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Integral representations of the Schrödinger Propagator

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Introduzione

Questa tesi di Dottorato indaga, da un punto di vista nuovo, l'equazione di Schrödinger e le sue soluzioni,

$$\begin{cases} i\hbar\partial_t\psi(t,x) = \left(-\dfrac{\hbar^2}{2m}\Delta + V(x)\right)\psi(t,x) \\ \\ \psi(0,x) = \varphi(x) \in H^2(\mathbb{R}^n) \end{cases} \tag{1}$$

dove $V \in C^2(\mathbb{R}^n)$ è una funzione di energia potenziale a supporto compatto, modellizzante per esempio problemi di scattering. Come è noto la soluzione di questo problema di Cauchy si esprime mediante la formula

$$\psi(t) = U(t)\varphi,$$

dove $U(t) = e^{-\frac{i}{\hbar}tH}$ è il ben noto Propagatore di Schrödinger, corrispondente al gruppo di operatori lineari unitari generato dall'Hamiltoniano quantistico $H = -\frac{\hbar^2}{2m}\Delta + V(x)$.
Lo scopo centrale di questa tesi è quello di costruire una classe di rappresentazioni integrali per una opportuna ε-regolarizzazione $U_\varepsilon(t)$, mostrando successivamente l'attesa convergenza $U_\varepsilon(t)\varphi \xrightarrow[\varepsilon\to 0^+]{} U(t)\varphi$. Precisamente, viene introdotto il Propagatore regolarizzato,

$$U_\varepsilon(t) := e^{-\frac{i+\varepsilon}{\hbar}tH_\varepsilon},$$

dove il generatore di tale semigruppo è definito da $H_\varepsilon := -\frac{\hbar^2}{2m}\Delta - \frac{V}{(i+\varepsilon)^2}$, e per il quale si dimostra la seguente proprietà di convergenza forte:

$$U(t)\varphi \overset{L^2(\mathbb{R}^n)}{=} \lim_{\varepsilon\to 0^+} U_\varepsilon(t)\varphi, \qquad \forall\varphi \in H^2(\mathbb{R}^n), \quad \forall t \geq 0. \tag{2}$$

Il risultato principale della tesi consiste nella rappresentazione,

$$U_\varepsilon(t)\varphi(x) = \int_{\mathbb{R}^n} U_\varepsilon(t,x,y)\varphi(y)\ dy,$$

il cui nucleo si costruisce mediante una classe di integrali oscillanti:

$$U_\varepsilon(t,x,y) = \int_{\mathbb{R}^k} e^{\frac{i}{(1+\varepsilon^2)\hbar}S(t,x,y,u)}\rho_\varepsilon^\hbar(t,x,y,u)\ du. \tag{3}$$

In questo tipo di rappresentazioni integrali risulta centrale l'utilizzo della classe delle *funzioni generatrici S (debolmente) quadratiche all'infinito* relative alla famiglia di sottovarietà Lagrangiane, grafico di Trasformazioni Canoniche,

$$\begin{aligned}\Lambda_t \quad &:= \big\{(y,\xi;x,p) \in T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n : (x,p) = \phi_H^t(y,\xi)\big\} \\ &= \big\{(y,\xi;x,p) \in T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n : p = \nabla_x S, \quad \xi = -\nabla_y S, \quad 0 = \nabla_u S\big\},\end{aligned} \tag{4}$$

Tali funzioni generatrici, introdotte e usate da Chaperon, Laudenbach, Sikorav e Viterbo, sono oggetti tipici della *topologia simplettica* e ricorrono in molte questioni di Calcolo delle Variazioni, di Teoria di Morse e di Lusternik-Schnirelman. Il loro uso sistematico nell'attuale ambiente (Schrödinger, Integrali Oscillanti) appare nuovo, anche rispetto alla vicina teoria degli Operatori Integrali di Fourier.
Nella (4) ϕ_H^t è il gruppo di trasformazioni canoniche da $T^\star\mathbb{R}^n$ in $T^\star\mathbb{R}^n$ che risolve le equazioni relative all'Hamiltoniana classica $H(x,p) = \frac{p^2}{2m} + V(x)$. In altre parole, $(x,p)(t) := \phi_H^t(y,\xi)$ risolve:

$$\begin{cases} \dot{x} = \nabla_p H(x,p), \\ \\ \dot{p} = -\nabla_x H(x,p). \end{cases} \tag{5}$$

La costruzione di questi integrali oscillanti si realizza per mezzo di serie di operatori fortemente convergenti al Propagatore regolarizzato,

$$U_\varepsilon(t)\varphi = \sum_{j=0}^{\infty} B_{\varepsilon,j}(t)\varphi, \tag{6}$$

i cui termini ammettono rappresentazioni integrali con nuclei

$$B_{\varepsilon,j}(t,x,y) = \int_{\mathbb{R}^k} e^{\frac{i}{(1+\varepsilon^2)\hbar} S(t,x,y,u)} \rho_{\varepsilon,j}^{\hbar}(t,x,y,u)\, du, \tag{7}$$

e dove le funzioni $\rho_{\varepsilon,j}^{\hbar} \in L^1(\mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^k;\mathbb{C})$, $\forall\varepsilon > 0$, $\forall j \geq 0$, definiscono una serie L^1 convergente:

$$\sum_{j=0}^{\infty} \rho_{\varepsilon,j}^{\hbar} = \rho_\varepsilon^{\hbar} \in L^1(\mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^k;\mathbb{C}).$$

Queste considerazioni permettono di dedurre che il nucleo del Propagatore regolarizzato $U_\varepsilon(t)$ si rappresenta mediante un'integrale oscillante di fase S e di ampiezza complessa $\rho_\varepsilon^{\hbar}$ dipendente dalla scelta di S, ottenendo cosí la rappresentazione (3) sopra annunciata.
Un'importante conseguenza dell'esistenza di questa ampia classe di rappresentazioni consiste in una formulazione finito-dimensionale di Path Integral del Propagatore. Precisamente, facendo riferimento ad un risultato dimostrato in [7], il Funzionale d'Azione classico del Calcolo delle Variazioni

$$A[\gamma] = \int_0^t \frac{1}{2} m\, |\dot{\gamma}(s)|^2 - V(\gamma(s))\, ds,$$

ammette una riduzione finito dimensionale (in cui lo spazio delle curve $\Gamma(t,x,y) \subset H^1([0,t];\mathbb{R}^n)$ ha la struttura di varietà finito-dimensionale $\Gamma \simeq \mathbb{R}^k$). Il funzionale così ridotto rappresenta una funzione generatrice S per Λ_t. Applicando i risultati generali esposti sopra a questo caso particolare di funzione generatrice dimostriamo la seguente formula di rappresentazione

$$U_\varepsilon(t,x,y) = \int_{\Gamma(t,x,y)} e^{\frac{i}{(1+\varepsilon^2)\hbar}A[\gamma]}\, P_\varepsilon^\hbar(d\gamma), \tag{8}$$

dove la misura $P_\varepsilon^\hbar(d\gamma)$ viene definita come immagine della misura di Lebesgue complessa $\rho_\varepsilon^\hbar(t,x,y,u)du$.

È importante sottolineare come la costruzione di questa classe di rappresentazioni integrali sia globale nel tempo avendo evitato, con questa tecnica, i problemi legati alla comparsa delle caustiche. Questo corrisponde al noto problema della non trasversalità delle sottovarietà Lagrangiane Λ_t rispetto alla varietà base $\mathbb{R}^n \times \mathbb{R}^n$, il quale compare dopo un tempo critico e che come conseguenza non permette l'esistenza di una funzione generatrice globale $S(t,x,y)$ (cioè senza parametri ausiliari). In questa tesi viene appunto risolto questo problema utilizzando la classe delle funzioni generatrici $S(t,x,y,u)$ con parametri ausiliari $u \in \mathbb{R}^k$, generanti la sottovarietà Lagrangiana Λ_t, anche in presenza di caustiche.

Differenti tecniche sono state usate per determinare rappresentazioni del Propagatore di Schrödinger. Nelle prime formulazioni del metodo WKB [20], [22] si rappresenta la soluzione ψ dell'equazione (1) nella forma

$$\psi(t,x) = A_\hbar(t,x)e^{\frac{i}{\hbar}S(t,x)}.$$

In questa formula la *funzione di fase* S, definita solamente per $t \in [0,t_0]$ con t_0 abbastanza piccolo (relativo alla non esistenza di caustiche), risolve l'equazione di Hamilton-Jacobi:

$$\frac{|\nabla S(t,x)|^2}{2m} + V(x) + \partial_t S(t,x) = 0,$$

e la *funzione ampiezza reale* ammette uno sviluppo formale $A_\hbar(t,x) = \sum_{j=0}^{\infty} \hbar^j A_j(t,x)$, nel quale i temini sono ottenuti per mezzo di una relazione ricorsiva e dove il termine di ordine zero risolve l'equazione del trasporto:

$$\partial_t A_0(t,x) + \nabla_x S(t,x)\cdot\nabla_x A_0(t,x) + \frac{1}{2}\Delta_x S(t,x)A_0(t,x) = 0.$$

Il problema delle soluzioni globali nel tempo è affrontato nella teoria dell'Operatore Canonico di Tunnel, [22], e nella teoria degli Operatori Integrali Fourier, sviluppatasi ad opera di Hörmander [11] e Duistermaat [9] (per i risultati più recenti ved.[5], [15], [17], [6], [10]). Altri approcci al problema impiegano le funzioni e misure di Wigner, e.g. [31]. Rispetto a queste tecniche una delle differenze salienti con questo lavoro consiste nel tipo di funzioni generatrici considerate. Mentre nella teoria degli Operatori Integrali di Fourier vengono utilizzate sistematicamente varietà Lagrangiane *coniche*, cioè generate da funzioni $1-$omogenee, in questo approccio, come già accennato, assumono un ruolo centrale le funzioni generatrici *quadratiche all'infinito*. In senso lato, mentre nel primo approccio si generalizza l'operazione di *trasformata di Fourier*, nel secondo il riferimento euristico lo si può ritrovare negli *integrali di Fresnel*.

Rispetto al problema di rappresentare il Propagatore di Schrödinger con integrali definiti su spazi di curve, noti come Path Integrals, vi sono numerosi approcci (e.g. [2], [25], [12]). In particolare Albeverio and Mazzucchi [2] hanno dimostrato recentemente una rappresentazione esatta mediante la teoria degli integrali di Fresnel infinito dimesionali, che rende rigorosa la formulazione dell'integrale di Feymann. Segnaliamo infine il lavoro di Robbin and Salomon, [25], che nel caso particolare di Hamiltoniani quadratici hanno ottenuto un Path Integral finito dimensionale in connessione con la rappresentazione metaplettica del Propagatore.

La struttura della tesi è la seguente. Dopo alcuni preliminari iniziali, il capitolo 1 sviluppa alcuni risultati generali circa l'espansione in serie per semigruppi C_0 di operatori lineari. Questi risultati non dipendono dalla particolare scelta del generatore e saranno applicati al capitolo 4 al caso centrale del Propagatore di Schrödinger. Prima di fare questo è necessario dimostrare alcuni teoremi riguardanti una larga classe di funzioni generatrici delle sottovarietà Lagrangiane Λ_t, che verranno usate come funzioni di fase per costruire gli integrali oscillanti. A questo scopo nel capitolo 2 si ricorda la definizione delle *funzioni generatrici debolmente quadratiche all'infinito* (GFWQI). Di seguito, utilizzando un risultato di Viterbo [34] che riguarda l'equivalenza di due funzioni GFWQI, si prova che per $V \in C^2(\mathbb{R}^n)$ a supporto compatto, esiste una GFWQI per la sottovarietà Lagrangiana Λ_t e ne viene mostrata la forma esplicita. Il passo successivo, il capitolo 3, è quello di introdurre una famiglia di operatori integrali associati alla classe funzioni generatrici studiate nel capitolo precedente, i quali ammettono kernel $b(t,x,y) = \int_{\mathbb{R}^k} e^{i\lambda S(t,x,y,u)} \rho(t,x,y,u)\; du$, $\lambda \in \mathbb{R}$. In particolare, vengono studiate alcune operazioni fra tali operatori, provando che questa famiglia è chiusa rispetto all'operazione di composizione. Infine, nel capitolo 4, vengono applicati i risultati ottenuti nei capitoli precedenti al Propagatore $e^{-\frac{i+\varepsilon}{\hbar} t H_\varepsilon}$, derivando l'esistenza di un insieme di sviluppi in serie di operatori i quali ammettono rappresentazioni mediante la famiglia degli integrali oscillanti introdotta. L'ultimo teorema riguarda il caso speciale nel quale viene utilizzato il funzionale d'Azione $A[\gamma]$ come funzione generatrice, che permette di realizzare, a partire dalla formulazione generale, una rappresentazione di Path Integral finito dimensionale per ψ_ε.

Introduction

In this Phd Thesis we consider the Schrödinger equation

$$\begin{cases} i\hbar\partial_t\psi(t,x) = \left(-\dfrac{\hbar^2}{2m}\Delta + V(x)\right)\psi(t,x), \\ \\ \psi(0,x) = \varphi(x) \in H^2(\mathbb{R}^n), \end{cases} \tag{9}$$

where $V \in C^2(\mathbb{R}^n)$ is a compact support energy potential function, e.g. modelizing a one particle scattering problem. As known the solution of this Cauchy problem can be represented by the formula

$$\psi(t) = U(t)\varphi,$$

where $U(t) = e^{-\frac{i}{\hbar}tH}$ is called Schrödinger Propagator, that corresponds to the group of unitary linear operators generated from the quantistic Hamiltonian $H = -\frac{\hbar^2}{2m}\Delta + V(x)$.
The central aim of this Thesis is to construct a class of integral representations for a suitable ε-regularization $U_\varepsilon(t)$, showing afterwards the expected convergence $U_\varepsilon(t)\varphi \xrightarrow[\varepsilon\to 0^+]{} U(t)\varphi$.
More precisely, it is introduced the regularized Propagator,

$$U_\varepsilon(t) := e^{-\frac{i+\varepsilon}{\hbar}tH_\varepsilon},$$

where the generator of this semigroup is defined as $H_\varepsilon := -\frac{\hbar^2}{2m}\Delta - \frac{V}{(i+\varepsilon)^2}$, and for which it is proved the following property of strong convergence:

$$U(t)\varphi \overset{L^2(\mathbb{R}^n)}{=} \lim_{\varepsilon\to 0^+} U_\varepsilon(t)\varphi, \qquad \forall\varphi \in H^2(\mathbb{R}^n), \quad \forall t \geq 0. \tag{10}$$

the main result of this Thesis consists in the representation,

$$U_\varepsilon(t)\varphi(x) = \int_{\mathbb{R}^n} U_\varepsilon(t,x,y)\varphi(y)\ dy,$$

where the kernel is constructed throught a class of oscillating integrals:

$$U_\varepsilon(t,x,y) = \int_{\mathbb{R}^k} e^{\frac{i}{(1+\varepsilon^2)\hbar}S(t,x,y,u)}\rho_\varepsilon^\hbar(t,x,y,u)\ du. \tag{11}$$

In this type of representation it is important the use of the class of *generating function S (weakly) quadratic at infinity* relative to the family of Lagrangian submanifolds, graph of Canonical Transformation,

$$\begin{aligned}\Lambda_t &:= \big\{(y,\xi;x,p) \in T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n : (x,p) = \phi_H^t(y,\xi)\big\} \\ &= \big\{(y,\xi;x,p) \in T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n : p = \nabla_x S, \quad \xi = -\nabla_y S, \quad 0 = \nabla_u S\big\},\end{aligned} \tag{12}$$

These generating function, introduced and used by Chaperon, Laudenbach, Sikorav e Viterbo, are tipical objects of *symplectic topology* and arises in many questions of Calculus of Variations, Morse Theory and Lusternik-Schnirelman Theory. Their frequent use in the actual framework (Schrödinger, Oscillating Integrals) is new, even respect to the near theory of Fourier Integral Operator.
In (12) ϕ_H^t is the group of canonical transformations from $T^\star\mathbb{R}^n$ in $T^\star\mathbb{R}^n$ that solves the related Hamilton's equations for $H(x,p) = \frac{p^2}{2m} + V(x)$. In others words, $(x,p)(t) := \phi_H^t(y,\xi)$ solves:

$$\begin{cases} \dot{x} = \nabla_p H(x,p), \\ \\ \dot{p} = -\nabla_x H(x,p). \end{cases} \tag{13}$$

The construction of this type of integrals it is realized by series of operators strongly convergent to the regularized Propagator,

$$U_\varepsilon(t)\varphi = \sum_{j=0}^{\infty} B_{\varepsilon,j}(t)\varphi, \tag{14}$$

where the terms admits integral representations with kernels

$$B_{\varepsilon,j}(t,x,y) = \int_{\mathbb{R}^k} e^{\frac{i}{(1+\varepsilon^2)\hbar}S(t,x,y,u)} \rho_{\varepsilon,j}^\hbar(t,x,y,u)\; du, \tag{15}$$

and where the functions $\rho_{\varepsilon,j}^\hbar \in L^1(\mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^k;\mathbb{C})$, $\forall\varepsilon > 0$, $\forall j \geq 0$, define an L^1-convergent series:

$$\sum_{j=0}^{\infty} \rho_{\varepsilon,j}^\hbar = \rho_\varepsilon^\hbar \;\in L^1(\mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^k;\mathbb{C}).$$

These considerations permit us to realize that the kernel of the regularized Propagator $U_\varepsilon(t)$ can be represented by an oscillating integral of phase function S and complex amplitude $\rho_\varepsilon^\hbar$ depending on the choice of S, obtaining in this way the representation (11) announced above.
An important conseguence of the existence of this type of representations consists in a finite dimensional Path Integral formulation of the Propagator. More precisely in [7] it has been proved that the classical mechanical Action functional

$$A[\gamma] = \int_0^t \frac{1}{2}m\,|\dot{\gamma}(s)|^2 - V(\gamma(s))\,ds,$$

evaluated on an suitable space of curves $\Gamma(t,x,y) \subset H^1([0,t];\mathbb{R}^n)$, that it is in fact a finite dimensional manifold, corresponds to a weakly quadratic global generating function S for Λ_t.

