturb the system greatly. The proof of this fact is based on the theory of *approximate inertial manifolds* developed by Temam, Manley and Foias [23, 13]: the original dynamics are confined to an *inertial manifold*, while the reduced dynamics to an approximate inertial manifold. Thus the proof of the adequacy of the reduction lies in proving that the two manifolds are close, at least for finite (long) times and in a neighborhood of equilibrium. Such proof follows the line of thought found in [19].

Even though the error committed by substituting the stationary tail is small, it still exists. In [5] the loss of information that occurs in the approximate form (3.21) has been compensated with the addition of some random Gaussian noise, leading to an SDE

$$\frac{\mathrm{d}\mu}{\mathrm{d}t} = -\nabla W + \sqrt{v}w \tag{3.22}$$

where w is the Gaussian noise and v the diffusion coefficient.

We can link (3.22) to a Fokker–Planck equation in a canonical way:

$$\frac{\partial p_\nu}{\partial t} - \nabla \cdot (p_\nu \nabla W) = \nu \Delta p_\nu \tag{3.23}$$

As it is well known, the stationary $\left(\frac{\partial p_\nu}{\partial t} \equiv 0\right)$ solution of the Fokker–Planck equation is

$$p_\nu^{eq}(\mu) = Z(\nu)^{-1} e^{-\frac{W(\mu)}{\nu}}, \quad Z(\nu) = \int_{\mathcal{U}_N} e^{-\frac{W(\mu)}{\nu}} d\mu \tag{3.24}$$

A *large deviation* reading of (3.22), on the line of thought of Friedlin and Wentzell [14], together with the Varadhan *contraction principle* (see e.g. [24]), leads us to an asymptotic probability density. The following development is borrowed from [5]. First set some notation. To be in line with the literature, pose $\mu = x$. Then we give the following

Definition 1.

(1) *Continuous paths of the SDE:*

$$\mathscr{C}_\nu^{(x_0,t)} = \{x_\nu(\tau) : \tau \in [0,t],\, x(0) = x_0,\, x_\nu \text{ continuous path of the SDE (3.22)}\}$$

(2) *Quasi-potential*

$$V(t,x,x_0) = \inf_{x(\cdot) \in \mathscr{C}_\nu^{(x_0,t)},\, x(t)=x} \left\{ \frac{1}{2} \int_0^t \left| \frac{dx}{dt}(\tau) + \nabla W(x(\tau)) \right|^2 d\tau \right\}$$

(3) *Lagrangian of the stochastic process*

$$L(x,\dot{x}) := \frac{1}{2} |\dot{x} + \nabla W(x)|^2$$

The aforementioned asymptotic probability density $p_\nu^{x_0}$, that is, relative to (3.23) with initial point x_0, is then found to satisfy (*Ellis logarithmic equivalence*):

$$\lim_{\nu\to 0} \nu \log p_\nu^{x_0}(t,x) = \lim_{\nu \to 0} \nu \log e^{-\frac{1}{\nu}V(t,x,x_0)} = \lim_{\nu\to 0} -V(t,x,x_0) \tag{3.25}$$

In a neighborhood of a critical point $\hat{x}$, $\nabla W(\hat{x}) = 0$, the equilibrium density $p_\nu^{eq}(x)$ has the form

$$\begin{aligned} &\lim_{\nu\to 0} \nu \log p_\nu^{eq}(x) = \lim_{\nu\to 0} \nu \log e^{-\frac{1}{\nu}V_\infty^{eq}(x,\hat{x})} = \lim_{\nu \to 0} -V_\infty^{eq}(x,\hat{x}), \\ &\text{where } V_\infty^{eq}(x,\hat{x}) = \lim_{t\to+\infty} V(t,x,\hat{x}), \end{aligned} \tag{3.26}$$

and a straightforward computation shows that

$$V_\infty^{eq}(x,\hat{x}) = W(x). \tag{3.27}$$

Therefore, as expected, in the infinite-time limit the large deviation description of the probability density tends to the equilibrium solution of the Fokker–Planck equation $p_\nu^{eq} = e^{-\frac{W}{\nu}}$.

Now, we have to recall the well known Lax–Oleinik representation formula

$$S(t,x,x_0) = \inf_{x(0)=x_0,\, x(t)=x} \left\{ \int_0^t L(x(\tau), \dot{x}(\tau))\, d\tau \right\} \tag{3.28}$$

for the viscosity solutions of the evolutive Hamilton–Jacobi problem, where the Hamiltonian is

$$H(x,\pi) = \frac{1}{2}|\pi|^2 - \nabla W(x)\cdot\pi \tag{3.29}$$

which is the Legendre transform of the Lagrangian of the stochastic process L of Definition 1–(4). Then we see that the quasi-potential (3) of Definition 1 is precisely the viscosity solution of the Hamilton–Jacobi equation, namely

$$\frac{\partial S}{\partial t} + \frac{1}{2}|\nabla S|^2 - \nabla W(x)\cdot\nabla S = 0, \quad S(0,x_0,x_0) = 0, \tag{3.30}$$

that is: $S(t,x,x_0) = V(t,x,x_0)$. Our circle of ideas is completed when we consider the Cole-Hopf transformation

$$p_\nu(t,x) = e^{-\frac{1}{\nu}\hat{S}_\nu(t,x)} \tag{3.31}$$

where we look for solutions of the Fokker–Planck equation that have a similar structure to the equilibrium solution, and again by a straightforward computation we see that, ν-asymptotically, $\hat{S}_\nu(t,x)$ solves the evolutive viscous Hamilton–Jacobi equation in (3.30) if and only if $p_\nu(t,x)$ solves Fokker–Planck. Standard results in weak KAM theory, see e.g. [9, 12], assure us that any viscosity solution of the *evolutive* H-J equation (3.30), for $t \to +\infty$, is $\mathscr{C}^0$-asymptotic (i.e. in the uniform convergence topology) to $\hat{S}(x) - ct$, where $\hat{S}$ is a suitable viscosity solution of the related *stationary* H-J equation, $\frac{1}{2}|\nabla\hat{S}|^2 - \nabla\hat{S}\cdot\nabla W = c$, at the (unique) real value

$$c := \inf_{u\in\mathscr{C}^1(\mathscr{D},\mathbb{R})} \sup_{x\in\mathscr{D}} H(x,\nabla u(x)) \tag{3.32}$$

called the *Mañé critical value*. A standard computation (see [5]), shows that in our case $c = 0$, so that, for time running to $+\infty$, we have that

$$\frac{1}{2}|\nabla V_\infty^{eq}|^2 - \nabla V_\infty^{eq}\cdot\nabla W = 0. \tag{3.33}$$

The above defined quasi potential V_∞^{eq} parallels (up to the inessential $1/2$) the definition of $\mathscr{F}$ by Jona-Lasinio and coworkers, the so-called *free energy of the* *system in the dynamic state* ρ,

$$\mathscr{F}(\rho) = -\inf_{\eta} \Big\{ I_\infty[\eta] : \eta(0) = \hat{\rho},\ \lim_{t\to\infty} \eta(t) = \rho \Big\} \tag{3.34}$$

which in their framework can be seen as the solution of an infinite dimensional Hamilton–Jacobi equation of the form (see [16])

$$\left\langle \nabla \frac{\delta \mathscr{F}}{\delta \rho} \cdot \chi(\rho) \nabla \frac{\delta \mathscr{F}}{\delta \rho} \right\rangle - \left\langle \frac{\delta \mathscr{F}}{\delta \rho} \nabla \cdot j(\rho) \right\rangle = 0, \tag{3.35}$$

where angular brackets stand for integration on the spatial domain.