Applying the general results descripted above in this particular case of generating function we prove the following representation:

$$U_\varepsilon(t,x,y) = \int_{\Gamma(t,x,y)} e^{\frac{i}{(1+\varepsilon^2)\hbar}A[\gamma]}\, P_\varepsilon^\hbar(d\gamma) \tag{16}$$

Where $P_\varepsilon^\hbar(d\gamma)$ is well defined, as the complex image measure of $\rho_\varepsilon^\hbar(t,x,y,u)du$ on $\Gamma(t,x,y)$. It is important to point out that the construction (11) is global in time, overcoming the problem related to the occurrence of caustics. This is the well known problem of the non-transversality of the Lagrangian submanifolds Λ_t that occours after a critical time, and this behaviour does not permit the existence of a global generating function $S(t,x,y)$ (without auxiliary parameters). We overtake this problem by using the direct generalizations of this function, namely the class of global generating functions $S(t,x,y,u)$ involving auxiliary parameters $u \in \mathbb{R}^k$ that permit, as shown in (12), to generate the entire Lagrangian submanifold even in the presence of non-transversality.

Different techniques have been used to find representations of the Schrödinger Propagator. First of all we mention the WKB methods [20], [22] where the solution of (9) is represented as

$$\psi(t,x) = A_\hbar(t,x)e^{\frac{i}{\hbar}S(t,x)}.$$

In this formula the *phase function* S, that it is defined only for $t \in [0,t_0]$ with t_0 small enough (relative to the nonexistence of caustics) solves the Hamilton-Jacobi's equation:

$$\frac{|\nabla S(t,x)|^2}{2m} + V(x) + \partial_t S(t,x) = 0,$$

and the *real amplitude function* admits a formal expansion $A_\hbar(t,x) = \sum_{j=0}^\infty \hbar^j A_j(t,x)$, where the terms are obtained through a ricoursive relation and where the zero order term solves the transport equation:

$$\partial_t A_0(t,x) + \nabla_x S(t,x)\cdot\nabla_x A_0(t,x) + \frac{1}{2}\Delta_x S(t,x)A_0(t,x) = 0.$$

The problem of the solution global in time it has been faced in the theory of Tunnel Canonical Operator, [22], and in the theory of Fourier Integral Operators developed by Hörmander [11] and Duistermaat [9](for more recently results see [5], [15], [17], [6], [10]). Other results have been obtained by the use of Wigner Functions and Wigner Measures, see for example [31]. With respect to this techniques one of the most important differents with this work corresponds to the type of generating functions considered. While in the theory of Fourier Integral Operators are always used conic Lagrangian manifold, that is generated by 1-omogeneous functions, in this approach the generating functions quadratic at infinity have a central role. While in the first approach it is generalized the operation of *Fourier transform*, in the second an heuristic connection can be found in *Fresnel integrals*.
Respect to the problem to represent the Schrödinger Propagator with integrals defined on spaces of curves, known as Path Integrals, there are several approaches (for example [2], [25], [12]). In particular Albeverio and Mazzucchi [2] proved an exact representation by the use of infinite dimensional Fresnel integrals, that provide a rigourus formulaton of Feynman integral.

We mention the work of Robbin and Salomon [25] that in the case of quadratic Hamiltonians obtained a finite dimensional phase space Path Integral in connection with metaplectic representation.

The plan of our paper is the following. In chapter 1, after some preliminaries, we developes some general results about series expansion for C_0-semigroup of linear operators. These results are not depending of the particular choice of the generator and will be applied in chapter 4 to the central case of the Schrödinger group. Before to do this we have to develop some machinery about generating functions, that are the basic ingredient in order to build the integral representation. To this purpose, in chapter 2 we first recall the definition of *generating function weakly quadratic ad infinity* (GFWQI). Then, following a result by Viterbo [34] about equivalence of two GFWQI, we prove that, under suitable assumption on potential V, there exists a GFWQI for the Lagrangian submanifold Λ_t. The next step, chapter 3, is to introduce a family of integral operators of the type we will use for our representation, that is, integral operators with kernel $b(t,x,y) = \int_{\mathbb{R}^k} e^{i\lambda S(t,x,y,u)}\rho(t,x,y,u)\ du$, $\lambda \in \mathbb{R}$. In particular, we study some operations among such operators, proving that this family is closed under these operations. Finally, in chapter 4, we apply the previous machinery to the semigroup $e^{-\frac{i+\varepsilon}{\hbar}tH_\varepsilon}$ and we derive the existence of $\rho_\varepsilon^\hbar$ by following the plane drawn above. The last theorem goes to the special case in which we apply the integral representation to the functional given by the classical mechanical action, that is, $A[\gamma]$. This allows us to derive a finite dimensional path integral representation of ψ_ε.

Chapter 1

Series expansions for semigroups of linear operators

1.1 Introduction

In all this chapter we will assume that $L : D(L) \subset \mathcal{X} \longrightarrow \mathcal{X}$ is a infinitesimal generator of a C_0-semigroup $\{e^{tL}\}_{t\geq 0}$ on a Banach space $\mathcal{X}$. In particular, L is a densely defined linear operator satisfying the hypotheses of Hille–Yoshida theorem.
It is well known that if $L \in \mathcal{L}(\mathcal{X})$ the series expansion,

$$e^{tL} = \sum_{j=0}^{\infty} \frac{(tL)^j}{j!}, \tag{1.1}$$

holds true (and, indeed, this is a way to define the semigroup). However, this series does not makes sense, generally, if L is an unbounded operator generating a C_0-semigroup.
The main aim of this first chapter is to prove that the semigroup of linear operators e^{tL}, generated by an arbitrary (generally unbounded) operator L, admits a general set of series expansions:

$$e^{tL} = \sum_{j=0}^{+\infty} B_j(t), \tag{1.2}$$

that of course, in the case of bounded L, contains the particular series (1.1). It will be shown that the set of all this series expansions has the structure of infinite dimesional affine space. Moreover we will show how each series (1.2) changes after bounded variation of the generator, namely if we consider $L + K$ where K is any bounded linear operator.

1.2 Preliminaries and settings

In the following $\mathcal{X}$ will denote a Banach space, $\mathcal{H}$ an Hilbert space. If $I \subset \mathbb{R}$ is an interval, $C(I;\mathcal{X})$ and $C^k(I;\mathcal{X})$ will be, respectively, the sets of all continuous and continuously k times differentiable functions $\psi : I \subset \mathbb{R} \to \mathcal{X}$. If I is closed and bounded such spaces will be endowed by the standard norms $\|\psi\|_{C(I;\mathcal{X})} := \sup_{t\in I} \|\psi(t)\|_{\mathcal{X}}$, $\|\psi\|_{C^k(I;\mathcal{X})} := \sum_{j=0}^{k} \|\psi^{(j)}\|_{C^0(I;\mathcal{X})}$ (here $\psi^{(j)}$ denotes the strong derivative of order j). Shortly, we will write $\|\psi\|_{C^0}, \|\psi\|_{C^1}, \dots$ for such norms. We will denote also by $C_b(I;\mathcal{X})$ the set of functions $\psi \in C(I;\mathcal{X})$ such that $\|\psi\|_{C^0} < +\infty$. Such notation is kept also in the case of classical spaces $C_b^k([a,b]\times\mathbb{R}^d;\mathbb{R}^m)$, that is the space of functions $F \in C^k([a,b]\times\mathbb{R}^d;\mathbb{R}^m)$ such that F with all his derivatives up to order k are bounded on $[a,b]\times\mathbb{R}^d$. The space of bounded linear operators on $\mathcal{X}$ will be denoted, as usual, by $\mathcal{L}(\mathcal{X})$. This is a Banach space endowed with the operator–norm that will be denoted by $\|L\|_{\mathcal{L}(\mathcal{X})}$ (or $\|L\|$ shortly if it is clear what do we intend with) for an operator $L \in \mathcal{L}(\mathcal{X})$. If $\psi \in C([0,T];\mathcal{X})$ then it is well-defined the Riemann Integral $\int_0^T \psi(s)\, ds$. Such integral is also well defined in the case of a ψ belonging to $C_b(]0,T];\mathcal{X})$, a case that we will need in what follows. We will need also to define convolutions. To this purpose let $G : [0,T] \to \mathcal{L}(\mathcal{X})$ and assume that G is strongly continuous (namely, $G(\cdot)\xi \in C([0,T];\mathcal{X})$ for any $\xi \in \mathcal{X}$). In this case, if $\psi \in C^0([0,T];\mathcal{X})$ is well defined the convolution $G * \psi(t) := \int_0^t G(t-s)\psi(s)\, ds$, $\forall t \in [0,T]$ and, in fact, this defines a map of $C([0,T];\mathcal{X})$ into itself. If, moreover, we assume that G is strongly differentiable and $G' : [0,T] \longrightarrow \mathcal{L}(\mathcal{X})$ we have that the above defined mapping takes values in $C^1([0,T];\mathcal{X})$. All these facts hold true also in the case of $G :]0,T] \longrightarrow \mathcal{L}(\mathcal{X})$ under the assumption, respectively, $G(\cdot)\varphi \in C_b(]0,T];\mathcal{X})$ and $G'(\cdot)\varphi \in C_b(]0,T];\mathcal{X})$.
The notation $\{e^{tL}\}_{t\geq 0}$ stands for the C_0−semigroup generated by a (generally unbounded) linear operator $L : D(L) \subset \mathcal{X} \longrightarrow \mathcal{X}$ which satisfies the hypotheses of Hille–Yosida theorem. For such matter we will refer to Pazy [23]. We recall that if $\varphi \in D(L)$, the function $\psi(t) = e^{tL}\varphi$ is a strong solution of the Cauchy problem

$$\begin{cases} \psi'(t) = L\psi(t), \quad t \geq 0, \\ \psi(0) = \varphi, \end{cases} \tag{1.3}$$

that is $\psi \in C^1([0,+\infty[;\mathcal{X}) \cap C([0,+\infty[;D(L))$ and satisfies (1.3).

1.3 Series expansions and Integral equations

In this section we prove a wide set of series expansions for $\{e^{tL}\}_{t\geq 0}$, and this is obtained by proving a bijective corrispondence with a set of integral equations solving the Cauchy problem (1.3).
To begin we introduce the definition of a mapping, related to the semigroup, that acts on a general space of linear operators.

Definition 1.1. *Over the space of linear operators*

$$\mathcal{G} := \{G :]0,T] \to \mathcal{L}(\mathcal{X}) \,|\, G(\cdot)\varphi \in C_b(]0,T];\mathcal{X}) \quad \forall \varphi \in \mathcal{X}\},$$

we define the mapping:

$$\Omega_L : \mathcal{G} \to \mathcal{G}, \quad [\Omega_L(G)(t)]\,\varphi := e^{tL}\varphi - \int_0^t G(s)e^{(t-s)L}\varphi\, ds, \quad \varphi \in \mathcal{X}.$$

Remark 1.2. *It is easy to check that $\Omega_L(\mathcal{G}) \subset \mathcal{G}$. We call $\mathcal{W}_L := \Omega_L(\mathcal{G})$, and observe that it is an infinite dimensional affine sub-space of $\mathcal{G}$. The space $\mathcal{W}_L$ contains lots of elements and in particular $\{e^{tL}\}_{t\geq 0}$ belongs to $\mathcal{W}_L$ (indeed $e^{tL} = \Omega_L(0)$).*

Now we provide a new characterization of $\mathcal{W}_L$ which is important because it is made by using the generator L instead of the semigroup $\{e^{tL}\}_{t\geq 0}$.

Theorem 1.3. *In order that $W \in \mathcal{G}$ belongs to $\mathcal{W}_L$ the following conditions must be satisfied by W: there exists $D \subset D(L)$ linear subspace dense in $\mathcal{X}$ such that*

i) $W(\cdot)\varphi \in C([0,T];\mathcal{X})$, $\forall \varphi \in \mathcal{X}$;

ii) $W(\cdot)\varphi \in C^1(]0,T];\mathcal{X})$, $\forall \varphi \in D$;

iii) $W(0)\varphi = \varphi$, $\forall \varphi \in \mathcal{X}$;

iv) there exists a constant $C_T \geq 0$ depending only by T such that

$$\|(W(t)L - W'(t))\varphi\| \leq C_T\|\varphi\|, \quad \forall \varphi \in D, \ \forall t \in]0,T].$$

Proof. Suppose first that $W(\cdot) \in \mathcal{W}_L$. Then, there exists $G \in \mathcal{G}$ such that

$$W(t)\varphi = e^{tL}\varphi - \int_0^t G(s)e^{(t-s)L}\varphi \, ds.$$

The first three properties are easily veryfied with $D := D(L)$. For the last, notice that

$$\begin{aligned} W(t)L\varphi - W'(t)\varphi \; &= e^{tL}L\varphi - \int_0^t G(s)e^{(t-s)L}L\varphi \, ds - Le^{tL}\varphi \\ &\quad + G(t)\varphi + \int_0^t G(s)Le^{(t-s)L}\varphi \, ds \\ &= G(t)\varphi, \quad \forall \varphi \in D(L). \end{aligned}$$

By the Banach–Steinhaus theorem it follows that $C_T := \sup_{t\in]0,T]} \|G(t)\| < +\infty$. Therefore

$$\|(W(t)L - W'(t))\varphi\| = \|G(t)\varphi\| \leq C_T\|\varphi\|, \quad \forall \varphi \in D(L), \ t \in]0,T].$$

Conversely, suppose the map $W(t) : [0,T] \to \mathcal{L}(\mathcal{X})$ satisfies i),…,iv). By iv) turns out that the operator $W(t)L - W'(t)$ can be extended from D to $\mathcal{X}$. Let be $G(t)$ such linear extention. Clearly, by definition, if $\varphi \in D$ we have $G(\cdot)\varphi \in C_b(]0,T];\mathcal{X})$. For general $\varphi \in \mathcal{X}$ there is a $\psi \in D$ such that $\|\varphi - \psi\| \leq \varepsilon$ (here $\varepsilon > 0$). Therefore

$$\begin{aligned} \|G(t)\varphi - G(t_0)\varphi\| \; &\leq \|G(t)(\varphi - \psi)\| + \|G(t)\psi - G(t_0)\psi\| + \|G(t_0)(\psi - \varphi)\| \\ &\leq 2C_T\|\varphi - \psi\| + \|G(t)\psi - G(t_0)\psi\| \\ &\leq 2C_T\varepsilon + \|G(t)\psi - G(t_0)\psi\| \,. \end{aligned}$$

Therefore we deduce that $\limsup_{t\to t_0} \|G(t)\varphi - G(t_0)\varphi\| \le 2C_T\varepsilon$. Because ε is arbitrary, by this $\{e^{tL}\}_{t\ge 0}$follows $G(\cdot)\varphi \in C(]0,T];\mathcal{X})$.
By the same argument it follows that $\|G(\cdot)\varphi\|_{C^0} \le C_T\|\varphi\|$ so that $G(\cdot)\varphi \in C_b(]0,T];\mathcal{X})$ for any $\varphi \in \mathcal{X}$. Now: take $\varphi \in D \subset D(L)$ and $\varepsilon > 0$. We have

$$\begin{aligned} e^{tL}\varphi - \int_\varepsilon^t G(s)e^{(t-s)L}\varphi\, ds &= e^{tL}\varphi - \int_\varepsilon^t [W(s)L - W'(s)]e^{(t-s)L}\varphi\, ds \\ &= e^{tL}\varphi + \int_\varepsilon^t \frac{d}{ds}\left[W(s)e^{(t-s)L}\varphi\right]\, ds \\ &= e^{tL}\varphi + \left[W(s)e^{(t-s)L}\varphi\right]_{s=\varepsilon}^{s=t} \\ &= e^{tL}\varphi + W(t)\varphi - W(\varepsilon)e^{(t-\varepsilon)L}\varphi. \end{aligned} \tag{1.4}$$

By the Banach–Steinhaus theorem it follows that $\sup_{s\in[0,T]}\|W(s)\| < +\infty$. Recalling that $W(\varepsilon)e^{tL}\varphi \longrightarrow W(0)e^{tL}\varphi = e^{tL}\varphi$ as $\varepsilon \to 0+$ and because

$$\left\|W(\varepsilon)e^{(t-\varepsilon)L}\varphi - W(\varepsilon)e^{tL}\varphi\right\| \le \sup_{s\in[0,T]}\|W(s)\|\left\|e^{(t-\varepsilon)L}\varphi - e^{tL}\varphi\right\| \longrightarrow 0,\ \varepsilon \to 0+,$$

we deduce that $W(\varepsilon)e^{(t-\varepsilon)L}\varphi \longrightarrow e^{tL}\varphi$ as $\varepsilon \to 0+$. Finally, by letting $\varepsilon \to 0+$ in (1.4) and bu using the property $W(0) = I$ we obtain that $\Omega_L(G) = W$, and this concludes the second part of the proof. □

Consider now the Cauchy problem

$$\begin{cases} \psi'(t) = L\psi(t),\ t \ge 0 \\ \psi(0) = \varphi, \end{cases} \tag{1.5}$$

where L is an infinitesimal generator of a C_0-semigroup e^{tL}. The next theorem will show that any couple $(G, W := \Omega_L(G))$ may be used to give an integral representation of the solution ψ (namely of the semigroup e^{tL}:

Proposition 1.4. *Let $L : D(L) \subseteq \mathcal{X} \to \mathcal{X}$ be a densely defined linear operator generating a C_0-semigroup, $G \in \mathcal{G}$ and $W = \Omega_L(G) \in \mathcal{W}_L$. Then $\psi \in C([0,T];\mathcal{X})$ is a strong solution of (1.5) if and only if ψ is the unique solution of*

$$\psi(t) = W(t)\varphi + \int_0^t G(t-s)\psi(s)\, ds. \tag{1.6}$$

Proof. If $\psi(t) = e^{tL}\varphi$ is a strong solution of (1.5) with $\varphi \in D(L)$, the conclusion follows immediately by the definition of $W = \Omega_L(G)$. Conversely: assume that ψ solves (1.6) with $W = \Omega_L(G)$. By a straightforward application of the Banach–Caccioppoli theorem it follows that (1.6) has a unique solution $C([0,T];\mathcal{X})$ for any $\varphi \in \mathcal{X}$. Indeed we observe that if $\varphi \in D(L)$ then a solution is $e^{tL}\varphi$, but it is also unique in view of the contraction property of an suitable iteration of map (1.6). □

The last proposition allows us to consider series expansion for ψ. Indeed, by the successive approximations, setting

$$\begin{aligned} B_0(t)\varphi &:= W(t)\varphi, \\ B_{j+1}(t)\varphi &:= \int_0^t G(t-s)B_j(s)\varphi\, ds, \quad \forall j \geq 0, \end{aligned} \tag{1.7}$$

we have

$$\psi(t) = \sum_{j=0}^{\infty} B_j(t)\varphi,$$

and this series is strongly convergent for any $\varphi \in \mathcal{X}$ fixed. In other words we have the

Theorem 1.5. *Let $L : D(L) \subseteq \mathcal{X} \to \mathcal{X}$ be a densely defined linear operator generating a C_0-semigroup, $G \in \mathcal{G}$ and $W = \Omega_L(G) \in \mathcal{W}_L$. Then*

$$e^{tL}\varphi = \sum_{j=0}^{+\infty} B_j(t)\varphi, \tag{1.8}$$

where the operators $B_j(t)$, $j \geq 0$, are defined by (1.7).

Notice that in the case $L = L_0 + K$ with arbitrary bounded operator K (for instance, $L = i\frac{\hbar}{2m}\Delta - \frac{i}{\hbar}V$ in the Schrödinger equation (1)), choosing $W(t) = e^{tL_0}$ (that is $W(t) = e^{i\frac{\hbar}{2m}t\Delta}$), the corresponding G is $G(t) = W(t)L - W'(t) = e^{tL_0}(L_0 + K) - L_0 e^{tL_0} = e^{tL_0}K$, and the series expansion becomes

$$\begin{aligned} e^{tL}\varphi \;&= e^{tL_0}\varphi + \int_0^t e^{(t-t_1)L_0} K e^{t_1 L_0}\varphi\, dt_1 \\ &+ \int_0^t \int_0^{t_1} e^{(t-t_1)L_0} K e^{(t_1-t_2)L_0} K e^{t_2 L_0}\varphi\, dt_2\, dt_1 + \dots \end{aligned} \tag{1.9}$$

This is one of the more classical perturbative method to construct the semigroup $e^{t(L_0+K)}$. However the choice of W is not necessarily linked to semigroups. Indeed we will use different kind of operators to represent the series of e^{tL} in a suitable way. This permits us, in the last chapter, to discover a Feynman like representation of the propagator for the solution.

Remark 1.6. *It is important to point out that for each $W \in \mathcal{W}_L$ it is constructed a different series expansion (1.8). But as we seen in the Remark (1.2), $\mathcal{W}_L$ has the structure of affine dimensional space, so we deduce the same structure for the set of all possible series contructed with this technique.*

1.4 Perturbations of Series expansions

We begin pointing out that expansion (1.9) allows us to prove a stability result for "lower order" perturbations of the generator L of the semigroup.

Theorem 1.7. *Let $L_0 : D(L_0) \subseteq \mathcal{X} \to \mathcal{X}$ be an infinitesimal generator of a C_0-semigroup e^{tL_0} and a family $\{K_\varepsilon\}_{\varepsilon>0} \subset \mathcal{L}(X)$ is such that $\lim_{\varepsilon\to 0} \|K_\varepsilon\| = 0$. Finally, let be $L_\varepsilon := L_0 + K_\varepsilon$ and e^{tL_ε} the C_0-semigroup generated by L_ε. Then, if $C_T := \sup_{t\in[0,T]} \|e^{tL_0}\|$,*

$$\left\|e^{tL_\varepsilon} - e^{tL_0}\right\| \leq e^{\|K_\varepsilon\|C_T t} - 1. \tag{1.10}$$

Proof. Indeed, recalling that there exists $M > 0$, $\omega \in \mathbb{R}$ such that $\|e^{tL_0}\| \leq Me^{\omega t}$, by (1.9) we have that

$$\begin{aligned}
\left\|e^{tL_\varepsilon}\varphi - e^{tL_0}\varphi\right\| &\leq \left\| \int_0^t e^{(t-t_1)L_0} K_\varepsilon e^{t_1 L_0}\varphi dt_1 \right\| \\
&\quad + \left\| \int_0^t \int_0^{t_1} e^{(t-t_1)L_0} K_\varepsilon e^{(t_1-t_2)L_0} K_\varepsilon e^{t_2 L_0}\varphi \; dt_2 \; dt_1 \right\| + \dots \\
&\leq \left(\sum_{j=1}^{\infty} \|K_\varepsilon\|^j \Big(\sup_{\tau\in[0,t]} \|e^{\tau L_0}\| \Big)^j \frac{t^j}{j!} \right) \|\varphi\| \\
&= \left(\sum_{j=1}^{\infty} \|K_\varepsilon\|^j C_T^j \frac{t^j}{j!} \right) \|\varphi\| \\
&= \left(e^{\|K_\varepsilon\|C_T t} - 1 \right) \|\varphi\|,
\end{aligned}$$

and the conclusion is straightforward. □

Now we notice that the class $\mathcal{W}_L$ does not depend by bounded variations of the operator L, namely perturbations made adding bounded linear operators. This concept is going to be defined in the following

Definition 1.8. *Let $\mathcal{X}$ be Banach space, $L_1 : D(L_1) \subseteq \mathcal{X} \to \mathcal{X}$ and $L_2 : D(L_2) \subseteq \mathcal{X} \to \mathcal{X}$ two densely defined linear operators. We say that $L_1 \sim L_2$ if and only if $D(L_1) \cap D(L_2)$ is dense in $\mathcal{X}$ and there exists some constant $C_{1,2}$ depending by L_1 and L_2 such that $\|(L_1 - L_2)\varphi\| \leq C_{1,2}\|\varphi\|$, $\forall \varphi \in D(L_1) \cap D(L_2)$.*

With respect to this definition we have the

Proposition 1.9. *Let be L_1 and L_2 two infinitesimal generators of C_0-semigroups such that $L_1 \sim L_2$. Then $\mathcal{W}_{L_1} = \mathcal{W}_{L_2}$, that is the set $\mathcal{W}_L$ depends only on the equivalence class $[L]$.*

Proof. We prove only that $\mathcal{W}_{L_1} \subset \mathcal{W}_{L_2}$, the opposite inclusion being the same. Let be $W_1 \in \mathcal{W}_{L_1}$. By the Proposition 1.3 we know that there exists a certain $D_1 \subset D(L_1)$ linear subspace dense in $\mathcal{X}$ on which W_1 satisfies properties i),. . . ,iv). By Banach–Steinhaus theorem $K_T := \sup_{t\in[0,T]} \|W(t)\|$ is finite. In order that $W_1 \in \mathcal{W}_{L_2}$ we have just to check the iv) with L_2 in place of L_1. Let be $D_2 := D_1 \cap D(L_2)$. Clearly D_2 is a dense linear subspace of $\mathcal{X}$. Moreover, by taking $\varphi \in D_2 \subset D(L_1) \cap D(L_2)$ we have

$$\begin{aligned} \|(W_1(t)L_2 - W'(t))\varphi\| &= \|(W_1(t)(L_2 - L_1 + L_1) - W_1'(t))\varphi\| \\ &\leq \|W_1(t)(L_2 - L_1)\varphi\| + \|(W_1(t)L_1 - W_1'(t))\varphi\| \\ &\leq \|W_1(t)\| \cdot \|(L_2 - L_1)\varphi\| + C_T\|\varphi\| \\ &\leq (K_T C_{1,2} + C_T)\|\varphi\|. \ \square \end{aligned}$$

In particular we have the straightforward

Corollary 1.10. *Let $\mathcal{X}$ Banach space, $L : D(L) \subseteq \mathcal{X} \to \mathcal{X}$ a linear operator generating C_0-semigroup. If $L_1 \sim L$, then $\exp\{tL_1\} \in \mathcal{W}_L$.*

We have shown that the set of all series expansions for e^{tL}, contructed with our technique, has a bijective mapping with the infinite dimesional affine space $\mathcal{W}_L$, moreover we have proved that this set depends only from the equivalent class $[L]$. Now we show how these series expansions changes after a bounded variation of the generator the semigroup. This is the subject of the following result:

Theorem 1.11. *Let $L : D(L) \subseteq \mathcal{X} \to \mathcal{X}$ be a densely defined linear operator generating a C_0-semigroup, $G \in \mathcal{G}$ and $W = \Omega_L(G) \in \mathcal{W}_L$. Then, if*

$$e^{tL} \stackrel{strongly}{=} \sum_{j=0}^{\infty} B_j(t),$$

and $K \in \mathcal{L}(\mathcal{X})$, we have that

$$e^{t(L+K)} \stackrel{strongly}{=} \sum_{j=0}^{\infty} \tilde{B}_j(t),$$

Then,

$$\begin{aligned} \widetilde{B}_0(t) &= B_0(t) = W(t), \\ \widetilde{B}_{j+1}(t) &= B_{j+1}(t) + \int_0^t W(t-s)KB_j(s)\ ds. \end{aligned} \tag{1.11}$$

Proof. We use the property that $\mathcal{W}_{L+K}$ does depend only from $[L+K]$ that of course it is the same of $[L]$, so we can use $W(t)$ to define $\widetilde{B}_0(t)$ and to determine $\widetilde{G}(t)$:

$$\begin{aligned} \widetilde{G}(t) &= W(t)(L+K) - \dot{W}(t) = W(t)L - \dot{W}(t) + W(t)K \\ &= G(t) + W(t)K. \end{aligned}$$

Now the conclusion follows easily:

$$\begin{aligned} \widetilde{B}_{j+1}(t) &= \int_0^t [G(t-s) + W(t-s)K]B_j(s)\ ds \\ &= B_{j+1}(t) + \int_0^t W(t-s)KB_j(s)\ ds. \end{aligned} \tag{1.12}$$

$\square$

Chapter 2

Generating functions for Lagrangian submanifolds

2.1 Introduction

In this chapter we first review some topics from the theory of generating functions for canonical transformations theory, where Symplectic geometry — symplectic manifolds and their Lagrangian submanifolds — is the natural framework to treat this subject.
Then, we begin by considering an important theorem of Viterbo [34] about quadratic at infinity generating functions of Lagrangian submanifolds contained in $T^\star\mathbb{R}^n$, and we prove the validity of this result also for weakly quadratic generating functions of the submanifold Λ_t, contained in $T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n$ and generated by a certain class of Hamiltonian flows.
Finally, as our main goal, we will prove the existence and the explicit representation of a global generating function weakly quadratic at infinity for Λ_t. But together with the previous result, we obtain in this way the explicit representations for all the weakly quadratic generating functions of Λ_t.

2.2 Some topics on the theory of generating functions

Adopting standard notations, as in [2], [4], we denote by $\omega = dp \wedge dx = \sum_{i=1}^n dp_i \wedge dx^i$ the natural symplectic 2-form on $T^\star\mathbb{R}^n$. The notion of Lagrangian submanifold of $T^\star\mathbb{R}^n$ can be introduced by thinking of it as a multivalued generalization of the graph of the differential of a function f on $\mathbb{R}^n$, $\mathrm{graph}(df) = \{(x,p) \in T^\star\mathbb{R}^n : p = \nabla_x f(x),\ x \in \mathbb{R}^n\}$. It is easy to see that: $\omega\big|_{\mathrm{graph}(f)} = \partial^2_{x^i x^j} f\ dx^i \wedge dx^j \equiv 0$, $\dim \mathrm{graph}(f) = n$, and $\mathrm{graph}(f)$ is globally transverse to the fibers of $T^\star\mathbb{R}^n \longrightarrow \mathbb{R}^n$. Thus, we say $\Lambda \subset T^\star\mathbb{R}^n$ is a Lagrangian submanifold if: $\omega\big|_\Lambda = 0$ and $\dim \Lambda = n\ = \frac{1}{2}\dim(T^\star\mathbb{R}^n)$.
Maslov [21] and Hörmander[11] theory draws the *local* (with respect the base manifold $\mathbb{R}^n = \{x\}$) description of the Lagrangian submanifold Λ by means of the generating functions $S(x,u)$. Here is the definition of *global* generating function:

Definition 2.1. *A generating function for a Lagrangian submanifold Λ is a smooth function $S = S(x,u) : \mathbb{R}^n \times \mathbb{R}^k \longrightarrow \mathbb{R}$ such that*

i) $\Lambda = \{(x,p) \in T^\star\mathbb{R}^n :\ \ p = \nabla_x S,\ \ 0 = \nabla_u S\ \}$,

ii) zero (in $\mathbb{R}^k$) is a regular value of the map $(x,u) \longmapsto \nabla_u S(x,u)$.

In many questions on symplectic topology the generating functions quadratic at infinity and weakly quadratic are of particular interest:

Definition 2.2. *A generating function $S : \mathbb{R}^n \times \mathbb{R}^k \to \mathbb{R}$ is called*

- **quadratic at infinity (GFQI)** *if there exists a compact set $K \subset \mathbb{R}^k$ and a nondegenerate quadratic function $a(x,u) = \langle a(x)u, u\rangle$ such that $S(x,u) = a(x,u)$ $\forall u \in \mathbb{R}^k \setminus K$.*

- **weakly quadratic at infinity (GFWQI)** *if there exists a non degenerate quadratic function $a(x,u)$ such that*

$$\|S(x,\cdot) - a(x,\cdot)\|_{C^1(\mathbb{R}^k)} < \infty, \quad \forall x \in \mathbb{R}^n.$$

Of course a GFQI is a GFWQI. GFQI are very important in the description of Lagrangian manifold. The basic reason is that there is a fundamental theorem due to Viterbo that says that any generating function $\tilde S$ of a Lagrangian manifold is obtained from a generating function quadratic at infinity S by a mixture of three basic operations that now we will introduce:

Definition 2.3. *Let $S = S(x,u)$ be a generating function for a Lagrangian submanifold Λ, $S : \mathbb{R}^n \times \mathbb{R}^k \longrightarrow \mathbb{R}$. We say that $\tilde S$ is obtained by*

- *a* **stabilization** *from S, if there exists a regular non degenerate quadratic function $a = a(x,v) \equiv \langle a(x)v, v\rangle$, $v \in \mathbb{R}^h$ and $\tilde S(x,u,v) \equiv S(x,u) + \langle a(x)v, v\rangle$.*

- *a* **fibered diffeomorphisms** *from S, if there exists a regular $u : \mathbb{R}^n \times \mathbb{R}^k \longrightarrow \mathbb{R}^k$ such that $u(x,\cdot)$ is a diffeomorphism and $\tilde S(x,v) \equiv S(x,u(x,v))$.*

- *an* **addition of constant** *from S, if there exists a constant $C \in \mathbb{R}$ such that $\tilde S(x,u) \equiv S(x,u) + C$.*

Remark 2.4. *Although it is trivial to check that each of these operations on S gives still a generating function $\tilde{S}$ for to the same Lagrangian submanifold, it is a rather intriguing fact that by means of these three operations we can exactly classify all the generating functions of a large enough class — see theorem (2.5) below — of Lagrangian submanifolds.*

The Hamiltonian vector field X_H, related to the Hamiltonian function $H : T^\star\mathbb{R}^n \to \mathbb{R}$, is defined by $i_{X_H}\omega = -dH$. Denoting curves by $\gamma = (x, p)$, the related Hamilton system $\dot{\gamma} = X_H(\gamma)$ reads:

$$\dot{\gamma} = J\nabla H(\gamma), \quad \Longleftrightarrow \quad \begin{cases} \dot{x} = \nabla_p H(x,p), \\ \\ \dot{p} = -\nabla_x H(x,p), \end{cases} \qquad \text{where } \; J = \begin{pmatrix} \mathbb{O} & \mathbb{I} \\ -\mathbb{I} & \mathbb{O} \end{pmatrix}.$$

We denote by $\phi_H^t : T^\star\mathbb{R}^n \to T^\star\mathbb{R}^n$ the flow generated by X_H, that is $\frac{d}{dt}\phi_H^t = J\nabla H(\phi_H^t)$. It is well known that Hamiltonian flows send Lagrangian submanifolds into Lagrangian submanifolds. Furthermore, for any Lagrangian submanifold Λ belonging to a regular fiber of a Hamiltonian H, $\Lambda \subset H^{-1}(e)$, we have: $X_H(x,p) \in T_{(x,p)}\Lambda$.