We think that the strong analogies between the original MFT with the present approximate reduction that have been found above support the physical interest of this framework, where the very gradient structure that is recovered in the reduction seems to play a determinant role.

4. Morse index and Morse index invariance

The reductions proposed above preserve a lot of the structure of the original equations. We have seen, in particular, that the equilibria are exactly preserved. In this section we will show in addition that the reductions *respect the stability properties* of the equilibria, that is, the stability of the equilibria of the original system (2.8) can be investigated via the stability of the equilibria of (3.21) with exactness. This is guaranteed by the fact that the reduction *preserves the Morse index* of the equilibria. The invariance of the Morse index can be computed directly by confronting the spectrum of the reduced and full actions, as has been first observed in [7].

Finally, in the next sections we will develop a symplectic environment for our elliptic PDE, appropriate to the presentation of a Morse–Smale–like theory in the background of our setting.

4.1. The Morse index

The Morse index can be defined for any bilinear form on a vector space. In our case, we want to define it for a solution of a dynamical system.

Definition 2 (Morse index). Let V be a vector space (eventually infinite-dimensional) and $\beta : V \times V \to \mathbb{R}$ a bilinear form. Then the Morse index $M(\beta)$ of β is the dimension of the negative space of β:

$$M(\beta) = \dim[\{v \in V : \beta(v,v) < 0\} \cup \{0\}] \tag{4.1}$$

In particular, we can define a Morse index for a stationary point starting from any variational problem: if a function u belongs to some functional (vector) space V and stationarizes a functional $I : V \to \mathbb{R}$, then its Morse index $m(u)$ is

$$m(u) = M(\mathrm{d}^2 I[u]|_{\mathrm{d}I[u]=0}) \tag{4.2}$$

In this sense the Morse index tells us about the *definiteness* of the Hessian of the action, evaluated on the stationary curve.

REMARK 4.1. Regarding the non-linear Poisson equation, the Morse index of a solution has a further meaning: the first variation of J gives us the Poisson equation, while the second variation gives us its linearization around a solution u^0, in the form of a selfadjoint bounded operator $A = F_Q'(u^0) - \triangle$:

$$\partial^2_{u^0} J[u^0, q](w, v) = \int_\Omega [-\triangle w + V''(u^0 + Q(q))w]v \,\mathrm{d}x \quad \forall v, w \in \mathscr{H}^0 \tag{4.3}$$

The Morse index at a solution $\bar{u}^0$ is then the number of *negative* eigenvalues of A at $\bar{u}^0$. If we consider Poisson equation as the search for equilibria in the reaction-diffusion system, this means that the Morse index of an equilibrium gives us information on the *unstable directions* that stem from such equilibrium. There is interest in these unstable directions because they flag the emergence of a possible *transition* in the system, for example, from an unstable equilibrium to a stable, $m(u) = 0$ equilibrium.

4.2. Morse index invariance

To make the notation lighter, in this section we will suppress the dependence of J from q and we will write the variation of the action functional as $\mathrm{d} := \partial_{u^0}$. We will show that the *negative space* of $\mathrm{d}^2 W(\mu)|_{\mathrm{d}W(\mu)=0}$ is the same of $\mathrm{d}^2 J[\mu + \tilde{\eta}_Q(\mu)]|_{\mathrm{d}J[\mu+\tilde{\eta}_Q(\mu)]=0}$. This will let us conclude immediately that the Morse index is preserved after the reduction.

Take the usual action functional $J : \mathscr{H}^0 \to \mathbb{R}$. We have seen that the introduction of the eigenfunctions of the Laplacian and the cutoff realizes the split $\mathscr{H}^0 = \mathscr{U}_N \oplus \mathscr{V}_N$. Consequently, the dual space splits into $(\mathscr{H}^0)^* = \mathscr{U}_N^* \oplus \mathscr{V}_N^*$, where

$$\begin{aligned} \mathscr{U}_N^* &:= \{\psi \in (\mathscr{H}^0)^* : \psi|_{\mathscr{V}_N} = 0\} \\ \mathscr{V}_N^* &:= \{\varphi \in (\mathscr{H}^0)^* : \psi|_{\mathscr{U}_N} = 0\} \end{aligned} \tag{4.4}$$

We may decompose the differential of J under this split:

$$\mathrm{d}J[u^0] = \partial_{\mathscr{U}_N} J[u^0] \oplus \partial_{\mathscr{V}_N} J[u^0] \in \mathscr{U}_N^* \oplus \mathscr{V}_N^* \tag{4.5}$$

By Riesz representation, we may identify

$$\partial_{\{\mathscr{U}_N, \mathscr{V}_N\}} J[u^0](\cdot) = \langle \{\mathbb{P}_N, \mathbb{Q}_N\} \nabla J[u^0], \cdot \rangle \tag{4.6}$$

In a similar way, we write $\partial^2_{\mathscr{U}_N} J = \mathbb{P}_N \mathrm{d}^2 J \mathbb{P}_N$, $\partial_{\mathscr{U}_N} \partial_{\mathscr{V}_N} J = \mathbb{Q}_N \mathrm{d}^2 J \mathbb{P}_N \ldots$ With this notation we can represent the second variation of J in block-matrix form on $\mathscr{U}_N \oplus \mathscr{V}_N$:

$$\mathrm{d}^2 J = \begin{pmatrix} \partial^2_{\mathscr{U}_N} J & \partial_{\mathscr{V}_N} \partial_{\mathscr{U}_N} J \\ \partial_{\mathscr{U}_N} \partial_{\mathscr{V}_N} J & \partial^2_{\mathscr{V}_N} J \end{pmatrix} \tag{4.7}$$

Moreover we can find an expression for $\mathrm{d}^2 W$ starting from J. Equation (3.17) shows us that $\mathrm{d}W(\mu) = \partial_{\mathscr{U}_N} J[\mu + \tilde{\eta}_Q(\mu)]$: then

$$(4.8)\quad \begin{aligned} &\mathrm{d}^2 W(\mu) = \partial^2_{\mathscr{U}_N} J[\mu + \tilde{\eta}_Q(\mu)] + \partial_{\mathscr{V}_N}\partial_{\mathscr{U}_N} J[\mu + \tilde{\eta}_Q(\mu)]\frac{\partial \tilde{\eta}_Q}{\partial \mu} \\ &\partial_{\mathscr{V}_N} J[\mu + \tilde{\eta}_Q(\mu)] = 0 \Rightarrow 0 = \partial_{\mathscr{U}_N}\partial_{\mathscr{V}_N} J[\mu + \tilde{\eta}_Q(\mu)] + \partial^2_{\mathscr{V}_N} J[\mu + \tilde{\eta}_Q(\mu)]\frac{\partial \tilde{\eta}_Q}{\partial \mu} \end{aligned}$$

From $(4.8)_2$ we can extract an expression for $\frac{\partial \tilde{\eta}}{\partial \mu}$, explicitly:

$$(4.9)\quad \frac{\partial \tilde{\eta}_Q}{\partial \mu} = -[\partial^2_{\mathscr{V}_N} J[\mu + \tilde{\eta}_Q(\mu)]]^{-1}\partial_{\mathscr{U}_N}\partial_{\mathscr{V}_N} J[\mu + \tilde{\eta}_Q(\mu)]$$