2.3 Equivalence of generating functions

The following theorem (see [34]) establishes the *equivalence*, in the sense of definition (2.3), between all the generating functions quadratic at infinity for the Lagrangian manifolds in $T^\star\mathbb{R}^n$ related to the class of Hamiltonian flow ϕ_H^t with H compact supported.

Theorem 2.5 (Viterbo)**.** *Let $p_0 \in \mathbb{R}^n$, $\Lambda_0 := \{(x, p_0) \in T^\star\mathbb{R}^n : x \in \mathbb{R}^n\}$ and $\Lambda_t = \phi_H^t(\Lambda_0) \subset T^\star\mathbb{R}^n$ the Lagrangian submanifold related to the Hamiltonian flow with a Hamiltonian H having compact support. Then Λ_t admits by a GFQI. Furthermore, assuming $S_j(t, x, u_j) : [0,T] \times \mathbb{R}^n \times \mathbb{R}^{k_j} \longrightarrow \mathbb{R}$, $j = 1, 2$ are two generating functions quadratic at infinity for Λ_t, then there exist two stabilizations $\tilde{S}_1(t,x,v)$ and $\tilde{S}_2(t,x,v)$ of S_1 and S_2, with same final parameter space $\mathbb{R}^k = \mathbb{R}^{k_1} \times \mathbb{R}^{h_1} = \mathbb{R}^{k_2} \times \mathbb{R}^{h_2}$, a fibered diffeomorphism*

$$R : \mathbb{R}^n \times \mathbb{R}^k \longrightarrow \mathbb{R}^n \times \mathbb{R}^k$$

and a constant C, such that $\tilde{S}_1$ and $\tilde{S}_2 + C$ are equivalent, that is the following diagram commutes:

$$\begin{tikzcd} \mathbb{R}^n \times \mathbb{R}^k \arrow[r, "R"] \arrow[d, "\tilde{S}_1(t,\cdot)"] & \mathbb{R}^n \times \mathbb{R}^k \arrow[d, "\tilde{S}_2(t,\cdot)+C"] \\ \mathbb{R} \arrow[r, "id"] & \mathbb{R} \end{tikzcd} \tag{2.1}$$

Remark 2.6. *The previous theorem has been generalized by Thèret (see [33]) for weakly quadratic generating functions and the same Lagrangian submanifold.*

The assumption about the support of H in Theorem 2.5 is naturally un-natural for the case of mechanical Hamiltonians of type $H(p,x) = \frac{1}{2m}p^2 + V(x)$. However, with some work we can extend the result also to this case under suitable assumption on V.
First, we begin to consider in some detail the product manifold $T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n$, and we will

equipe it by a suitable symplectic structure $\bar{\omega}$ in order to deal with canonical transformations as Lagrangian submanifolds in such a 'graph structure'. Let us consider the standard projections

$$T^\star\mathbb{R}^n \overset{pr_1}{\longleftarrow} T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n \overset{pr_2}{\longrightarrow} T^\star\mathbb{R}^n$$

and we carry out a symplectic structure $\bar{\omega}$ on $T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n \cong T^\star(\mathbb{R}^n \times \mathbb{R}^n)$ by the following twofold pull-back of the standard symplectic 2-form on $T^\star\mathbb{R}^n$,

$$\bar{\omega} := pr_2^\star\omega - pr_1^\star\omega = dp_2 \wedge dx_2 - dp_1 \wedge dx_1.$$

We point out that for any fixed time $t \in [0,T]$ the set

$$\Lambda_t := \left\{(y,\xi,x,p) \in T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n \ : \ (x,p) = \phi_H^t(y,\xi)\right\} \tag{2.2}$$

is a Lagrangian submanifold of $(T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n, \bar{\omega})$, that is:

$$\bar{\omega}\big|_{\Lambda_t} = 0, \quad \dim \Lambda_t = 2n = \frac{1}{2}\dim(T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n).$$

Therefore we can try to determine a global generating function:

$$\Lambda_t = \{(y,\xi;x,p) \in T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n \ : \ p = \nabla_x S, \quad \xi = -\nabla_y S, \quad 0 = \nabla_u S\ \}.$$

Before to do this, we first recall a classical result on Hamiltonian flows.

Proposition 2.7 (Hamilton)**.** *Let $H(x,p) := H_0(x,p) + H_1(x,p)$ and denote $\phi_H^t(x,p)$, $\phi_{H_0}^t(x,p)$ related Hamiltonian flows. Define the time-dependent Hamiltonian $K(t,x,p) := (\phi_{H_0}^t)^\star(H_1)$ and consider the related flow $\phi_K^{t,0}(x,p)$. We have:*

$$\phi_H^t = \phi_{H_0}^t \circ \phi_K^{t,0}. \tag{2.3}$$

Now we prove that Theorem of Viterbo (2.5) can be applied also for the Lagrangian submanifold $\Lambda_t \subset T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n$ and involving the general class of weakly quadratic at infinity generating functions.

Theorem 2.8. *Th.2.5, for (weakly) GFQI, does work also for the canonical transformation Lagrangian submanifold $\Lambda_t \subset T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n$, related to the non-compact supported (in $T^\star\mathbb{R}^n$) mechanical Hamiltonian $H(x,p) := \frac{p^2}{2m} + V(x)$, where the potential energy V is compact supported (in $\mathbb{R}^n$).*

Proof. Define the map, by Viterbo [34]:

$$h : T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n \longrightarrow T^\star(\mathbb{R}^n \times \mathbb{R}^n),$$

$$(y,\xi;x,p) \longmapsto (\hat{X};\hat{P}) := \Big(\frac{x+y}{2}, \frac{\xi+p}{2}; p-\xi, y-x\Big),$$

and observe that it is a symplectic isomorphism, sending the diagonal into the zero section. Indeed the invertibility is straightforward, while:

$$\begin{aligned} h^\star\omega^{(2n)} &= \frac{1}{2}(dp-d\xi)\wedge(dy+dx) + \frac{1}{2}(dy-dx)\wedge(d\xi+dp) \\ &= dp\wedge dx - d\xi\wedge dy = \omega_2^{(n)} - \omega_1^{(n)} = \bar{\omega}, \end{aligned}$$

tells us that the pull back of the 2-form ω^{2n} on $T^\star(\mathbb{R}^n\times\mathbb{R}^n)$ is exactly $\bar\omega$ on $T^\star\mathbb{R}^n\times T^\star\mathbb{R}^n$, so it is a symplectic map. We consider the set $\hat\Lambda_t := h(\Lambda_t)$ that is a Lagrangian submanifold of $T^\star(\mathbb{R}^n\times\mathbb{R}^n)$ because the map h is a symplectic and Λ_t is Lagrangian. In view of this relation, we can find a generating function for $\hat\Lambda_t$ if we know S for Λ_t:

$$\hat S(t,\hat X_1,\hat X_2,\xi) := S(t,\alpha,\beta,u)+(\alpha+\beta-2\hat X_1)\gamma+\hat X_2(\alpha-\beta),\quad \xi=(\alpha,\beta,\gamma,u). \tag{2.4}$$

For the same reason, if we compute h^{-1},

$$h^{-1}: T^\star(\mathbb{R}^n\times\mathbb{R}^n)\longrightarrow T^\star\mathbb{R}^n\times T^\star\mathbb{R}^n,$$

$$(\hat X_1,\hat X_2;\hat P_1,\hat P_2)\longmapsto (y,\xi;x,p) := \Big(\hat X_1+\frac12\hat P_2,\hat X_2-\frac12\hat P_1;\hat X_1-\frac12\hat P_2,\hat X_2+\frac12\hat P_1\Big),$$

we can determine S if we know $\hat S$:

$$S(t,x,y,\chi) := \hat S(t,\alpha,\beta,u)-y\Big(\beta-\frac12\mu\Big)+x\Big(\beta+\frac12\mu\Big)-\mu\alpha,\quad \chi=(\alpha,\beta,\mu,u). \tag{2.5}$$

This two transformations preserves the property of quadraticity at infinity, so we deduce that the existence and the unicity (modulo stabilitazions and fibered diffeomorphims) that we are going to prove for generating function $\hat S$ it is proved also for S.
We easily observe that $\hat\Lambda_t=\phi^t_{\hat H}(\hat\Lambda_0)$, namely it is generated by an Hamiltonian flow, where:

$$\begin{aligned}\hat H(\hat X_1,\hat X_2;\hat P_1,\hat P_2) &:= H\Big(\hat X_1-\frac12\hat P_2,\hat X_2+\frac12\hat P_1\Big)\\ &= \frac{1}{2m}\Big(\hat X_2+\frac12\hat P_1\Big)^2+V\Big(\hat X_1-\frac12\hat P_2\Big)=:\hat H_0+\hat H_1.\end{aligned}$$

Note that this Hamiltonian is the sum of quadratic and compact supported terms. Now we apply Proposition (2.7) to represent its flow:

$$\phi^t_{\hat H}(\hat X_1,\hat X_2;\hat P_1,\hat P_2)=\phi^t_{\hat H_0}\circ\phi^{t,0}_{\hat K}(\hat X_1,\hat X_2;\hat P_1,\hat P_2), \tag{2.6}$$

with $\hat K=(\phi^t_{\hat H_0})^\star(\hat H_1)$. If we define $\widetilde\Lambda_t:=\phi^{t,0}_{\hat K}(\hat\Lambda_0)$ then $\hat\Lambda_t=\phi^t_{\hat H_0}(\widetilde\Lambda_t)$ and consequently $\widetilde\Lambda_t:=\phi^{-t}_{\hat H_0}(\hat\Lambda_t)$. Now we write down the explicit structure of $\phi^t_{\hat H_0}$:

$$\phi^t_{\hat H_0}(\hat X_1,\hat X_2;\hat P_1,\hat P_2) \;=\; \Big(\hat X_1+\frac{t}{2m}\Big(\hat X_2+\frac{\hat P_1}{2}\Big),\hat X_2;\hat P_1,\hat P_2+\frac{t}{m}\Big(\hat X_2+\frac{\hat P_1}{2}\Big)\Big). \tag{2.7}$$

This transformation is linear and symplectic, so admits a non degenerate quadratic generating function $\mathcal{S}_1=\mathcal{S}_1(q_1,q_2,Q_1,Q_2)$; For this reason, given a genenrarating function $\widetilde S$ for $\widetilde\Lambda_t$ for $\widetilde\Lambda_t$, we can immediatly determine $\hat S(t,\hat Q_1,\hat Q_2,u)$ in this way:

$$\hat S(t,\hat Q_1,\hat Q_2,\mu,z,u)=\widetilde S(t,\mu,z,u)+\mathcal{S}_1(\mu,z,\hat Q_1,\hat Q_2). \tag{2.8}$$

By the same argument, by $\mathcal{S}_2$ generating $(\phi^t_{\hat H_0})^{-1}$, we can determine $\hat S$ if we know $\widetilde S$:

$$\widetilde S(t,\widetilde Q_1,\widetilde Q_2,\alpha,\beta,u)=\hat S(t,\alpha,\beta,u)+\mathcal{S}_2(\alpha,\beta,\widetilde Q_1,\widetilde Q_2). \tag{2.9}$$

In view of the compactness of K we can now apply Th. (2.5) to have the existence and unicity (modulo stabilitazions and fibered diffeomorphism) for generating functions weakly quadratic at infinity $\widetilde S$ of $\widetilde\Lambda_t$, but the transformations (2.8) and (2.9) preserves the property of quadraticity at infinity, so we conclude the validity of the theorem also for $\hat\Lambda_t$. □

2.4 Representations of generating functions

In this section we provide a result of existence and representation for the class of weakly quadratic generating functions of Λ_t described in the previous section. We begin proving a simple Lemma about the "partial reduction" of a generating function; this will be useful in the next theorem, where it is possible to prove the property of weakly quadraticity at infinity (see definition 2.2) only after this type of particular reduction.

Lemma 2.9. *Consider the stationary condition for a generating function $\mathcal{S}$ of $\Lambda \subset T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n$, with respect to the group of the parameters u:*

$$0 = \nabla_u \mathcal{S}(x, y, u, v), \tag{2.10}$$

Suppose that there exists a smoot function $g : \mathbb{R}^{2n} \times \mathbb{R}^k \to \mathbb{R}^k$ such that

$$u = g(x, y, v),$$

realize the relation (2.10); then it is possible to determine a reduced new generating function S,

$$S(x, y, v) = \mathcal{S}(x, y, g(x, y, v), v).$$

Proof. Indeed

$$\begin{aligned}
&\{(y, \xi, x, p) \in T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n : \xi = -\nabla_y S \;\; p = \nabla_x S, \;\; 0 = \nabla_v S\} \\
&= \;\; \{(y, \xi, x, p) : \xi = -\nabla_y S + \nabla_u \mathcal{S} \cdot \nabla_y g, \;\; p = \nabla_x \mathcal{S} + \nabla_u \mathcal{S} \cdot \nabla_x g, \;\; 0 = \nabla_u \mathcal{S} \cdot \nabla_v g, \;\; 0 = \nabla_v \mathcal{S}\} \\
&= \;\; \{(y, \xi, x, p) : \xi = -\nabla_y S \;\; p = \nabla_x \mathcal{S}, \;\; 0 = \nabla_u \mathcal{S}, \;\; 0 = \nabla_v \mathcal{S}\} = \Lambda
\end{aligned}$$

□

The following theorem establishes the existence and the explicit representation for a weakly quadratic generating function for Λ_t.

Theorem 2.10. *Suppose that $V \in C^2(\mathbb{R}^n)$ with compact support, and let be $H(x, p) := \frac{p^2}{2m} + V(x)$. Then there exists a generating function $S(t, x, y, u)$ weakly quadratic at infinity for the Lagrangian submanifold Λ_t, such that in the interval $t \in [0, T]$ assumes this form:*

$$S(t, x, y, u) = m\frac{|x - y|^2}{2t} + \frac{m}{2}|u|^2 + c(t, x, y, u), \tag{2.11}$$

where the auxiliary parameters $u \in \mathbb{R}^k$ with $k = k(T, V) \in \mathbb{N}$ and the remaining term $c \in C^2_b([0, T] \times \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^k; \mathbb{R})$.

Proof. We start borrowing a result by [7]. In order to do this we have first to introduce some notations. Let $N \in \mathbb{N}$ and $\mu := 2n(2N + 1)$. In the space $L^2([0, t]; \mathbb{R}^{2n})$, given $v \in \mathbb{R}^\mu \equiv (\mathbb{R}^{2N+1})^{2n}$, $v = (v_{-N}, \ldots, v_N)$ with $v_j \in \mathbb{R}^{2n}$, let $p_N(v) := \sum_{|j| \le N} v_j e_j(r)$, $e_j(r) = \frac{1}{\sqrt{t}} e^{i\frac{2\pi}{t} jr}$ be the trigonometric polynomial with coefficients v and $\mathbb{P}_N L^2([0, t]; \mathbb{R}^{2n})$ the linear subspace of $L^2([0, t]; \mathbb{R}^{2n})$ whose elements are $\{p_N(v)\}_{v \in \mathbb{R}^k}$. We will use the notation $p_N(v) = (v^x, v^p)$, where $v^x, v^p \in L^2([0, t]; \mathbb{R}^n)$. Finally, define $\mathbb{Q}_N L^2([0, t]; \mathbb{R}^{2n}) := \mathbb{P}_N L^2([0, t]; \mathbb{R}^{2n})^\perp$.

In [7] has been proved that, if N is big enough [1], namely if N is such that

$$\|\nabla^2 H\|_{L^\infty} \cdot \frac{(1+\sqrt{2N})T}{2\pi N} < 1,$$

then it is possible construct a global generating function for any Lagrangian submanifold Λ_t, $t \in [0,T]$, of type

$$\mathcal{S}(t,x,y,v) = \mathcal{A}[\gamma(t,x,y,v)] = \int_0^t [\gamma^p(s)\dot{\gamma}^x(s) - H(\gamma^x(s),\gamma^p(s))]\, ds, \tag{2.12}$$

where $\mathcal{A}[\cdot]$ is the action functional evaluated on a suitable set of curves$^{(2)}$ $\gamma = (\gamma^x,\gamma^p) \in H^1([0,t];\mathbb{R}^{2n})$ depending of $(t,x,y,v) \in [0,T]\times\mathbb{R}^n\times\mathbb{R}^n\times\mathbb{R}^k$ (where $k = k(T,V,n) = 2n(2N+1)$). The curves (γ^x,γ^p) have the following structure

$$\begin{cases} \gamma^x(s) := y + \dfrac{x-y}{t}s + \displaystyle\int_0^s \phi^x(r)\, dr - \frac{s}{t}\int_0^t \phi^x(r)\, dr, & \phi^x := u^x + f^x_u, \\[2ex] \gamma^p(s) := m\dfrac{x-y}{t} + \dfrac{1}{t}\displaystyle\int_0^t \phi^x(r)\, dr + \int_0^s \phi^p(r)\, dr, & \phi^p := v^p + f^p_v, \end{cases} \tag{2.13}$$

where $(f^x,f^p) \equiv (f^x_N(t,x,y,v), f^p_N(t,x,y,v)) \in \mathbb{Q}_N L^2([0,t];\mathbb{R}^{2n})$ solves the fixed point equation:

$$(f^x,f^p) = \mathbb{Q}_N J\nabla H\left(h(t,x,y,(v^x,v^p)+(f^x,f^p))\right). \tag{2.14}$$

About (f^x,f^p) we have precisely that

$$\begin{cases} f^x(\cdot) = \dfrac{1}{m}\mathbb{Q}_N h^p(t,x,y,v^p+f^p)(\cdot) = \dfrac{1}{m}\mathbb{Q}_N \displaystyle\int_0^\bullet f^p(r)\, dr, \\[2ex] f^p(\cdot) = -\mathbb{Q}_N \nabla V(h^x(t,x,y,v^x+f^x)(\cdot)). \end{cases} \tag{2.15}$$

It is easy to check that (2.15) can be rewritten in the form:

$$\begin{cases} \mathbb{Q}_N\dot{\gamma}^x(t,x,y,v) = \dfrac{1}{m}\mathbb{Q}_N\gamma^p(t,x,y,v), \\[2ex] \mathbb{Q}_N\dot{\gamma}^p(t,x,y,v) = -\mathbb{Q}_N\nabla V(\gamma^x(t,x,y,v)). \end{cases} \tag{2.16}$$

Generally, f^x and f^p they are non linear functional$^{(3)}$, of v, and [7] provides some good information on them that will be useful in what follows. In particular, there exists constant $C, C' \geq 0$ such that

$$\|f(t,x,y,v)(\cdot)\|_{L^2} \leq Ct, \quad \|\nabla_v f(t,x,y,v)(\cdot)\|_{L^2} \leq C't. \tag{2.17}$$

[1] in order to equation (2.14) is generated by a contraction map

[2] Clearly $H^1([0,t];\mathbb{R}^{2n})$ is the usual Sobolev space.

[3] We stress the fact that the upper indexes x and p are just labels that recall to us on which component we are working. On the other side the lower indexes are true variables for the various functions involved. In particular, v^x, v^p are elements of $L^2([0,t];\mathbb{R}^n)$ that depends only by $v \in \mathbb{R}^k$ whereas $f^{x,p}_N(t,x,y,v)$ is again in $L^2([0,t];\mathbb{R}^n)$ and it depends by x, y, u and t explicitly.

Moreover it is important to observe that the $f^x(t,x,y,v)(s)$, and then $\gamma^x(t,x,y,v)(s)$, depends only of $(v^x_{-N},..v^x_{-1},v^x_1,...v^x_N)$, so they are not depending of v^p and v^x_0. Indeed by the second of (2.15) we deduce that f^p does not depend of v^p and v^x_0, and because the first of (2.15) shows a linear relation between f^x and f^p, the same holds true also for f^x. Finally, in view of the definition of $\gamma^x(t,x,y,v)(s)$, it is straightforward to recognize that the same conclusion holds for it. The utility of this observations will be clear below.
We now come back to (2.12),

$$\begin{aligned}
\mathcal{S}(t,x,y,v) &= \int_0^t \gamma^p(s)\dot\gamma^x(s) - H(\gamma^x(s),\gamma^p(s))\,ds \\
&= \int_0^t \gamma^p(s)\dot\gamma^x(s) - \frac{1}{2m}|\gamma^p(s)|^2 - V(\gamma^x(s))\,ds \\
&= \int_0^t (\mathbb{P}_N+\mathbb{Q}_N)\gamma^p(s)\cdot(\mathbb{P}_N+\mathbb{Q}_N)\dot\gamma^x(s) - \frac{1}{2m}|(\mathbb{P}_N+\mathbb{Q}_N)\gamma^p(s)|^2 - V(\gamma^x(s))\,ds \\
&= \int_0^t \mathbb{P}_N\gamma^p(s)\cdot\mathbb{P}_N\dot\gamma^x(s) + \mathbb{Q}_N\gamma^p(s)\cdot\mathbb{Q}_N\dot\gamma^x(s) \\
&- \frac{1}{2m}|\mathbb{P}_N\gamma^p(s)|^2 - \frac{1}{2m}|\mathbb{Q}_N\gamma^p(s)|^2 - V(\gamma^x(s))\,ds.
\end{aligned} \tag{2.18}$$

By the first of (2.16) we have that

$$\mathcal{S}(t,x,y,v) = \int_0^t \mathbb{P}_N\gamma^p(s)\cdot\mathbb{P}_N\dot\gamma^x(s) - \frac{1}{2m}|\mathbb{P}_N\gamma^p(s)|^2 + \frac{m}{2}|\mathbb{Q}_N\dot\gamma^x(s)|^2 - V(\gamma^x(s))\,ds. \tag{2.19}$$

We recall now that the function $\mathcal{S}$ so constructed generates the Lagrangian submanifold Λ_t:

$$\begin{aligned}
\Lambda_t &:= \left\{(y,\xi;x,p)\in T^\star\mathbb{R}^n\times T^\star\mathbb{R}^n : (x,p)=\phi^t_H(y,\xi)\right\} \\
&= \{(y,\xi;x,p)\in T^\star\mathbb{R}^n\times T^\star\mathbb{R}^n : p=\nabla_x\mathcal{S},\quad \xi=-\nabla_y\mathcal{S},\quad 0=\nabla_v\mathcal{S}\}\,.
\end{aligned}$$

Therefore, the stationary condition,

$$0=\nabla_v\mathcal{S}(v)=(\nabla_{v^x}\mathcal{S}(v),\nabla_{v^p}\mathcal{S}(v)), \tag{2.20}$$

we derive the following relations:

$$\begin{cases}
\mathbb{P}_N\dot\gamma^x(t,x,y,v) = \dfrac{1}{m}\mathbb{P}_N\gamma^p(t,x,y,v), \\[2ex]
\mathbb{P}_N\dot\gamma^p(t,x,y,v) = -\mathbb{P}_N\nabla V(\gamma^x(t,x,y,v)).
\end{cases} \tag{2.21}$$

Recalling the parametrizations (2.13), the previous relations becomes

$$\begin{cases}
v^x(s) + \dfrac{x-y}{t} - \dfrac{v^x_0}{\sqrt{t}} = \dfrac{1}{m}\mathbb{P}_N\gamma^p(t,x,y,v)(s), \\[2ex]
v^p(s) = -\mathbb{P}_N\nabla V(\gamma^x(t,x,y,v))(s).
\end{cases} \tag{2.22}$$

In view of the Lemma 2.9, we can insert the first (2.21) in (2.19), and obtain a reduced generating function:

$$\begin{aligned}
S &= \int_0^t m\mathbb{P}_N\dot{\gamma}^x(s)\cdot\mathbb{P}_N\dot{\gamma}^x(s) + m\mathbb{Q}_N\dot{\gamma}^x(s)\cdot\mathbb{Q}_N\dot{\gamma}^x(s) \\
&- \frac{m}{2}|\mathbb{P}_N\dot{\gamma}^x(s)|^2 - \frac{m}{2}|\mathbb{Q}_N\dot{\gamma}^x(s)|^2 - V(\gamma^x(s))\,ds \\
&= \int_0^t \frac{m}{2}|\mathbb{P}_N\dot{\gamma}^x(s)|^2 + \frac{m}{2}\,|\mathbb{Q}_N\dot{\gamma}^x(s)|^2 - V(\gamma^x(s))\,ds \\
&= \int_0^t \frac{m}{2}|\mathbb{P}_N\dot{\gamma}^x(s)|^2 + \frac{m}{2}\,|f^x(s)|^2 - V(\gamma^x(s))\,ds.
\end{aligned} \tag{2.23}$$

We realize that the new associated parameter space is $u := (v^x_{-N}, ..v^x_{-1}, v^x_1, ...v^x_N) \in \mathbb{R}^{2N\cdot n} = \mathbb{R}^k \subset \mathbb{R}^\mu$ because, in wiev of the observation made above, f^x and γ^x have the dependence only on u and not on all the other parameter $(v^x_0; v^p)$, and obviuosly we have that $\mathbb{P}_N\dot{\gamma}^x(s)$ depends only from u parameters, because the derivative eliminate the dependence from the mean term v^x_0. In this way we obtain a more detailed representation of the generating function:

$$\begin{aligned}
S(t,x,y,u) &= \int_0^t \frac{m}{2}\left|v^x(s) + \frac{x-y}{t} - \frac{v_0}{\sqrt{t}}\right|^2 + \frac{m}{2}\,|f^x(s)|^2 - V(\gamma^x(s))\,ds \\
&= m\frac{|x-y|^2}{2t} + \frac{m}{2}\int_0^t \left|v^x(s) - \frac{v_0}{\sqrt{t}}\right|^2 ds + \frac{m}{2}\int_0^t |f^x(s)|^2\,ds - \int_0^t V(\gamma^x(s))\,ds \\
&= m\frac{|x-y|^2}{2t} + \frac{m}{2}\sum_{0<|j|\le N}|u_j|^2 + \frac{m}{2}\int_0^t |f^x(t,x,y,u)(s)|^2 - V(\gamma^x(t,x,y,u)(s))\,ds.
\end{aligned} \tag{2.24}$$

Finally, by defining

$$c(t,x,y,u) := \int_0^t \frac{m}{2}|f^x(t,x,y,u)(s)|^2 - V(\gamma^x(t,x,y,u)(s))\,ds,$$

we conclude that

$$S(t,x,y,u) = m\frac{|x-y|^2}{2t} + \frac{m}{2}|u|^2 + c(t,x,y,u),$$

generate the same Lagrangian submanifold Λ_t and it is the expected generating function weakly quadratic at infinity. In order to check this final sentence, it is enough consider the non degenerate quadratic form $P(u) := \frac{m}{2}|u|^2$, for which

$$\|S-P\|_{C^1} = \|\nabla_u S - \nabla_u P\|_{C^0} = \|\nabla_u c\|_{C^0} < +\infty. \tag{2.25}$$

Moreover by using the C^2_b-regularity property of $f(t,x,y,u)(\tau)$ and $\gamma^x(t,x,y,u)(\tau)$ in the variables (t,x,y,u) we obtain the C^2_b-regularity of $c(t,x,y,u)$ and so of $S(t,x,y,u)$. □

Remark 2.11. *We remark that for $(t,x,y) \in [0,T]\times\mathbb{R}^n\times\mathbb{R}^n$ fixed the space of curves $\Gamma(t,x,y) := \{\gamma^x(t,x,y,u) \in H^1([0,t];\mathbb{R}^{2n}) : u \in \mathbb{R}^k\}$ has a structure of finite dimensional manifold induced by the map $\gamma(t,x,y,\cdot) : \mathbb{R}^k \longrightarrow H^1([0,t];\mathbb{R}^{2n})$. Indeed the inverse of this injective map, together with $\Gamma(t,x,y)$, represents exactly the unique local chart needed to define the structure of manifold.*

As a conseguence of Theorems (2.8) and (2.10) we prove the representation for a generic weakly quadratic generating function of Λ_t.

Theorem 2.12. *Suppose that $V \in C^2(\mathbb{R}^n)$ with compact support, and let be $H(x,p) := \frac{p^2}{2m} + V(x)$. Then any generating function $\mathcal{S}(t,x,y,v_1)$ weakly quadratic for the Lagrangian submanifold Λ_t verifies the relation:*

$$\mathcal{S}(t,x,y,v_1)+\Omega(t,x,y)w_1\cdot w_1 = m\frac{|x-y|^2}{2t}+\frac{m}{2}|v_2|^2+c(t,x,y,v_2)+Q(t,x,y)w_2\cdot w_2+C, \quad (2.26)$$

Proof. We consider the generating function of Theorem (2.10):

$$S(t,x,y,u) = m\frac{|x-y|^2}{2t} + \frac{m}{2}|u|^2 + c(t,x,y,u), \quad u \in \mathbb{R}^k. \quad (2.27)$$

Appling Thereom (2.8) we deduce that any other generating function is connected with this one by combinations of three operations: stabilization by suitable nondegenerate matrix $Q(t,x,y)$ and $\Omega(t,x,y)$ on some $\mathbb{R}^{k_1}$ and $\mathbb{R}^{k_2}$, a composition with a fibered diffeomorphism $\Phi(t,x,y,\cdot) : \mathbb{R}^\mu \to \mathbb{R}^\mu$, sum of a constant C, (see definition 2.3). From the composition of S with these operations we obtain the expected result. $\square$

Chapter 3

Integral operators related to generating functions

3.1 Introduction

In this chapter we construct a family of integral operators related to the class of generating functions studied in the previous chapter. More precisely we made a direct link between the representations of the kernel for this operators and weakly quadratic at infinity generating functions of the Lagrangian submanifolds $\Lambda_t = \phi_H^t \Lambda_0$. For these operators we will show some important properties, that are due to the use of Hamiltonian flow ϕ_H^t to define the set Λ_t. In particular, we study some operations among such operators, proving that this family is closed under these operations. In the next chapter we will use a particular subset of these operators, that are more strictly connected to ϕ_H^t and that will be foundamental to determine the integral representations of Schrödinger Propagator .

3.2 A family of integral operators

In this section we define a large class of Integral operators that exibits interesting properties related to generating functions.
Consider a generating function $S : [0,T] \times \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^k \longrightarrow \mathbb{R}$ weakly quadratic at infinity for Λ_t. The existence of such functions was proved in Theorem 2.10. We are interested here to study integral operators of type

$$[B(t)\varphi](x) := \int_{\mathbb{R}^n} b(t,x,y)\varphi(y)\, dy, \quad \text{where} \quad b(t,x,y) := \int_{\mathbb{R}^k} e^{i\lambda S(t,x,y,u)}\rho(t,x,y,u)\, du, \tag{3.1}$$

where $\lambda \in \mathbb{R}$ and ρ is some complex amplitude function. Among all the several possible hypotheses on ρ that makes $B(t)$ a bounded linear operator on $L^2(\mathbb{R}^n)$ we will introduce the following class of densities:

Definition 3.1. *Let Ξ_k be the class of all the complex functions $\rho : [0,T]\times\mathbb{R}^n\times\mathbb{R}^n\times\mathbb{R}^k \longrightarrow \mathbb{C}$, $\rho = \rho(t,x,y,u)$ such that*

i) $\sup_{x\in\mathbb{R}^n} \|\rho(t,x,\cdot,\cdot)\|_{L^1(\mathbb{R}^n\times\mathbb{R}^k)} \le C_T < +\infty$, $\forall t \in [0,T]$;

ii) $\sup_{y\in\mathbb{R}^n} \|\rho(t,\cdot,y,\cdot)\|_{L^1(\mathbb{R}^n\times\mathbb{R}^k)} \le C_T$, $\forall t \in [0,T]$.

It is easy to check that if $\rho \in \Xi_k$ then $B(t)$ is well defined and $B(t) \in \mathcal{L}(L^2(\mathbb{R}^n))$. Moreover

Lemma 3.2. *The family of operators $\{B(t)\}_{t\in[0,T]}$ is uniformly bounded on $L^2(\mathbb{R}^n)$, that is $\|B(t)\| \le C_T$ for all $t \in [0,T]$.*

Proof. By Schur Lemma and the properties of $\rho \in \Xi_k$ we have

$$\begin{aligned}
\|B(t)\|^2 &\le \Big(\sup_{x\in\mathbb{R}^n}\int_{\mathbb{R}^n} |b(t,x,y)|dy\Big)\cdot\Big(\sup_{y\in\mathbb{R}^n}\int_{\mathbb{R}^n} |b(t,x,y)|dx\Big) \\
&\le \Big(\sup_{x\in\mathbb{R}^n}\int_{\mathbb{R}^n}\int_{\mathbb{R}^k} |\rho(t,x,y,u)|dudy\Big)\cdot\Big(\sup_{y\in\mathbb{R}^n}\int_{\mathbb{R}^n}\int_{\mathbb{R}^k} |\rho(t,x,y,u)|dudx\Big) \\
&= \sup_{x\in\mathbb{R}^n} \|\rho(t,x,\cdot,\cdot)\|_{L^1(\mathbb{R}^n\times\mathbb{R}^k)} \cdot \sup_{y\in\mathbb{R}^n} \|\rho(t,\cdot,y,\cdot)\|_{L^1(\mathbb{R}^n\times\mathbb{R}^k)}. \\
&\le C_T^2
\end{aligned}$$

□

3.3 Properties of operators

Here we establish some important properties about the family of integral operators defined in the previous section. Operators of type (3.1) are the base to construct the integral representations (3). The next theorem is a crucial step because it allows us to prove that their kernel admits the same type of representation for each generating function S.