This way we can represent $\mathrm{d}^2 W$ in block-matrix form on $\mathscr{U}_N \oplus \mathscr{V}_N$:

$$(4.10)\quad \mathrm{d}^2 W = \begin{pmatrix} \partial^2_{\mathscr{U}_N} J - [\partial^2_{\mathscr{V}_N} J]^{-1}\partial_{\mathscr{U}_N}\partial_{\mathscr{V}_N} J & \mathbb{O} \\ \mathbb{O} & \partial^2_{\mathscr{V}_N} J \end{pmatrix}$$

We are ready for

Theorem 1 (Proposition 4 of [7]). *The negative space of* $\mathrm{d}^2 W(\mu)|_{\mathrm{d}W(\mu)=0}$ *is the same of* $\mathrm{d}^2 J[\mu + \tilde{\eta}_Q(\mu)]|_{\mathrm{d}J[\mu+\tilde{\eta}_Q(\mu)]=0}$.

Proof. To simplify notation, let

$$(4.11)\quad \mathrm{d}^2 J = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$$

We can block-diagonalize $\mathrm{d}^2 J$ with a technique called *Schur's complement*, namely, via the matrix

$$(4.12)\quad T = \begin{pmatrix} \mathbb{1}_{\mathscr{U}_N} & \mathbb{O} \\ -D^{-1}C & \mathbb{1}_{\mathscr{V}_N} \end{pmatrix}$$

Setting $\widetilde{\mathrm{d}^2 J} = T^*\mathrm{d}^2 J T$, which is the block-diagonalized form of $\mathrm{d}^2 J$, we have that $\widetilde{\mathrm{d}^2 J} = \mathrm{d}^2 W$. Then, at least the negative spaces of the two bilinear forms must coincide. Note that the positive and null spaces will in general not be the same, since $\mathrm{d}^2 J$ is infinite-dimensional. $\square$

4.3. Towards a symplectic non-homogeneous Morse–Smale theory

Morse theory was first developed by M. Morse as a technique to investigate the stability properties of the solutions of variational problems, precisely, geodesic problems, with applications in differential topology. Such theory has been considerably extended by S. Smale in the seminal paper [22], where instead of a one-dimensional geodesic problem, n-dimensional elliptic boundary deformation problems are considered. The results that are obtained are remarkable: we may study the spectrum of an elliptic operator on an n-dimensional Riemannian manifold Ω, by shrinking its boundary $\partial\Omega$ until it is small in measure. To be precise, the result can be explained in steps: first of all Smale studies how the eigenvalues of the elliptic operator vary when the boundary is smoothly deformed, showing that they depend continuously on the deformation and that they are strictly increasing if the deformation is towards a boundary that is small in measure, on which the eigenvalues must be all positive. Next, *conjugate instants* are defined, namely, the instants of the deformation at which the elliptic operator has at least one null eigenvalue. Finally, the original boundary is shrunk until it is small in measure: since the eigenvalues must all become positive, and since they strictly increase continuously, the negative ones on the original boundary must pass by zero. The negative eigenvalues on the initial boundary are equal in number to the conjugate instants. This theory, which has the right to be called Morse–Smale theory, is a real extension of the Morse theory, as remarked in Smale's article: in the geodesic case, Ω is simply the geodesic curve, the elliptic operator is defined by Jacobi's equation, and the boundary shrinking is the procedure of moving one extremal point of the curve towards the other.

This theory finds a further expansion in the articles [10, 8], where the Morse index is translated in its natural cohomological language, by the identification of a symplectic environment for the boundary deformation procedure. A Maslov index is used to prove the Morse index theorem. The theory is genuinely extended not only because of the identification of the symplectic environment, but also because the deformation now does not have to go towards a small boundary necessarily.

In this section we wish to develop the first steps towards a generalization of this environment to a non-homogeneous one. In fact, Deng and Jones' theory is done for *homogeneous* Robin conditions (linear combination of Neumann and Dirichlet conditions). We wish to borrow the cohomological language used in that theory, and use it to formulate a Morse theorem for, this time, *smooth variations of boundary data functions* (*curves in* $\mathscr{H}^{\partial\Omega}$), realizing a true non-homogeneous extension. What we want to capture is that the *intersection index* of such curves with the Maslov cycle of a certain Lagrangian submanifold in phase space carries with it all the stability properties of the underlying system.

4.3.1. Symplectic view of the nonlinear Poisson equation. The first thing that has to be done is set our elliptic boundary value problem in an infinite-dimensional symplectic environment. In this section we construct such phase space, in the spirit of [10], and show that the solutions of (2.9) play the role of the infinite parameters of a generating function for a Lagrangian submanifold. Such generating function, or Morse family, results to be the action functional of the equation. These ideas originate from the tractation found in [6], on the line of thought of Weinstein and Tulczyjew.

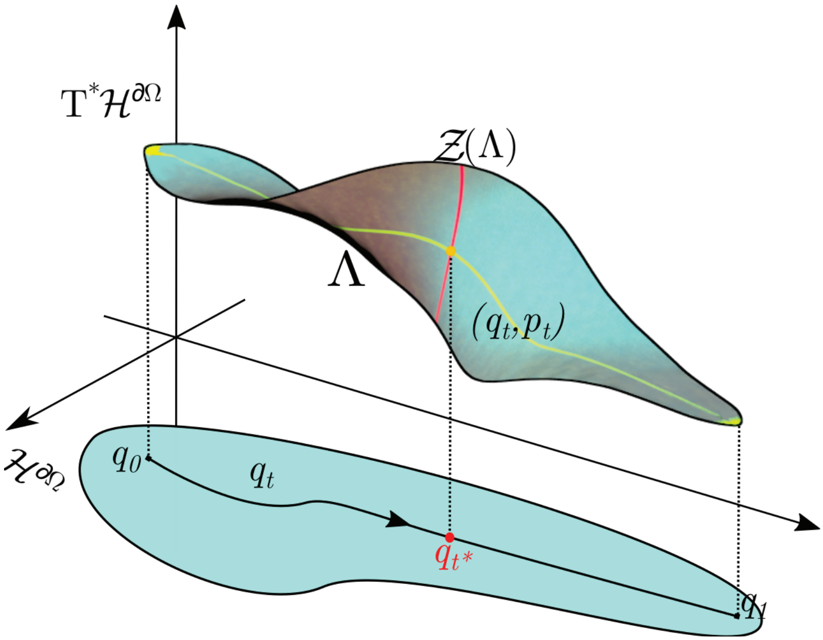

Figure 1. The Lagrangian submanifold Λ of equation (4.16), the path q_t in phase space, the lifted path on Λ (in yellow) and Λ's Maslov cycle (in red)

Consider the variational formulation via J. We may look at the $q \in \mathscr{H}^{\partial\Omega}$ as points in configuration space. Thus a reasonable choice for a phase space seems to be the formal cotangent bundle of $\mathscr{H}^{\partial\Omega}$ (see Remark 2.2):

$$\mathbf{H} = \mathrm{T}^* \mathscr{H}^{\partial\Omega} = \mathscr{H}^{\partial\Omega} \times (\mathscr{H}^{\partial\Omega})^* (= H^{\frac{3}{2}} \times H^{-\frac{3}{2}}) \tag{4.13}$$

The canonical (strong) symplectic form on $\mathbf{H}$ can be defined starting from the natural pairing between $\mathscr{H}^{\partial\Omega}$ and $(\mathscr{H}^{\partial\Omega})^*$, as seen in [18, Chap. 5, Par. 7], and also in Appendix A

$$\begin{gathered}\omega_{(q,p)}((Q_1, P_1), (Q_2, P_2)) = P_1(Q_2) - P_2(Q_1), \\ \forall (q, p) \in \mathbf{H}, \ \forall (Q_i, P_i) \in \mathrm{T}_{(q,p)}\mathbf{H}\end{gathered} \tag{4.14}$$

We want to obtain a Lagrangian submanifold description of the set of solutions. To do this, define

$$p(\cdot) = \partial_q J[u^0, q](\cdot) \tag{4.15}$$

Now clearly the set of solutions is

$$\Lambda = \{(q, p) \in \mathbf{H} : p = \partial_q J[u^0, q], \ 0 = \partial_{u^0} J[u^0, q], \ u^0 \in \mathscr{H}^0\} \tag{4.16}$$

which is a Lagrangian submanifold of $\mathbf{H}$, with J acting as a generating function with infinite parameters u^0. To see the proof of this, refer to Theorem 2 in Appendix A.

4.3.2. Conjugate instants and the Morse–Smale theorem. We now want to take a path in the configuration space $\mathscr{H}^{\partial\Omega}$, lift it on the Lagrangian submanifold, then look at its Maslov index, defined as the intersection index of the path with the Maslov cycle on Λ. The Morse index of the solutions will thus be brought back to such Maslov index.

The main result used in this section is the existence of the map $u^0 = \tilde{u}^0(q,p)$, guaranteed for our Lagrangian submanifold Λ by point (1) of Theorem 2.

Suppose that $0 \in (\mathscr{H}^0)^*$ is a *regular value* (see Theorem 2) for the map $(u^0, q) \mapsto \partial_{u^0} J[u^0, q]$. This is a structural hypotheses, that makes Λ a well-behaving submanifold of the cotangent fiber bundle. Then we are in the hypotheses of Theorem 2, and we may find a function $u^0 = \tilde{u}^0(q,p)$ that, in particular satisfies

$$\begin{cases} \partial_{u^0} J[\tilde{u}^0(q,p), q] \equiv 0 \\ \partial_q J[\tilde{u}^0(q,p), q] - p \equiv 0 \end{cases} \tag{4.17}$$

Now suppose that we know that for a generic fixed q_1 a certain $\hat{u}^0 \in \mathscr{H}^0$ is a global minimum for the map

$$u^0 \mapsto \partial_{u^0} J[u^0, q_1] \tag{4.18}$$

Conditions on J for which such minimizer exists can be found in [11, Theorem 2, Par. 8.2]. Then, locally, it must be that $\hat{u}^0 = \tilde{u}^0(q_1, p_1)$ for $(q_1, p_1) \in \Lambda$. We may connect q_1 in configuration space with a q_0 constructing a path $[0,1] \ni \tau \mapsto q_\tau \in \mathscr{H}^{\partial\Omega}$, and we can lift it to Λ setting $p_\tau = \partial_q J[u^0, q_\tau]$ (where we take u^0 such that $0 = \partial_{u^0} J[u^0, q_\tau]$) for all τ. The idea is that the Morse index at $\bar{u}^0 = \tilde{u}^0(q_0, p_0)$ can be extracted from the topological features of such path.

Consider the linearized dynamics on Λ along the path (q_τ, p_τ) as found in (4.3):

$$\begin{cases} -A_\tau w := \triangle w - F_Q'(\tilde{u}^0(q_\tau, p_\tau))w = 0 \\ w|_{\partial\Omega} = 0 \end{cases} \tag{4.19}$$

Definition 3 (Conjugate Instant). If equation (4.19) has a nontrivial solution for $\tau = \tau^*$, then we say that τ^* is a *conjugate instant* to $\tau = 0$, and q_{τ^*} is a *conjugate point* to q_0. The *multiplicity* of the conjugate instant is the dimension of the solution space:

$$\alpha(\tau^*) = \dim\ker A_{\tau^*} \tag{4.20}$$

Remark 4.2. Restating the definition of a conjugate instant via the second variation of the action functional, once we restrict on the subspace $\mathscr{H}^0$ to suppress the boundary conditions, we see that what we are looking for is a fall in the rank of the "Hessian" of the generating function:

$$\partial^2_{u^0} J[\tilde{u}^0(q_{\tau^*}, p_{\tau^*}), q_{\tau^*}](w, v) = 0 \quad \forall v \tag{4.21}$$

When such system has only $w = 0$ as a solution, we can actually find a function $u^0 = \check{u}^0(q)$ that satisfies $\partial_{u^0} J[\check{u}^0(q), q] \equiv 0$, and thus we find that around q, Λ is *transversal* to the fibers of the cotangent bundle.

On the contrary, when such system has a nontrivial solution for a time τ^*, we *cannot* locally explicit a function $u^0 = \check{u}^0(q)$ from $\partial_{u^0} J[u^0, q_\tau] = 0$, but we must be satisfied with the function prompted by Theorem 2. It is well known in the finite-dimensional theory of generating functions that these are also the instants at which the curve $\tau \mapsto (q_\tau, p_\tau)$ crosses a *non-transversal* locus on Λ, that is, its *Maslov cycle*. This can be extended also to infinite dimensions, as has been presented in [15], through the spectral theory of Fredholm operators. In other words, when we look at the linearized dynamics along the path $\tau \mapsto (q_\tau, p_\tau)$, we produce a flow of operators $\tau \mapsto A_\tau$. This can be seen as a path in the subset of the Grassmanian of Lagrangian subspaces of $\mathbf{H}$, called Fredholm Lagrangian Grassmanian, which is the natural habitat for the current treatment of the Morse and Maslov indices.

Rephrase the definition given in (4.2) as:

$$m(\tilde{u}^0(q_\tau, p_\tau)) = \dim(\{w \in \mathscr{H}^0 : \langle A_\tau w, w\rangle < 0\} \cup \{0\}) \tag{4.22}$$

that is, the number of *negative* eigenvalues of A_τ. The eigenvalue problem for A_τ is

$$A_\tau w = \lambda(\tau) w \tag{4.23}$$

Such eigenvalue problem is well defined on $\mathscr{H}^0$, since A_τ is selfadjoint with compact resolvent on it ([10]).

What we want to prove is that the number of negative eigenvalues at the instant $\tau = 0$ is the number of null eigenvalues found at some conjugate instants $\tau_1^*, \tau_2^* \ldots$, which correspond to the times at which $\tau \mapsto (q_\tau, p_\tau)$ crosses the Maslov cycle. The multiplicity of the conjugate instant is precisely the degree of the crossing. Suppose, as before, that $\hat{u}^0 = \tilde{u}^0(q_1, p_1)$ is a global minimum for J. This means that the spectrum of A_1 is composed of only positive eigenvalues: its Morse index is zero. Now, proceeding in analogy to Smale's construction carried out above, starting from a generic point (q_0, p_0) – from which we want to extract the Morse index of $\tilde{u}^0(q_0, p_0)$ – we construct a path $[0, 1] \ni \tau \mapsto (q_\tau, p_\tau) \in \Lambda$. Along (q_τ, p_τ), by crossing time by time $\mathscr{Z}(\Lambda)$, the spectrum looses or gains negative eigenvalues, correspondingly to the sign of the crossing, to produce some null eigenvalues. Since the final point corresponds to a minimum, we must have lost all the negative eigenvalues of the beginning in this crossing phenomenon. The natural homological invariance inherited in this environment offers us that the Morse index of $\tilde{u}^0(q_0, p_0)$ is *precisely* such Maslov index of the path with the Maslov cycle $\mathscr{Z}(\Lambda)$.