Theorem 3.3. *Assume that S_1 and S_2 be two generating functions for Λ_t weakly quadratic at infinity with space of parameters, respectively, $\mathbb{R}^{k_1}$ and $\mathbb{R}^{k_2}$. Then, for any $(t,x,y) \in [0,T] \times \mathbb{R}^n \times \mathbb{R}^n$ and $\lambda \in \mathbb{R}$, there exists a bounded linear operator*

$$N = N_{t,x,y,\lambda} : L^1(\mathbb{R}^{k_1};\mathbb{C}) \longrightarrow L^1(\mathbb{R}^{k_2};\mathbb{C}), \tag{3.2}$$

such that

$$\int_{\mathbb{R}^{k_1}} e^{i\lambda S_1(t,x,y,u)} \rho(u)\ du = \int_{\mathbb{R}^{k_2}} e^{i\lambda S_2(t,x,y,v)} \left[N\rho\right](v)\ dv, \quad \forall \lambda \in \mathbb{R}.$$

Moreover

$$\|N_{t,x,y,\lambda}\|_{\mathcal{L}(L^1(\mathbb{R}^{k_1});L^1(\mathbb{R}^{k_2}))} \leq 1. \tag{3.3}$$

In particular: if $\rho \in \Xi_{k_1}$, then $\tilde{\rho} = N\rho$, that is $\tilde{\rho}(t,x,y,v) := \left[N_{t,x,y,\lambda}\rho(t,x,y,\cdot)\right](v)$ belongs to Ξ_{k_2} for all $\lambda \in \mathbb{R}$.

Proof. By Viterbo's theorem 2.5 there exists stabilizations

$$\widetilde{S}_1 = S_1(t,x,y,u) + \langle Q_1(t,x,y)\bar{u},\bar{u}\rangle,$$

$$\widetilde{S}_2 = S_2(t,x,y,v) + \langle Q_2(t,x,y)\bar{v},\bar{v}\rangle,$$

of the generating functions S_1 and S_2 on the same space of parameters $(u,\bar{u}),(v,\bar{v}) \in \mathbb{R}^k = \mathbb{R}^{k_1} \times \mathbb{R}^{\bar{k}_1} = \mathbb{R}^{k_2} \times \mathbb{R}^{\bar{k}_2}$. We will call w the new parameters, that is $u = \Pi_{k_1} w$, $\bar{u} = \Pi_{\bar{k}_1} w$. Moreover there exists a fibered diffeomorphism

$$R_{t,x,y} : \mathbb{R}^k \longrightarrow \mathbb{R}^k$$

such that $\widetilde{S}_1$ and $\widetilde{S}_2$ are equivalent, that means

$$\widetilde{S}_1(t,x,y,w) = \widetilde{S}_2(t,x,y,R_{t,x,y}(w)), \quad \forall w \in \mathbb{R}^k.$$

Now, define

$$\sigma^1_{t,x,y,\lambda}(\bar{u}) := \frac{1}{(2\pi)^{k/2}} e^{-\frac{|\bar{u}|^2}{2} - i\lambda\langle Q_1(t,x,y)\bar{u},\bar{u}\rangle}.$$

This function clearly fulfills the following identity:

$$\int_{\mathbb{R}^{\bar{k}_1}} e^{i\lambda\langle Q_1(t,x,y)\bar{u},\bar{u}\rangle} \sigma^1_{t,x,y,\lambda}(\bar{u})\ d\bar{u} = 1.$$

Then, for any $\rho \in L^1(\mathbb{R}^{k_1};\mathbb{C})$, we have

$$\int_{\mathbb{R}^{k_1}} e^{i\lambda S_1(t,x,y,u)}\rho(u)\ du = \int_{\mathbb{R}^{k_1}\times\mathbb{R}^{\bar{k}_1}} e^{i\lambda(S_1(t,x,y,u)+\langle Q_1(t,x,y)\bar{u},\bar{u}\rangle)}\rho(u)\sigma^1_{t,x,y,\lambda}(\bar{u})\ du\ d\bar{u}$$

$$= \int_{\mathbb{R}^{k_1}\times\mathbb{R}^{\bar{k}_1}} e^{i\lambda\tilde{S}_1(t,x,y,w)}\rho(\Pi_{k_1}w)\sigma^1_{t,x,y,\lambda}(\Pi_{\bar{k}_1}w)\ dw$$

$$= \int_{\mathbb{R}^{k_1}\times\mathbb{R}^{\bar{k}_1}} e^{i\lambda\widetilde{S}_2(t,x,y,R_{t,x,y}(w))}\rho(\Pi_{k_1}w)\sigma^1_{t,x,y,\lambda}(\Pi_{\bar{k}_1}w)\ dw$$

$$= \int_{\mathbb{R}^{k_2}\times\mathbb{R}^{\bar{k}_2}} e^{i\lambda\widetilde{S}_2(t,x,y,w)}\rho\left(\Pi_{k_1}R^{-1}_{t,x,y}(w)\right)\sigma^1_{t,x,y,\lambda}\left(\Pi_{\bar{k}_1}R^{-1}_{t,x,y}(w)\right)|JR^{-1}_{t,x,y}(w)|\ dw$$

$$= \int_{\mathbb{R}^{k_2}} e^{i\lambda S_2(t,x,y,v)}\left[N_{t,x,y,\lambda}\ \rho\right](v)\ dv,$$

where, of course,

$$\left[N_{t,x,y,\lambda}\ \rho\right](v) := \int_{\mathbb{R}^{\bar{k}_2}} e^{i\lambda\langle Q_2(t,x,y)\bar{v},\bar{v}\rangle}\rho\left(\Pi_{k_1}R^{-1}_{t,x,y}(v,\bar{v})\right)\sigma^1_{t,x,y,\lambda}\left(\Pi_{\bar{k}_1}R^{-1}_{t,x,y}(v,\bar{v})\right)|JR^{-1}_{t,x,y}(v,\bar{v})|\ d\bar{v}. \tag{3.4}$$

It remains to prove that $N \equiv N_{t,x,y,\lambda} \in \mathcal{L}(L^1(\mathbb{R}^{k_1}); L^1(\mathbb{R}^{k_2}))$. This is straightforward because,

$$|N\rho(v)| \leq \int_{\mathbb{R}^{\bar{k}_2}} \left|\rho\left(\Pi_{k_1}R^{-1}_{t,x,y}(v,\bar{v})\right)\right|\sigma^1_{t,x,y,\lambda}\left(\Pi_{\bar{k}_1}R^{-1}_{t,x,y}(v,\bar{v})\right)|JR^{-1}_{t,x,y}(v,\bar{v})|\ d\bar{v}$$

hence,

$$\begin{aligned}
\|N\rho\|_{L^1(\mathbb{R}^{k_2})} &= \int_{\mathbb{R}^{k_2}} |N\rho(v)|\ dv \\
&\leq \int_{\mathbb{R}^{k_2}}\left(\int_{\mathbb{R}^{\bar{k}_2}} \left|\rho\left(\Pi_{k_1}R^{-1}_{t,x,y}(v,\bar{v})\right)\right|\sigma^1_{t,x,y,\lambda}\left(\Pi_{\bar{k}_1}R^{-1}_{t,x,y}(v,\bar{v})\right)|JR^{-1}_{t,x,y}(v,\bar{v})|\ d\bar{v}\right)dv \\
&= \int_{\mathbb{R}^{k_1}\times\mathbb{R}^{\bar{k}_1}} |\rho\left(\Pi_{k_1}w\right)|\sigma^1_{t,x,y,\lambda}\left(\Pi_{\bar{k}_1}w\right)\ dw \\
&= \left(\int_{\mathbb{R}^{k_1}}|\rho(u)|\ du\right)\left(\int_{\mathbb{R}^{\bar{k}_1}}\sigma^1_{t,x,y,\lambda}(\bar{u})\ d\bar{u}\right) \\
&= \|\rho\|_{L^1(\mathbb{R}^{k_1})}.
\end{aligned}$$

For the last part of the statement, just the last inequality shows that

$$\|\tilde{\rho}(t,x,y,\cdot)\|_{L^1(\mathbb{R}^{k_2})} \leq \|\rho(t,x,y,\cdot)\|_{L^1(\mathbb{R}^{k_1})},$$

and by this and the fact that $\rho \in \Xi_{k_1}$ it follows immediately that $\tilde{\rho} \in \Xi_{k_2}$, for any $\lambda \in \mathbb{R}$. $\square$

We now consider two operators of type (3.1) based upon two different ρ and different S, generating functions for Λ_t weakly quadratic at infinity. By the previous theorem, modulo a linear transformation, we can assume that the two kernels are of type

$$b_{1,2}(t,x,y) = \int_{\mathbb{R}^k} e^{i\lambda S(t,x,y,u)} \rho_{1,2}(t,x,y,u)\, du.$$

The next corollary, that indeed is an immediate consequence of the Theorem 3.3, shows that the convolution of the two operators generated in this way is still of the same type:

Corollary 3.4. *Consider $\lambda \in \mathbb{R}$, $S(t,x,y,u)$ GFQI of Λ_t, $\rho_{1,2} \in \Xi_k$ and let $b_{1,2}$ be the corresponding kernels for the operators $B_{1,2}$ defined as in (3.1). Moreover, suppose that $\|\rho_1(t,x,y,\cdot)\|_{L^1(\mathbb{R}^k)}$ is uniformly bounded in $t \in [0,T]$ and $y \in \mathbb{R}^n$, that is* [1]

$$\sup_{t\in[0,t]} \sup_{y\in\mathbb{R}^n} \|\rho_1(t,x,y,\cdot)\|_{L^1(\mathbb{R}^k)} < +\infty.$$

Finally, the operator

$$B(t)\varphi := \int_0^t B_1(t-s)B_2(s)\varphi\, ds.$$

is well defined and is of type (3.1) with corresponding ρ given by

$$\rho(t,x,z,u) = \int_0^t N_{t,x,z,\lambda} b_s(t,x,z,\cdot)\ ds,$$

where

$$b_s(t,x,z,w) = \rho_1(t-s,x,y,u)\rho_2(s,y,z,v), \quad w=(y,u,v).$$

Proof. First notice that, by definition,

$$\begin{aligned} B(t)\varphi &= \int_0^t B_1(t-s)B_2(s)\varphi\ ds \\ &= \int_0^t \left(\int_{\mathbb{R}^n} b_1(t-s,x,y) \int_{\mathbb{R}^n} b_2(s,y,z)\varphi(z)\ dz\ dy \right)\ ds \\ &= \int_{\mathbb{R}^n} \left(\int_0^t \int_{\mathbb{R}^n} b_1(t-s,x,y) b_2(s,y,z)\ dy\ ds \right) \varphi(z)\ dz. \end{aligned}$$

Now, by definition of $b_{1,2}$,

$$\begin{aligned} &\int_{\mathbb{R}^n} b_1(t-s,x,y)b_2(s,y,z)\ dy \\ &= \int_{\mathbb{R}^n} \left(\int_{\mathbb{R}^k} e^{i\lambda S(t-s,x,y,u)} \rho_1(t-s,x,y,u)\ du \right) \left(\int_{\mathbb{R}^k} e^{i\lambda S(s,y,z,v)} \rho_2(s,y,z,v)\ dv \right)\ dy \\ &= \int_{\mathbb{R}^k\times\mathbb{R}^k} \left(\int_{\mathbb{R}^n} e^{i\lambda [S(t-s,x,y,u)+S(s,y,z,v)]} \rho_1(t-s,x,y,u)\rho_2(s,y,z,v)\ dy \right)\ dudv, \end{aligned}$$

[1]This is striclty more than $\rho_1 \in \Xi_k$, but enough for our purpose.

all the exchanges in the integrals being justified by the application of Fubini–Tonelli theorem, that holds true in our hypotheses.

Define now the space of parameters $w := (y, u, v) \in \mathbb{R}^n \times \mathbb{R}^k \times \mathbb{R}^k = \mathbb{R}^{n+2k}$, and notice that the function

$$\tilde{S}_s(t, x, z, w) := S(t-s, x, y, u) + S(s, y, z, v)$$

is still a generating function of Λ_t, with parameters w and for $0 < s < t$. Introducing the auxiliary kernel $b_s(t, x, z, w) := \rho_1(t-s, x, y, u)\rho_2(s, y, z, v)$, and applying (3.2) the theorem 3.3 we can write

$$\begin{aligned}\int_{\mathbb{R}^n} b_1(t-s, x, y) b_2(s, y, z)\ dy &= \int_{\mathbb{R}^{n+2k}} e^{i\lambda \tilde{S}_s(t,x,z,w)} b_s(t, x, z, w)\ dw \\ &= \int_{\mathbb{R}^k} e^{i\lambda S(t,x,z,u)} N b_s(u)\ du,\end{aligned}$$

where N was defined in (3.4). We have to precise that Nb_s stands for $N_{t,x,z,\lambda} b_s(t, x, z, \cdot)$, and moreover that N depends upon s. We can finally write the form for the kernel of $B(t)$, being

$$b(t, x, z) = \int_0^t \int_{\mathbb{R}^k} e^{i\lambda S(t,x,z,u)} N b_s(u)\ du = \int_{\mathbb{R}^k} e^{i\lambda S(t,x,z,u)} \left(\int_0^t N b_s(u)\ ds \right)\ du,$$

so that the dependance on s disappear in $\rho(t, x, z, u) := \int_0^t N b_s(u)\ ds$. We have just finally to check that $\rho \in \Xi_k$. To this purpose, by (3.3), we have that

$$\|\rho(t, x, z, \cdot)\|_{L^1(\mathbb{R}^k)} \leq \int_0^t \|N b_s(\cdot)\|_{L^1(\mathbb{R}^k)}\ ds \leq \int_0^t \|b_s\|_{L^1(\mathbb{R}^{n+2k})}\ ds.$$

Now

$$\begin{aligned}\|b_s\|_{L^1(\mathbb{R}^{n+2k})} &\leq \int_{\mathbb{R}^n} \int_{\mathbb{R}^k} \int_{\mathbb{R}^k} |\rho_1(t-s, x, y, u)\rho_2(s, y, z, v)|\ dv\ du\ dy \\ &\leq \sup_{r \in [0,T], y \in \mathbb{R}^n} \|\rho_1(r, x, y, \cdot)\|_{L^1(\mathbb{R}^k)} \|\rho_2(s, y, \cdot, \cdot)\|_{L^1(\mathbb{R}^n \times \mathbb{R}^k)}\end{aligned}$$

and since $\rho_2 \in \Xi_k$ the conclusion is immediate. □

Chapter 4

The Schrödinger Propagator

4.1 Introduction

We briefly recall some well known facts about Schrödinger equation. First, if the potential $V \in L^\infty(\mathbb{R}^n) \cap L^p(\mathbb{R}^n)$ with $p > \frac{n}{2}$ and $p > 2$, it is well defined the selfadjoint operator $H := -\frac{\hbar^2}{2M}\Delta_x + V(x)$ on the domain $H^2(\mathbb{R}^n)$ (here $H^2(\mathbb{R}^n)$ stands for the usual Sobolev space $W^{2,2}(\mathbb{R}^n)$). Also in the case of $V \in L^\infty(\mathbb{R}^n;\mathbb{R})$ the same conclusions hold; in particular, as we have done in the previous sections, there will be considered $V \in C^2(\mathbb{R}^n;\mathbb{R})$ with compact support. This class of potentials arises in many problems of quantum mechanics, for example in problems of scattering and molecular modelling.
By Stone theorem it follows that it is well defined the unitary group of linear operators $e^{-\frac{i}{\hbar}tH}$, and for any $\varphi \in H^2(\mathbb{R}^n)$ the function $\psi(t,x) := e^{-\frac{i}{\hbar}tH}\varphi(x)$ is a strong solution for the Schrödinger equation

$$\begin{cases} i\hbar\partial_t\psi(t,x) = \left(-\frac{\hbar^2}{2m}\Delta + V(x)\right)\psi(t,x), & t \in \mathbb{R},\ x \in \mathbb{R}^n, \\ \psi(0,x) = \varphi(x), & x \in \mathbb{R}^n. \end{cases}$$

The starting point for a derivation of Feynman Path Integral representation is the following well known perturbative series expansion:

$$e^{-\frac{i}{\hbar}tH}\varphi = e^{\frac{i\hbar}{2}t\Delta}\varphi + \int_0^t e^{\frac{i\hbar}{2}(t-s)\Delta}Ve^{\frac{i\hbar}{2}s\Delta}\varphi\, ds + \dots \tag{4.1}$$