The very difference with Smale's construction consists in the fact that the deformations that are considered in his work are deformations of the domain Ω_τ, while our deformations are of the boundary data q_τ for a fixed Ω.

4.3.3. Finite reduction as finite parameters. The point of view of taken in the previous sections shifts the attention from the solution of the Poisson equation to the boundary conditions. The boundary conditions, in fact, make up the configuration space of the system, which is quite natural. In this section the ACZ finite reduction is reinterpreted as the identification of a finite set of parameters that describe the *same* Lagrangian submanifold Λ.

As has been done multiple times throughout this paper, consider the natural splitting of the dynamics in the "boundary-less" and "boundary" parts:

$$\begin{cases} \triangle Q = 0 \\ Q|_{\partial\Omega} = q \end{cases} \quad \text{and} \quad \begin{cases} \triangle u^0 = F_Q(u^0) \\ u^0|_{\partial\Omega} = 0 \end{cases} \tag{4.24}$$

The boundary-less part admits a finite-dimensional description, once the fixed-point function $\tilde{\eta}_Q(\mu)$ has been found. This also prompts a reduction of the action functional, by defining

$$W(\mu, q) = J[\mu + \tilde{\eta}_{Q(q)}(\mu), q] \tag{4.25}$$

We have added the functional dependence of W from q for convenience, while in the preceding treatment it seemed superfluous.

Since the variational character of the equation is preserved by the reduction, such finite-dimensional description reflects itself onto the Lagrangian submanifold defined by the action. Through the reduction we have identified a set of finite parameters that describe Λ in this sense:

$$\Lambda \equiv \left\{ (q, p) \in \mathbf{H} : p = \partial_q W(\mu, q),\ 0 = \frac{\partial W}{\partial \mu}(\mu, q) \right\} \tag{4.26}$$

The p-component of Λ is left unchanged, while the auxiliary parameters are now *in a finite number*.

4.3.4. Finite reduction and the Morse index. There is a strong synergy between the reduction and the Morse–Smale setting we put our theory in. The Lagrangian submanifold is still described, once the fixed-point function $\tilde{\eta}_Q$ has been found, by the *finite* parameters μ, as has been shown in the previous section. Thus the path $\tau \mapsto q_\tau$ can be still lifted on the Lagrangian submanifold Λ, in the exact same way we have constructed it in the infinite-parameters case, with the caution of inverting the equation $\mathrm{d}W(\mu) = 0$ to obtain a function $\mu = \check{\mu}(q)$ away from the degenerate points for which $\mathrm{d}^2 W(\mu) = 0$, that will act as conjugate points for this finite description. Around the points where the rank of $\mathrm{d}^2 W$ *falls*, exactly at the conjugate points q_{τ^*}, we have the function $\mu = \tilde{\mu}(q, p)$ whose existence is assured by Theorem 2, where $\mathscr{H}^0$ is replaced by $\mathscr{U}_N$ and $J[u^0, q]$ is substituted by $W(\mu, q)$.

In fact, the proof of the Morse theorem we gave does *not* concern itself on the structure of the *auxiliary parameters*, while the reduction does *not* concern itself with the *boundary conditions*.

Since the finite parameters μ are obtained via a spectral decomposition, and considering the negative-space invariance proved above, we are at least sure that the spectrum of $d^2 W(\mu)$ is composed of positive eigenvalues when $\mu = \check{\mu}(q_1)$ corresponds to the aforementioned minimum $\check{u}^0(q_1) = \mu + \tilde{\eta}_Q(\check{\mu}(q_1))$ for J. So if we want to know the Morse index at a point $\mu_0 = \tilde{\mu}(q_0, p_0)$, we construct the usual smooth path $\tau \mapsto q_\tau$ from q_0 to q_1 and we lift it on the finitely-described Lagrangian submanifold Λ. The proof then proceeds as in the infinite-dimensional case, with the conjugate points substituted by the finitely-described conjugate points defined above (points for which $d^2(W \circ \tilde{\mu})$ has a nonempty kernel). This fact underlines how the stability properties of the system are intrinsically tied with the topology of the Lagrangian submanifold, which admits a description through finite parameters.

5. Conclusions

In this article we have reproposed the reduction elaborated in [5], extending it to the non-homogeneous Dirichlet case. The extension also underlines that the non-homogeneous boundary conditions can be loaded completely on an easier, linear PDE, the heat equation, thanks to its existence and uniqueness theorem.

The Morse index invariance of the reduction, first found in [7], is extended to this thermodynamical theory. In such spirit, we wish to give a more thermodynamical interpretation to the Morse index of any critical solution: it is a sort of qualitative *chemical affinity*, since it measures the tendency of a certain configuration of the system to undergo a transition. The viscous component given by the Laplacian also suggests that a stable, null-Morse index might attract other instable, positive Morse index equilibrium configurations, in the sense that any solution close to an instable equilibrium will eventually "fall" into the stable equilibrium.

We propose two ways to compute the Morse index of an equilibrium:

- The direct way, passing from the finite-dimensional reduction.
- The geometric way, constructing a path in the space of boundary data towards a minimizer for the action, counting the intersection of the lifted path with the Maslov cycle of the Lagrangian submanifold Λ that summarizes the equilibrium solutions. Such path also has a remarkable thermodynamical interpretation: we are actuating a *quasistatic transformation*, moving the boundary conditions while keeping the system at equilibrium. The topological features of such transformation, in the dynamical landscape of the system, influence the stability of the equilibrium in exam.

These two computation schemes combined propose some insight on the properties of the system, namely, that the stability of the equilibria of the system is a "shadow" of the topology of the Lagrangian submanifold constructed in the cotangent bundle of the space of boundary data. Also, such topological structure does not depend significantly from the *solutions* of the equations, that act as auxiliary parameters: to be precise, the dimension of the parameter space, finite or infinite may it be, does not influence the topological features of the Lagrangian submanifold, thus, does not influence the stability properties of the system.

To conclude, we wish to remark that the finite reduction also carries some information on the *global* stability properties of the system. In fact, the *appropriate* cutoff N that has to be chosen to make the reduction possible depends only on the spectral properties of $\triangle$ on Ω and the Lipschitz constant C of V'. The cutoff then tells us the minimal number of parameters that must be used to describe the system. Consequently, since the reduction preserves the Morse index, such dimension of the space of parameters gives us a *strict, global upper bound* for the Morse indexes of *every* equilibrium of the system.

These features signal that the reduction is indeed a robust procedure, that gives a faithful skeleton of the thermodynamical theory in study.

Appendix A. A weak infinite-dimensional Maslov–Hörmander theorem

In this section, we state and prove a theorem, that is the infinite-dimensional analogous of the well-known Maslov–Hörmander theorem. The finite-dimensional result is a necessary and sufficient condition that characterizes Lagrangian submanifolds of the cotangent fiber bundle of a manifold, with the introduction of a *generating function* in the sense of Weinstein and Tulczyjew.

Our result is weaker, in the sense that it only provides a necessary condition, which is what we need for the development of the Morse–Smale theory. The reason is that to find a sufficient condition, it is customary to integrate the Liouville 1-form on the submanifold, which cannot be done in infinite dimensions for the lack of a theory of integration of forms.

As far as we know, this theorem is original. Our treatment relies heavily on the infinite-dimensional differential geometry developed in the book by S. Lang [18]. The theory of differential forms on Banach manifolds in the form we need is also proposed and utilized in [18, Chap. V].

Theorem 2. *Let $\mathscr{H}^0$, $\mathscr{H}^{\partial\Omega}$ be two Hilbert spaces, and $J : \mathscr{H}^0 \times \mathscr{H}^{\partial\Omega} \to \mathbb{R}$ a $\mathscr{C}^2$-Fréchet map. Consider the subset of the formal cotangent bundle of $\mathscr{H}^{\partial\Omega}$, $\mathrm{T}^*\mathscr{H}^{\partial\Omega} = (\mathscr{H}^{\partial\Omega}) \times (\mathscr{H}^{\partial\Omega})^* \ni (q, p)$*

$$\Lambda := \{(q,p) : p = \partial_q J[u^0, q],\ 0 = \partial_{u^0} J[u^0, q]\} \tag{A.1}$$

Suppose that the map

$$\mathscr{H}^0 \times \mathscr{H}^{\partial\Omega} \ni (u^0, q) \mapsto \partial_{u^0} J[u^0, q] \in (\mathscr{H}^0)^* \tag{A.2}$$

admits $0 \in (\mathscr{H}^0)^*$ as a regular value*, namely the following condition holds:*

$$\ker \mathrm{d}_{(u^0,q)}(\partial_{u^0} J[u^0, q])|_{0=\partial_{u^0} J[u^0,q]} = \{0\} \tag{A.3}$$

Then:

(1) *There exist locally maps* $\tilde{u}^0 : \mathrm{T}^*\mathscr{H}^{\partial\Omega} \to \mathscr{H}^0$, $\mathscr{C}^2$*-Fréchet, that identically nullify the map defined in* (A.2)*, for the* $(q, p) \in \Lambda$

(2) Λ *is a* Lagrangian submanifold *of* $\mathrm{T}^*\mathscr{H}^{\partial\Omega}$*. This means that every tangent space to* Λ, $\mathrm{T}_\lambda\Lambda$*, is a* maximal isotropic subspace*, or* Lagrangian subspace*, of* $\mathrm{T}_{\iota(\lambda)}\mathrm{T}^*\mathscr{H}^{\partial\Omega}$*, where* $\iota : \Lambda \to \mathrm{T}^*\mathscr{H}^{\partial\Omega}$ *is the embedding defined by* (A.1).

REMARK A.1. The first point of the thesis of the theorem is telling us that the submanifold Λ, that may be tangled up and wildly non-transversal to the fibers of $\mathrm{T}^*\mathscr{H}^{\partial\Omega}$, gets "straightened out" once we see it as a submanifold of the *augmented space* $\mathscr{H}^0 \times \mathrm{T}^*\mathscr{H}^{\partial\Omega}$, namely, it is (locally) the graph of a function $\tilde{u}^0$, and thus, transversal to the fibers.

As a note, we keep the notation we set in the rest of the paper for clarity, but the result is general and does not rely on the particular Hilbert spaces that are chosen.

LEMMA A.2. *If* $0 \in (\mathscr{H}^0)^*$ *is a regular value for the map in* (A.2)*, then* $(0, 0) \in (\mathscr{H}^0)^* \times (\mathscr{H}^{\partial\Omega})^*$ *is a regular value for the map*

$$(u^0, q, p) \mapsto (\partial_{u^0} J[u^0, q], \partial_q J[u^0, q] - p) \tag{A.4}$$

PROOF. First of all, we observe that the differential of the map in (A.2) can be written in block-matrix form

$$\mathrm{d}_{(u^0,q)}(\partial_{u^0} J[u^0, q]) = (\partial^2_{u^0} J[u^0, q] \quad \partial_q\partial_{u^0} J[u^0, q]) \tag{A.5}$$

so that the hypotheses is equivalent to asking that any $(h_{u^0}, h_q) \in \mathscr{H}^0 \times \mathscr{H}^{\partial\Omega}$ that solve the linear system

$$\begin{cases} \partial^2_{u^0} J[u^0, q]|_{0=\partial_{u^0} J[u^0,q]}(h_{u^0}, \cdot) = 0 \\ \partial_q\partial_{u^0} J[u^0, q]|_{0=\partial_{u^0} J[u^0,q]}(h_q, \cdot) = 0 \end{cases} \tag{A.6}$$

are in fact both zero: $(h_{u^0}, h_q) = (0, 0)$. Then, we also write the differential of the map in (A.4):

$$\mathrm{d}_{(u^0,q,p)}(\partial_{u^0} J[u^0, q],\ \partial_q J[u^0, q] - p) = \begin{pmatrix} \partial^2_{u^0} J[u^0, q] & \partial_q\partial_{u^0} J[u^0, q] & \mathbb{O} \\ \partial_{u^0}\partial_q J[u^0, q] & \partial^2_q J[u^0, q] & -\mathbb{1} \end{pmatrix} \tag{A.7}$$

So, $(h_{u^0}, h_q, h_p) \in \ker \mathrm{d}_{(u^0,q,p)}(\partial_u J[u, q], \partial_q J[u, q] - p)|_{0=\partial_u J[u,q]}$ if, and only if, it solves the linear system

$$\begin{cases} \partial^2_{u^0} J[u^0, q]|_{0=\partial_{u^0} J[u^0,q]}(h_{u^0}, \cdot) + \partial_q\partial_{u^0} J[u^0, q]|_{0=\partial_{u^0} J[u^0,q]}(h_q, \cdot) = 0 \\ \partial_{u^0}\partial_q J[u^0, q]|_{0=\partial_{u^0} J[u^0,q]}(h_{u^0}, \cdot) + \partial^2_q J[u^0, q]|_{0=\partial_{u^0} J[u^0,q]}(h_q, \cdot) - h_p = 0 \end{cases} \tag{A.8}$$

But the first equation is solved only for $(h_{u^0}, h_q) = (0, 0)$ by the hypotheses, so that the only surviving term in the second equation is h_p, forcing $h_p = 0$. The only vector in the kernel is $(0,0,0)$, thus $(0,0)$ is a regular value for the map defined in (A.4). □

We also must invoke the following theorem, that can be found in [18, Chap. I, 5.9]

THEOREM 3 (Implicit function). *Let X, Y, Z be Banach spaces, $A \subseteq X \times Y$ open in $X \times Y$ and $f : A \to Z$ a $\mathscr{C}^k$-Fréchet function, $k \geq 1$. Take $(u_0, v_0) \in A$ such that $f(u_0, v_0) = 0$. If $\mathrm{d}_u(f(\cdot, v_0))(u_0)$ is an isomorphism between X and Z, then there exists locally a function $\tilde{u} : Y \to X$ such that*

(1) *$\tilde{u}$ is $\mathscr{C}^k$-Fréchet*
(2) *Locally $f(\tilde{u}(v), v) = 0$*
(3) *Locally, if some u is such that $f(u, v) = 0$, then $u = \tilde{u}(v)$*

We are now ready for the proof of Theorem 2.