Unfortunately, the Feynman Path Integral,

$$e^{-\frac{i}{\hbar}tH}\varphi = \int_{\gamma(t)=x} e^{\frac{i}{\hbar}A[\gamma]}\ \varphi(\gamma(0))\ D\gamma, \tag{4.2}$$

that arises by this expansion is purely formal.
In order to obtain a rigorous Feynman like formula together with a wide class of integral representations, we apply the results of chapter 1 to determine a general set of series expansions for the regularized Propagator $U_\varepsilon(t) := e^{-\frac{i+\varepsilon}{\hbar}tH_\varepsilon}$, with $H_\varepsilon := -\frac{\hbar^2}{2m}\Delta - \frac{V}{(i+\varepsilon)^2}$:

$$U_\varepsilon(t)\varphi = \sum_{j=0}^{\infty} B_{\varepsilon,j}(t)\varphi.$$

It will be shown the connection between these series of operators and the class of generating functions S for the Lagrangian submanifold Λ_t by an appropriate integral representation. Indeed each terms of the series has the representation

$$B_{\varepsilon,j}(t)\varphi = \int_{\mathbb{R}^n} \int_{\mathbb{R}^k} e^{\frac{i}{(1+\varepsilon^2)\hbar} S(t,x,y,u)} \rho^{\hbar}_{\varepsilon,j}(t,x,y,u)\ du\ \varphi(y)\ dy. \tag{4.3}$$

The convergence of the series:

$$\sum_{j=0}^{\infty} \rho^{\hbar}_{\varepsilon,j} = \rho^{\hbar}_{\varepsilon}\ \in L^1(\mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^k; \mathbb{C}),$$

related to the series of the integral operators, permits us to obtain the representation:

$$U_{\varepsilon}(t)\varphi(x) = \int_{\mathbb{R}^n} \int_{\mathbb{R}^k} e^{\frac{i}{(1+\varepsilon^2)\hbar} S(t,x,y,u)} \rho^{\hbar}_{\varepsilon}(t,x,y,u)\ du\ \varphi(y)\ dy. \tag{4.4}$$

We point out that this representation is obtained for any generating function weakly quadratic at infinity S studied in chapter 2. In particular the generating function constructed in the Theorem 2.10 corresponds to the use of the Action functional $A[\gamma] = \int_0^t \frac{1}{2} m\,|\dot\gamma(s)|^2 - V(\gamma(s))\,ds$ evaluated on a suitable finite dimensional space of curves $\Gamma(t,x,y)$. This permits us to obtain a finite dimensional Path Integral formulation:

$$U_{\varepsilon}(t)\varphi(x) = \int_{\mathbb{R}^n} \int_{\Gamma(t,x,y)} e^{\frac{i}{(1+\varepsilon^2)\hbar} A[\gamma]}\, P^{\hbar}_{\varepsilon}(d\gamma)\ \varphi(y)\ dy.$$

This will be the subject of the last theorem of the chapter.

4.2 Series expansions of the Propagator

In this section we apply the results of chapter 1, about the series expansions of semigroups of linear operators, to the case of the regularized Schrodinger Propagator.
Now we begin by proving that a suitable ε-regularitazion of the Hamiltonian allows to approximate the unitary group $e^{-\frac{i}{\hbar}tH}$.

Theorem 4.1. *Assume that $V \in L^\infty(\mathbb{R}^n) \cap L^p(\mathbb{R}^n)$, $p > \frac{n}{2}$ and $p > 2$ and set*

$$H_\varepsilon := -\frac{\hbar^2}{2m}\Delta - \frac{V}{(i+\varepsilon)^2}.$$

Then $e^{-\frac{i}{\hbar}tH}$ is the strong limit of $e^{-\frac{i+\varepsilon}{\hbar}tH_\varepsilon}$, that is

$$\lim_{\varepsilon\to 0^+} e^{-\frac{i+\varepsilon}{\hbar}tH_\varepsilon}\varphi \overset{L^2(\mathbb{R}^n)}{=} e^{-\frac{i}{\hbar}tH}\varphi, \quad \forall\varphi \in H^2(\mathbb{R}^n). \tag{4.5}$$

Proof. By triangular inequality we have

$$\begin{aligned}\limsup_{\varepsilon\to 0^+}\left\|e^{-\frac{i+\varepsilon}{\hbar}tH_\varepsilon}\varphi - e^{-\frac{i}{\hbar}tH}\varphi\right\|_{L^2} &\le \limsup_{\varepsilon\to 0^+}\left\|e^{-\frac{i+\varepsilon}{\hbar}tH_\varepsilon}\varphi - e^{-\frac{i+\varepsilon}{\hbar}tH}\varphi\right\|_{L^2}\\ &+\limsup_{\varepsilon\to 0^+}\left\|e^{-\frac{i+\varepsilon}{\hbar}tH}\varphi - e^{-\frac{i}{\hbar}tH}\varphi\right\|_{L^2}\end{aligned}$$

For the first term in the right hand side we observe that

$$K_\varepsilon := H_\varepsilon - H = -\frac{\hbar^2}{2m}\Delta - \frac{V}{(i+\varepsilon)^2} - \Big(-\frac{\hbar^2}{2m}\Delta + V\Big) = -\Big[1 + \frac{1}{(i+\varepsilon)^2}\Big]V$$

it is a bounded operator on $L^2(\mathbb{R}^n)$ $\forall\varepsilon > 0$, and verifies $\lim_{\varepsilon\to 0+}\|K_\varepsilon\| = 0$. Therefore, applying Theorem 1.7 we conclude that

$$\left\|e^{-\frac{i+\varepsilon}{\hbar}tH_\varepsilon}\varphi - e^{-\frac{i+\varepsilon}{\hbar}tH}\varphi\right\|_{L^2} \le \Big(e^{\|K_\varepsilon\|C_T t} - 1\Big)\|\varphi\|_{L^2} \overset{\varepsilon\to 0+}{\longrightarrow} 0,$$

where $C_T = \sup_{\varepsilon\in]0,1]}\left\|e^{-\frac{i+\varepsilon}{\hbar}tH}\right\| < +\infty$ for any t fixed. For the second term

$$\left\|e^{-\frac{i+\varepsilon}{\hbar}tH}\varphi - e^{-\frac{i}{\hbar}tH}\varphi\right\|_{L^2} = \left\|e^{-\frac{\varepsilon}{\hbar}tH}\varphi - \varphi\right\|_{L^2} \overset{\varepsilon\to 0+}{\longrightarrow} 0,$$

by the strong continuity of the semigroup $e^{-\frac{\varepsilon}{\hbar}tH}$. □

In the following definition we will assume that S is the generating function constructed in Theorem (2.10), where it is proved the decomposition $S = m\frac{|x-y|^2}{2t} + \frac{m}{2}|u|^2 + c(t,x,y,u)$, with the remaining term $c \in C^2_b$.

Definition 4.2. *We introduce the set*

$$\Sigma^\hbar_\varepsilon := \left\{\sigma \in L^1(\mathbb{R}^k;\mathbb{C}) \ : \ \int_{\mathbb{R}^k}\sigma(u)e^{-\frac{1}{(i+\varepsilon)\hbar}\frac{m}{2}|u|^2}du = 1\right\}. \tag{4.6}$$

Then, given $\sigma_\varepsilon^\hbar \in \Sigma_\varepsilon^\hbar$, we define the integral operator with parameters $t \in]0,T]$ and $\varepsilon > 0$:

$$W_\varepsilon(t)\varphi(x) := \int_{\mathbb{R}^n} \int_{\mathbb{R}^k} \frac{1}{(2\pi t(i+\varepsilon)\hbar)^{n/2}} e^{-\frac{1}{(i+\varepsilon)\hbar}S(t,x,y,u)} \sigma_\varepsilon^\hbar(u)\ du\ \varphi(y)\ dy. \tag{4.7}$$

We will denote by $W_\varepsilon(t,x,y)$ the kernel of $W_\varepsilon(t)$, that is,

$$W_\varepsilon(t,x,y) := \int_{\mathbb{R}^k} \frac{1}{(2\pi t(i+\varepsilon)\hbar)^{n/2}} e^{-\frac{1}{(i+\varepsilon)\hbar}S(t,x,y,u)} \sigma_\varepsilon^\hbar(u)\ du. \tag{4.8}$$

Remark 4.3. *This set of operators, defined as the conseguence of the different choice of the function $\sigma_\varepsilon^\hbar \in \Sigma_\varepsilon^\hbar$, is contained in the family of operators studied in the previous chapter. For this reason the operators $W_\varepsilon(t)$ are not directly related to the particular function S because, in view of Theorem 3.2, this representation of the kernel is possible for any generating function weakly quadratic at infinity. Moreover we observe that the functions $\sigma_\varepsilon^\hbar$ depends only from the auxiliary parameters $u \in \mathbb{R}^k$. As a conseguence we can say that these operators are related to the entire class of weakly quadratic generating functions, and with respect to this we can say that they are directly connected to the group of canonical transfomations ϕ_H^t generating Λ_t. As we will see in next theorems, these operators represent the main tool to contruct series expansions converging to the Schrödinger Propagator.*

With this settings, we have the following theorem about properties of these operators:

Theorem 4.4. *Let $\sigma_\varepsilon^\hbar \in \Sigma_\varepsilon^\hbar$, $\{W_\varepsilon(t)\}_{t\in[0,T]}$, $\varepsilon > 0$ defined by (4.2). Then $W_\varepsilon(t) \in \mathcal{L}(L^2(\mathbb{R}^n))$ and verifies the properties of Theorem 1.3, that is:*

i) $W_\varepsilon(\cdot)\varphi \in C^0([0,T]; L^2(\mathbb{R}^n))$, $\forall \varphi \in L^2(\mathbb{R}^n)$;

ii) $W_\varepsilon(\cdot)\varphi \in C^1(]0,T]; L^2(\mathbb{R}^n))$, $\forall \varphi \in H^2(\mathbb{R}^n)$;

iii) $\lim_{t\to 0^+} W_\varepsilon(t)\varphi = \varphi$, $\forall \varphi \in L^2(\mathbb{R}^n)$;

iv) there exists a constant $C_T \geq 0$ depending only by T such that

$$\|(W_\varepsilon(t)L_\varepsilon - W'_\varepsilon(t))\varphi\|_{L^2} \leq C_T\|\varphi\|_{L^2}, \quad \forall\varphi \in H^2(\mathbb{R}^n),\ \forall t \in]0,T];$$

where $L_\varepsilon := -\frac{i+\varepsilon}{\hbar}H_\varepsilon = -\frac{i+\varepsilon}{\hbar}\left(-\frac{\hbar^2}{2m}\Delta - \frac{V}{(i+\varepsilon)^2}\right)$.

Proof. We first prove that $W_\varepsilon(t) \in \mathcal{L}(L^2(\mathbb{R}^n))$ for all $t \in]0,T]$ ($W_\varepsilon(0) = I$). Due to the Schur lemma, we prove that

$$\sup_{x\in\mathbb{R}^n} \int_{\mathbb{R}^n} |W_\varepsilon(t,x,y)|\ dy < +\infty, \quad \sup_{y\in\mathbb{R}^n} \int_{\mathbb{R}^n} |W_\varepsilon(t,x,y)|\ dx < +\infty.$$

Because these two estimates are similar, we will limit to prove only the first one. To do this first notice that

$$\int_{\mathbb{R}^n} |W_\varepsilon(t,x,y)|\ dy \leq \int_{\mathbb{R}^n} \int_{\mathbb{R}^k} \left| \frac{1}{(2\pi t(i+\varepsilon)\hbar)^{n/2}} e^{-\frac{1}{\hbar(i+\varepsilon)}S(t,x,y,u)} \sigma_\varepsilon^\hbar(u) \right|\ du\ dy.$$

Now, we recall that a particular generating function S, constructed in theorem 2.10, has the decomposition:

$$S(t,x,y,u) = m\frac{|x-y|^2}{2t} + \frac{m}{2}|u|^2 + c(t,x,y,u). \tag{4.9}$$

But all the others are obtained by fibered diffeomorphism, stabilizations and sum of constants so they the proof in what follows does not change so much in the general case. However in this case we can obtain the estimate:

$$\left| e^{-\frac{1}{\hbar(i+\varepsilon)}S} \right| \leq e^{-\frac{\varepsilon}{\hbar(1+\varepsilon^2)}\left(\frac{|x-y|^2}{2t}+\frac{m}{2}|u|^2+c(t,x,y,u)\right)}, \quad \forall t\in[0,T], \tag{4.10}$$

Therefore,

$$\begin{aligned}
&\int_{\mathbb{R}^n} |W_\varepsilon(t,x,y)|\ dy \\
&\leq \int_{\mathbb{R}^n} \frac{1}{\left(2\pi\hbar t\sqrt{1+\varepsilon^2}\right)^{n/2}} e^{-\frac{\varepsilon}{\hbar(1+\varepsilon^2)}\frac{|x-y|^2}{2t}} \left[\int_{\mathbb{R}^k} e^{-\frac{\varepsilon}{\hbar(1+\varepsilon^2)}\left(\frac{m}{2}|u|^2+c(t,x,y,u)\right)}|\sigma_\varepsilon^\hbar(u)|\ du\ \right] dy \\
&\leq M_\varepsilon^\hbar \int_{\mathbb{R}^n} \frac{1}{\left(2\pi\hbar t\sqrt{1+\varepsilon^2}\right)^{n/2}} e^{-\frac{\varepsilon}{\hbar(1+\varepsilon^2)}\frac{|x-y|^2}{2t}} dy
\end{aligned}$$

Indeed, in view of the definition (4.6) of $\sigma_\varepsilon^\hbar$ and by using the property $c(t,\cdot)\in L^\infty$ with respect all variables, we have:

$$M_\varepsilon^\hbar := \sup_{(t,x,y)\in[0,T]\times\mathbb{R}^{2n}} \int_{\mathbb{R}^k} e^{-\frac{\varepsilon}{\hbar(1+\varepsilon^2)}\left(\frac{m}{2}|u|^2+c(t,x,y,u)\right)}|\sigma_\varepsilon^\hbar(u)|\ du < +\infty \tag{4.11}$$

Henceforth, noticing moreover that

$$\int_{\mathbb{R}^n} \frac{1}{\left(2\pi\hbar t\sqrt{1+\varepsilon^2}\right)^{n/2}} e^{-\frac{\varepsilon}{\hbar(1+\varepsilon^2)}\frac{|x-y|^2}{2t}} dy = \left(\frac{\sqrt{1+\varepsilon^2}}{\varepsilon}\right)^{n/2},$$

we finally conclude that, ,

$$\int_{\mathbb{R}^n} |W_\varepsilon(t,x,y)|\ dy \leq M_\varepsilon^\hbar \left(\frac{\sqrt{1+\varepsilon^2}}{\varepsilon}\right)^{n/2}, \quad \forall\ 0<\varepsilon<1, \quad t\in[0,T],$$

and by this the conclusion is immediate. For the remaining statements of the Lemma, the unique serious part is the proof of point iv). Let $\varphi\in H^2(\mathbb{R}^n)$. By direct computation and integration by parts, we have

$$\begin{aligned}
&W_\varepsilon(t)L_\varepsilon\varphi - W_\varepsilon'(t)\varphi = \\
&= \int_{\mathbb{R}^n} \left[W_\varepsilon(t,x,y)\left(-\frac{i+\varepsilon}{\hbar}\left(-\frac{\hbar^2}{2m}\Delta_y\varphi(y) - \frac{V(y)}{(i+\varepsilon)^2}\varphi(y)\right)\right) - \partial_t W_\varepsilon(t,x,y)\varphi(y)\right] dy \\
&= \int_{\mathbb{R}^n} \left[\frac{(i+\varepsilon)\hbar}{2m}\Delta_y W_\varepsilon(t,x,y) + W_\varepsilon(t,x,y)\frac{V(y)}{(i+\varepsilon)\hbar} - \partial_t W_\varepsilon(t,x,y)\right]\varphi(y)\ dy \\
&=: \int_{\mathbb{R}^n} G_\varepsilon(t,x,y)\varphi(y)\ dy.
\end{aligned} \tag{4.12}$$