PROOF. (1) We must verify that we are in the hypotheses of Theorem 3. The Lemma will be important for this purpose, and also the request that the spaces are not only Banach, but also Hilbert, giving us reflexivity and in particular the Riesz representation theorem.

First of all, we compose the map (A.2) with the Riesz isomorphism, defining $\partial_{u^0} J[u^0, q]h =: \langle \nabla_{u^0} J[u^0, q], h \rangle_{\mathscr{H}^0}$, $\forall h \in \mathscr{H}^0$, obtaining:

$$\mathscr{H}^0 \times \mathscr{H}^{\partial\Omega} \ni (u^0, q) \mapsto \nabla_{u^0} J[u^0, q] \in \mathscr{H}^0 \tag{A.9}$$

We know that the differential of this map is at least injective, when evaluated on the set $\{(u^0, q) : 0 = \nabla_{u^0} J[u^0, q]\}$. The Lemma assures us that this fact also translates to the map in the augmented space, namely, also via Riesz representation, the following map

$$\mathscr{H}^0 \times \mathrm{T}^*\mathscr{H}^{\partial\Omega} \ni (u^0, q, p) \mapsto (\nabla_{u^0} J[u^0, q], \nabla_q J[u^0, q] - p^\#) \in \mathscr{H}^0 \times \mathscr{H}^{\partial\Omega} \tag{A.10}$$

where we have defined $\langle p^\#, q \rangle_{\mathscr{H}^{\partial\Omega}} = p(q)$ (in this case, the "musical isomorphism" is the same as Riesz isomorphism), is injective on the set

$$\{(u^0, q, p) : p^\# = \nabla_q J[u^0, q],\ 0 = \nabla_{u^0} J[u^0, q]\} \tag{A.11}$$

which is simply Λ seen in the augmented space.

To use Theorem 3 to extract a map $\tilde{u}^0 : \mathrm{T}^*\mathscr{H}^{\partial\Omega} \to \mathscr{H}^0$ from the function defined in (A.10), we have to verify that the differential, evaluated on the $(q, p) \in \Lambda$, is not only injective (guaranteed by the Lemma), but also surjective. To do this, consider the evaluated map

$$\Phi := \mathrm{d}_{(u^0, q, p)}(\nabla_{u^0} J[u^0, q], \nabla_q J[u^0, q] - p^\#)(\cdot, h_q, h_p) : \mathscr{H}^0 \to \mathscr{H}^0 \tag{A.12}$$

We know that $\ker\Phi = 0$. Also, using the first isomorphism theorem (which also holds in infinite dimensions),

$$\mathscr{H}^0 = \ker\Phi \oplus \operatorname{im}\Phi \tag{A.13}$$

and thus in our case $\mathscr{H}^0 = \operatorname{im}\Phi$, proving surjectivity. We are in the hypotheses of Theorem 3, so we know there exists locally a function $\tilde{u}^0 : \mathrm{T}^*\mathscr{H}^{\partial\Omega} \to \mathscr{H}^0$ that satisfies

(1) $\tilde{u}^0$ is $\mathscr{C}^2$-Fréchet
(2) locally on Λ, $(\partial_{u^0} J[\tilde{u}^0(q,p),q] \equiv 0,\ \partial_q J[\tilde{u}^0(q,p),q] - p \equiv 0])$
(3) also if the preceding equations are satisfied by some u, then u is the image under $\tilde{u}^0$ of some (q,p)

and in particular, we have that the submanifold defined by such equations in $\mathscr{H}^0 \times \mathrm{T}^*\mathscr{H}^{\partial\Omega}$ is the graph of $\tilde{u}^0 : \{\tilde{u}^0(q,p) : (q,p) \in \Lambda\}$

(2) We now show that, given the existence of the function $\tilde{u}^0$, the pull-back on Λ of the canonical symplectic form

$$\begin{aligned}\omega_{(q,p)}((Q_1,P_1),(Q_2,P_2)) &= P_1(Q_2) - P_2(Q_1)\\ &= \langle P_1^\#, Q_2\rangle_{\mathscr{H}^{\partial\Omega}} - \langle P_2^\#, Q_1\rangle_{\mathscr{H}^{\partial\Omega}}\end{aligned} \tag{A.14}$$

where $(q,p) \in \mathrm{T}^*\mathscr{H}^{\partial\Omega}$ is thought as a base point and $(Q_i,P_i) \in \mathrm{T}_{(q,p)}\mathrm{T}^*\mathscr{H}^{\partial\Omega}$ are thought as tangent vectors, is identically zero, showing that at least, the tangent spaces to Λ are all *isotropic*.

The situation is the following:

$$\begin{tikzcd} \Lambda \arrow[r, hook, "\imath"] & \mathrm{T}^*\mathscr{H}^{\partial\Omega} \\ \mathrm{T}\Lambda \arrow[u, "\pi_\Lambda"] \arrow[r, "\mathrm{T}\imath"] & \mathrm{TT}^*\mathscr{H}^{\partial\Omega} \arrow[u, "\pi_{\mathrm{T}^*\mathscr{H}^{\partial\Omega}}"'] \end{tikzcd} \qquad \begin{cases} \lambda \mapsto \imath(\lambda) = (q(\lambda), \partial_q J[\tilde{u}^0(q,p), q(\lambda)]) \\ (\lambda, h_\lambda) \mapsto \mathrm{T}\imath(\lambda,h_\lambda) = (\imath(\lambda), \mathrm{d}\imath(\lambda)h_\lambda) \end{cases} \tag{A.15}$$

where h_λ denotes a vector in $\mathrm{T}_\lambda\Lambda$ and $\mathrm{d}\imath(\lambda)$ the Fréchet differential of $\imath$, calculated in λ. The pull-back of ω under $\imath$ is

$$\imath^*\omega_\lambda(h_\lambda,k_\lambda) = \omega_{\imath(\lambda)}(\mathrm{d}\imath(\lambda)h_\lambda, \mathrm{d}\imath(\lambda)k_\lambda) \tag{A.16}$$

Denote with $\mathrm{d}_q\tilde{u}^0$ the Fréchet differential of $\tilde{u}^0$ in the q component. First, notice that $\mathrm{d}\imath(\lambda)h_\lambda$ has a q and a p component. The q component is clearly $\mathrm{d}q(\lambda)h_\lambda$, while the p component is

$$\partial_{u^0}\partial_q J[\tilde{u}^0(q,p),q](\mathrm{d}_q\tilde{u}^0(q,p)\,\mathrm{d}q(\lambda)h_\lambda,\cdot) + \partial_q^2 J[\tilde{u}^0(q,p),q](\mathrm{d}q(\lambda)h_\lambda,\cdot) \tag{A.17}$$

Now, $\partial_{u^0} J[\tilde{u}^0(q,p),q] \equiv 0$ by the definition of $\tilde{u}^0$, so we are left with

$$\mathrm{d}\imath(\lambda)h_\lambda = (\mathrm{d}q(\lambda)h_\lambda, \partial_q^2 J[\tilde{u}^0(q,p),q](\mathrm{d}q(\lambda)h_\lambda,\cdot)) \tag{A.18}$$

and now we substitute:

$$
\begin{aligned}
\imath^*\omega_\lambda(h_\lambda,k_\lambda) &= -\langle \partial_q^2 J|_{\dots}(\mathrm{d}q(\lambda)h_\lambda,\cdot)^\#, \mathrm{d}q(\lambda)k_\lambda\rangle_{\mathscr{H}^{\partial\Omega}} \\
&\quad + \langle \partial_q^2 J|_{\dots}(\mathrm{d}q(\lambda)k_\lambda,\cdot)^\#, \mathrm{d}q(\lambda)h_\lambda\rangle_{\mathscr{H}^{\partial\Omega}} \\
&= -\partial_q^2 J[\tilde{u}^0(q,p),q](\mathrm{d}q(\lambda)h_\lambda, \mathrm{d}q(\lambda)k_\lambda) \\
&\quad + \partial_q^2 J[\tilde{u}^0(q,p),q](\mathrm{d}q(\lambda)k_\lambda, \mathrm{d}q(\lambda)h_\lambda) \\
&\equiv 0
\end{aligned} \tag{A.19}
$$

where J is evaluated in $(\tilde{u}^0(q,p),q)$.

To prove maximality, we use the following characterization, given in the form of a

LEMMA A.3. *Let H be a Hilbert space and $\omega: H\times H\to\mathbb{R}$ the canonical symplectic form. Take a subspace L of H and define its ω*-annihilator

$$
L^\S := \{h\in H : \omega(h,l)=0,\ \forall l\in L\} \tag{A.20}
$$

Then L is a Lagrangian subspace, namely, the maximal isotropic subspace of H, if and only if $L^\S = L$.

PROOF. The proof is based on the ideas found in the beginning of [15]. Some preliminary remarks: first of all, it is a well known fact that the existence of a symplectic form on H implies that there is an orthogonal isomorphism $\mathbb{J}: H\to H$ that satisfies $\omega(h,k)=\langle \mathbb{J}h,k\rangle$ and $\mathbb{J}^2=-\mathbb{1}$ ([18, Chap. 5, Par. 6]). Notice that through such isomorphism clearly $L^\S=(\mathbb{J}L)^\perp$, where $\perp$ is the orthogonality with respect to the scalar product $\langle\cdot,\cdot\rangle$. Secondly, for any subspace K, $K^\S$ is closed, and for any subset $S\subset H$, $(S^\S)^\S=\overline{S}$.

Now, suppose $L^\S=L$, and, by absurd, that there is another isotropic subspace $\hat{L}$ of H that contains it: $L\subset\hat{L}$. This implies $\hat{L}^\perp\subset L^\perp$. Now, since $\hat{L}$ is isotropic, necessarily $\hat{L}\perp\mathbb{J}\hat{L}$, that is, $\mathbb{J}\hat{L}\subset\hat{L}^\perp$. This means that $\mathbb{J}\hat{L}\subset L^\perp$, and passing to the orthogonals, $L^\S=L\subset(\mathbb{J}\hat{L})^\perp=\hat{L}^\S$, which is equivalent to saying $\mathbb{J}\hat{L}\subset\mathbb{J}L$. But $\mathbb{J}$ is bijective, so $\hat{L}\subset L$, bringing us to the conclusion that $\hat{L}=L$.

Conversely, suppose L maximally isotropic. Also $L^\S$ is isotropic, and as before we have that $L\perp\mathbb{J}L\Rightarrow\mathbb{J}L\subset L^\perp\Rightarrow L\subset(\mathbb{J}L)^\perp\Rightarrow L\subset L^\S$ and for maximality we may conlude $L^\S=L$. □

To finish the proof it suffices to control that $\forall\lambda\in\Lambda$, $\mathrm{T}_\lambda\Lambda$ coincides with its ω-annihilator when seen as a subspace of $\mathrm{T}_{\imath(\lambda)}\mathrm{T}^*\mathscr{H}^{\partial\Omega}$, that is, we must control that $[\mathrm{d}\imath(\lambda)(\mathrm{T}_\lambda\Lambda)]^\S=\mathrm{d}\imath(\lambda)(\mathrm{T}_\lambda\Lambda)$. To simplify notation: $H=\mathrm{T}_{\imath(\lambda)}\mathrm{T}^*\mathscr{H}^{\partial\Omega}$, $L=\mathrm{d}\imath(\lambda)(\mathrm{T}_\lambda\Lambda)$. Surely $L\subset L^\S$ because ω pulled-back on Λ is identically zero. Finally, restate $L=L^\S$ as $L^\perp=\mathbb{J}L$. Since we are dealing with Hilbert spaces, and not with genuine Hilbert manifolds, $\mathbb{J}$ can be written in a block-matrix form, starting from its action on two generic vectors:

$$
\omega((Q_1,P_1),(Q_2,P_2)) = P_1(Q_2)-P_2(Q_1) \equiv (Q_1\ P_1)\begin{pmatrix}\mathbb{0} & \mathbb{1}\\ -\mathbb{1} & \mathbb{0}\end{pmatrix}\begin{pmatrix}Q_2\\ P_2\end{pmatrix} \tag{A.21}
$$

thus the image of L under $\mathbb{J}$ is characterized this way:

$$(Q, P) \in \mathbb{J}L \Leftrightarrow Q = \partial_q^2 J[\tilde{u}^0(q, p), q](\mathrm{d}q(\lambda)h_\lambda, \cdot)^\#, \quad P^\# = -\mathrm{d}q(\lambda)h_\lambda \ \forall h_\lambda \tag{A.22}$$

Moreover, the natural Hilbert structure on H is the cartesian product one, namely

$$\begin{aligned} H &\cong \mathscr{H}^{\partial\Omega} \times (\mathscr{H}^{\partial\Omega})^* \\ &\Rightarrow \langle (Q_1, Q_2), (P_1, P_2) \rangle_H = \langle Q_1, Q_2 \rangle_{\mathscr{H}^{\partial\Omega}} + \langle P_1^\#, P_2^\# \rangle_{\mathscr{H}^{\partial\Omega}} \end{aligned} \tag{A.23}$$

The orthogonal to L now can be explicited: take

$$\begin{aligned} &(\mathrm{d}q(\lambda)h_\lambda, \partial_q^2 J[\tilde{u}^0(q, p), q]) \in L, \quad \text{so } (Q, P) \in L^\perp \\ &\Rightarrow \langle Q, \mathrm{d}q(\lambda)h_\lambda \rangle_{\mathscr{H}^{\partial\Omega}} = -\langle P^\#, \partial_q^2 J[\tilde{u}^0(q, p), q](\mathrm{d}q(\lambda)h_\lambda, \cdot)^\# \rangle_{\mathscr{H}^{\partial\Omega}} \\ &\Rightarrow Q = \partial_q^2 J[\tilde{u}^0(q, p), q](\mathrm{d}q(\lambda)h_\lambda, \cdot)^\#, \quad P^\# = -\mathrm{d}q(\lambda)h_\lambda \ \forall h_\lambda \end{aligned} \tag{A.24}$$

thus surely $L^\perp \subset \mathbb{J}L \Leftrightarrow L \supset (\mathbb{J}L)^\perp = L^\S$. This concludes the proof. □

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