By computing all the derivatives in $W_\varepsilon(t,x,y)$ we deduce:

$$
\begin{aligned}
G_\varepsilon(t,x,y) &= \int_{\mathbb{R}^k}\left[\frac{V(y)}{(i+\varepsilon)\hbar}-\frac{\Delta_y S}{2m}+\frac{1}{(i+\varepsilon)\hbar}\frac{|\nabla_y S|^2}{2m}+\frac{n}{2t}+\frac{1}{(i+\varepsilon)\hbar}\partial_t S\right]\sigma_\varepsilon^\hbar(u)e^{-\frac{\varepsilon}{1+\varepsilon^2}S}e^{i\lambda_{\varepsilon,\hbar}S}du \\
&=: \int_{\mathbb{R}^k} g_\varepsilon(t,x,y,u)e^{i\lambda_{\varepsilon,\hbar}S}\,du,
\end{aligned}
\tag{4.13}
$$

for $\lambda_{\varepsilon,\hbar}=\frac{1}{(1+\varepsilon^2)\hbar}$. By using (4.9) in (4.13) we obtain

$$
\begin{aligned}
&g_\varepsilon(t,x,y,u)= \\
&= \left[\frac{V(y)}{(i+\varepsilon)\hbar}-\frac{\Delta_y c}{2M}-\frac{n}{2t}+\frac{1}{(i+\varepsilon)\hbar}\frac{|\nabla_y c|^2}{2m}+\frac{1}{(i+\varepsilon)\hbar}\frac{|\nabla_y S_0|^2}{2m}+\frac{1}{(i+\varepsilon)\hbar}\frac{\nabla_y S_0\cdot\nabla_y c}{m}\right. \\
&+ \left.\frac{n}{2t}+\frac{1}{(i+\varepsilon)\hbar}\partial_t S_0+\frac{1}{(i+\varepsilon)\hbar}\partial_t c\right]\frac{\sigma_\varepsilon^\hbar(u)}{(2\pi t(i+\varepsilon)\hbar)^{n/2}}e^{-\frac{\varepsilon}{1+\varepsilon^2}S} \\
&= \left[\frac{V(y)}{(i+\varepsilon)\hbar}-\frac{\Delta_y c}{2m}+\frac{1}{(i+\varepsilon)\hbar}\frac{|\nabla_y c|^2}{2m}+\frac{1}{(i+\varepsilon)\hbar}\frac{\nabla_y S_0\cdot\nabla_y c}{m}+\frac{1}{(i+\varepsilon)\hbar}\partial_t c\right]\frac{\sigma_\varepsilon^\hbar(u)e^{-\frac{\varepsilon}{1+\varepsilon^2}S}}{(2\pi t(i+\varepsilon)\hbar)^{n/2}}
\end{aligned}
$$

because, if we denote as $S_0 := m\frac{|x-y|^2}{2t}$, then we have:

$$
\frac{|\nabla S_0|^2}{2m}+\partial_t S_0=0.
$$

We can now proceed with the estimates: it is easy to check that for $\varepsilon\le 1$ we have that

$$
|g_\varepsilon(t,x,y,u)|\le\left[C_1+\frac{C_2}{\hbar}+\frac{C_3}{\hbar}|x-y|\right]\frac{|\sigma_\varepsilon^\hbar(u)|}{\left(2\pi\hbar\sqrt{1+\varepsilon^2}t\right)^{n/2}}\left|e^{-\frac{\varepsilon}{1+\varepsilon}S}\right|, \tag{4.14}
$$

The constants $C_{1,2,3}$ are also depending upon T:

$$
C_1 := \frac{1}{2m}\sup_{t\in[0,T]}\|\Delta_y c(t,\cdot)\|_\infty \tag{4.15}
$$

$$
C_2 := \sup_{t\in[0,T]}\left\|V(\cdot)+\frac{|\nabla_y c(t,\cdot)|^2}{2m}+\nabla_y c(t,\cdot)+\partial_t c(t,\cdot)\right\|_\infty \tag{4.16}
$$

$$
C_3 := \sup_{t\in[0,T]}\left\|\frac{\nabla_y c(t,\cdot)}{t}\right\|_\infty \tag{4.17}
$$

where $\|\cdot\|_\infty$ is evaluated with respect to $(x,y,u)\in\mathbb{R}^n\times\mathbb{R}^n\times\mathbb{R}^k$.

Therefore, recalling also (4.10),

$$\begin{aligned}
&\sup_{x\in\mathbb{R}^n}\int_{\mathbb{R}^n}|G_\varepsilon(t,x,y)|dy \\
&\quad\le \sup_{x\in\mathbb{R}^n}\int_{\mathbb{R}^n}\left|\int_{\mathbb{R}^k} g_\varepsilon(t,x,y,u)e^{i\lambda_{\varepsilon,\hbar}S(t,x,y,u)}\ du\right|\ dy \\
&\quad\le \sup_{x\in\mathbb{R}^n}\int_{\mathbb{R}^n}\int_{\mathbb{R}^k}|g_\varepsilon(t,x,y,u)|\ du\ dy \\
&\quad\le \sup_{x\in\mathbb{R}^n}\int_{\mathbb{R}^n}\int_{\mathbb{R}^k}\left[C_1+\frac{C_2}{\hbar}+\frac{C_3}{\hbar}|x-y|\right]\frac{|\sigma_\varepsilon^\hbar(u)|}{\left(2\pi\hbar t\sqrt{1+\varepsilon^2}\right)^{n/2}}\left|e^{-\frac{\varepsilon}{1+\varepsilon}S}\right|du\ dy \\
&\quad= \sup_{x\in\mathbb{R}^n}\int_{\mathbb{R}^n}\int_{\mathbb{R}^k}\left[C_1+\frac{C_2}{\hbar}+\frac{C_3}{\hbar}|x-y|\right]\frac{|\sigma_\varepsilon^\hbar(u)|}{\left(2\pi\hbar t\sqrt{1+\varepsilon^2}\right)^{n/2}}\ e^{-\frac{\varepsilon}{\hbar(1+\varepsilon^2)}\left(\frac{|x-y|^2}{2t}+\frac{m}{2}|u|^2+c(t,x,y,u)\right)}dudy \\
&\quad\le M_\varepsilon^\hbar\sup_{x\in\mathbb{R}^n}\int_{\mathbb{R}^n}\left[C_1+\frac{C_2}{\hbar}+\frac{C_3}{\hbar}|x-y|\right]\frac{1}{\left(2\pi\hbar t\sqrt{1+\varepsilon^2}\right)^{n/2}}\ e^{-\frac{\varepsilon}{\hbar(1+\varepsilon^2)}\frac{|x-y|^2}{2t}}\ dy
\end{aligned}$$

where $M_\varepsilon^\hbar$ it is defined in (4.11). Integrating the others terms we have:

$$\sup_{x\in\mathbb{R}^n}\int_{\mathbb{R}^n}|G_\varepsilon(t,x,y)|dy \le M_\varepsilon^\hbar\left(C_1+\frac{C_2}{\hbar}+\frac{C_3}{2\hbar}\right)\left(\frac{\sqrt{1+\varepsilon^2}}{\varepsilon}\right)^{\frac{n}{2}},\quad \forall t\in]0,T], \tag{4.18}$$

Because:

$$\int_{\mathbb{R}^n}|x-y|\frac{1}{\left(2\pi\hbar t\sqrt{1+\varepsilon^2}\right)^{n/2}}\ e^{-\frac{\varepsilon}{\hbar(1+\varepsilon^2)}\frac{|x-y|^2}{2t}}\ dy=\frac{1}{2}\left(\frac{\sqrt{1+\varepsilon^2}}{\varepsilon}\right)^{\frac{n}{2}}$$

In the same way

$$\sup_{y\in\mathbb{R}^n}\int_{\mathbb{R}^n}|G_\varepsilon(t,x,y,\hbar)|dx\le M_\varepsilon^\hbar\left(C_1+\frac{C_2}{\hbar}+\frac{C_3}{2\hbar}\right)\left(\frac{\sqrt{1+\varepsilon^2}}{\varepsilon}\right)^{\frac{n}{2}},\quad \forall t\in]0,T], \tag{4.19}$$

Finally, by (4.18) and (4.19),

$$\begin{aligned}
\|W_\varepsilon(t)L_\varepsilon\varphi-W'_\varepsilon(t)\varphi\|_{L^2}^2 &\le \left(\sup_{x\in\mathbb{R}^n}\int_{\mathbb{R}^n}|G_\varepsilon(t,x,y)|\ dy\right)\left(\sup_{y\in\mathbb{R}^n}\int_{\mathbb{R}^n}|G_\varepsilon(t,x,y)|\ dx\right)\|\varphi\|_{L^2}^2 \\
&\le \left[M_\varepsilon^\hbar\left(C_1+\frac{C_2}{\hbar}+\frac{C_3}{2\hbar}\right)\right]^2\left(\frac{\sqrt{1+\varepsilon^2}}{\varepsilon}\right)^n,\quad \forall t\in]0,T].
\end{aligned}$$

which is the conclusion. □

In the previous theorem we have proved that operators $W_\varepsilon(t)$ satisfy the properties of Thereom 1.3; this is important because now we can apply Theorem 1.5 and use these operators to construct series that converges directly to the semigroup of linear operators corresponding to regularized Propagator $U_\varepsilon(t)$.

Theorem 4.5. *Let $\sigma_\varepsilon^\hbar \in \Sigma_\varepsilon^\hbar$ fixed, $\Sigma_\varepsilon^\hbar$ being defined by (4.6), $W_\varepsilon(t)$ defined by (4.7) and $G_\varepsilon(t) := W_\varepsilon(t)L_\varepsilon - W'_\varepsilon(t)$ with $L_\varepsilon := -\frac{i+\varepsilon}{\hbar}H_\varepsilon$. Then, the semigroup of bounded operators generated by the operator $H_\varepsilon = -\frac{\hbar^2}{2m}\Delta - \frac{V}{(i+\varepsilon)^2}$ admits the strongly convergent series expansion:*

$$e^{-\frac{(i+\varepsilon)}{\hbar}tH_\varepsilon}\varphi = \sum_{j=0}^{\infty} B_{\varepsilon,j}(t)\varphi, \quad \forall \varphi \in H^2(\mathbb{R}^n), \tag{4.20}$$

where $B_{\varepsilon,0}(t) := W_\varepsilon(t)$, and

$$B_{\varepsilon,j+1}(t)\varphi = \int_0^t G_\varepsilon(t-s)B_{\varepsilon,j}(s)\varphi \; ds, \quad \forall j \geq 0.$$

□

Remark 4.6. *Notice that there is not a unique series expansion (4.20), because this depends on the choice of $\sigma_\varepsilon^\hbar \in \Sigma_\varepsilon^\hbar$. In this way we have a set of different series that converges to the same semigroup, that anyway is not the entire set of possible series that arises in the setting of chapter 1. This is due to the choice we made about the definition of the set $\Sigma_\varepsilon^\hbar$, in order to contruct in a simple way a set of operators $W_\varepsilon(t)$ that it is intrisically related to the Hamiltonian flow, as we have pointed out in Remark 4.3.*

4.3 Integral Representations of the Propagator

The next step is to study the form of series espansion (4.20). In particular, we want to show that there is an appropriate integral representation of $e^{-\frac{(i+\varepsilon)}{\hbar}tH_\varepsilon}\varphi$. In order to do this we have to study the convergence of the kernels of the operators $B_{\varepsilon,j}(t)$:

Theorem 4.7. *Let $\varepsilon, \hbar > 0$, $\sigma_\varepsilon^\hbar \in \Sigma_\varepsilon^\hbar$ fixed. Choose a generating function S weakly quadratic at infinity for the submanifold Λ_t. There exists then a function $\rho_\varepsilon^\hbar = \rho_\varepsilon^\hbar(t,x,y,u)$ such that*

$$e^{-\frac{(i+\varepsilon)}{\hbar}tH_\varepsilon}\varphi(x) = \int_{\mathbb{R}^n} U_\varepsilon(t,x,y)\varphi(y)\; dy, \quad \forall \varphi \in H^2(\mathbb{R}^n), \tag{4.21}$$

where

$$U_\varepsilon(t,x,y) := \int_{\mathbb{R}^k} e^{\frac{i}{(1+\varepsilon^2)\hbar}S(t,x,y,u)}\rho_\varepsilon^\hbar(t,x,y,u)\; du. \tag{4.22}$$

Proof. By (4.20) we have

$$e^{-\frac{(i+\varepsilon)}{\hbar}tH_\varepsilon}\varphi = \sum_{j=0}^{\infty} B_{\varepsilon,j}(t)\varphi, \quad \forall \varphi \in H^2(\mathbb{R}^n).$$

We recall that

$$B_{\varepsilon,j}(t)\varphi(x) = \int_{\mathbb{R}^n}\left(\int_{\mathbb{R}^k}\frac{1}{(2\pi t(i+\varepsilon)\hbar)^{n/2}}e^{-\frac{1}{(i+\varepsilon)\hbar}S(t,x,y,u)}\sigma_\varepsilon^\hbar(u)\; du\right)\varphi(y)\; dy.$$

Defining

$$\rho^{\hbar}_{\varepsilon,0}(t,x,y,u) := \frac{1}{(2\pi t(i+\varepsilon)\hbar)^{n/2}} e^{-\frac{\varepsilon}{(1+\varepsilon^2)\hbar}S(t,x,y,u)}\sigma^{\hbar}_{\varepsilon}(u),$$

we have that

$$B_{\varepsilon,0}(t)\varphi(x) = \int_{\mathbb{R}^n}\left(\int_{\mathbb{R}^k} e^{i\lambda_{\varepsilon,\hbar}S(t,x,y,u)}\rho^{\hbar}_{\varepsilon,0}(t,x,y,u)\ du\right)\varphi(y)\ dy,$$

where $\lambda_{\varepsilon,\hbar} = \frac{1}{(1+\varepsilon^2)\hbar}$. It is easy to check that $\rho^{\hbar}_{\varepsilon,0} \in \Xi_k$, where the class Ξ_k is defined by 3.1. Moreover, by definition of the operator $G_\varepsilon(t)$ and (4.13),

$$G_\varepsilon(t)\varphi(x) = \int_{\mathbb{R}^n}\left(\int_{\mathbb{R}^k} e^{i\lambda_{\varepsilon,\hbar}S} g_\varepsilon(t,x,y,u)\sigma^{\hbar}_{\varepsilon}(u)\ du\right)\varphi(y)\ dy,$$

It is easily verified that, by (4.14), $g_\varepsilon \times \sigma^{\hbar}_{\varepsilon} \in \Xi_k$. Furthermore, by (4.18), $\|g_\varepsilon(t,x,y,\cdot)\sigma^{\hbar}_{\varepsilon}(\cdot)\|_{L^1}$ is uniformly bounded in $(t,y) \in [0,T]\times\mathbb{R}^n$. Therefore, applying corollary 3.4 j-times we obtain that

$$B_{\varepsilon,j}(t)\varphi(x) = \int_{\mathbb{R}^n}\left(\int_{\mathbb{R}^k} e^{i\lambda_{\varepsilon,\hbar}S(t,x,y,u)}\rho^{\hbar}_{\varepsilon,j}(t,x,y,u)\ du\right)\varphi(y)\ dy,$$

where

$$\rho^{\hbar}_{\varepsilon,j}(t,x,y,u) = \int_0^t N_{t,x,y,\lambda_{\varepsilon,\hbar}}\left[g_\varepsilon(t-s,x,\flat,\sharp)\sigma^{\hbar}_{\varepsilon}(\sharp)\rho^{\hbar}_{\varepsilon,j-1}(s,\flat,y,\natural)\right]\ ds. \tag{4.23}$$

Therefore

$$e^{-\frac{(i+\varepsilon)}{t}\hbar H_\varepsilon}\varphi(x) \quad = \sum_{j=0}^{\infty}\int_{\mathbb{R}^n}\int_{\mathbb{R}^k} e^{i\lambda_{\varepsilon,\hbar}S(t,x,y,u)}\rho^{\hbar}_{\varepsilon,j}(t,x,y,u)\varphi(y)\ du\ dy. \tag{4.24}$$

Our aim is now to exchange the sum with the two integrals in (4.24). In order to do this it is enough to prove the total convergence of the series $\sum_{j=0}^{\infty} e^{i\lambda_{\varepsilon,\hbar}S(t,x,y,u)}\rho^{\hbar}_{\varepsilon,j}(t,x,y,u)\varphi(y)$, that is the convergence in norm $L^1(\mathbb{R}^n\times\mathbb{R}^k)$. With this respect, note that

$$\begin{aligned}\sum_{j=0}^{\infty}\left\| e^{i\lambda_{\varepsilon,\hbar}S(t,x,\cdot,\bullet)}\rho^{\hbar}_{\varepsilon,j}(t,x,\cdot,\bullet)\varphi(\cdot)\right\|_{L^1(\mathbb{R}^n\times\mathbb{R}^k)} &\leq \sum_{j=0}^{\infty}\left\|\rho^{\hbar}_{\varepsilon,j}(t,x,\cdot,\bullet)\varphi(\cdot)\right\|_{L^1(\mathbb{R}^n\times\mathbb{R}^k)} \\ &= \sum_{j=0}^{\infty}\int_{\mathbb{R}^n}\int_{\mathbb{R}^k}|\rho^{\hbar}_{\varepsilon,j}(t,x,y,u)|du\ |\varphi(y)|\ dy\end{aligned}$$

Now, by (3.3) and (4.23) we have that

$$\|\rho^{\hbar}_{\varepsilon,j}(t,x,y,\cdot)\|_{L^1(\mathbb{R}^k)} \leq \int_0^t \left\| g_\varepsilon(t-s,x,\flat,\sharp)\sigma^{\hbar}_{\varepsilon}(\sharp)\rho^{\hbar}_{\varepsilon,j-1}(s,\flat,y,\natural)\right\|_{L^1(\mathbb{R}^n\times\mathbb{R}^k\times\mathbb{R}^k)}\ ds.$$

Recalling (4.14),

$$\begin{aligned}
&\left\| g_\varepsilon(t-s,x,\flat,\sharp)\sigma^\hbar_\varepsilon(\sharp)\rho^\hbar_{\varepsilon,j-1}(s,\flat,y,\natural)\right\|_{L^1(\mathbb{R}^n\times\mathbb{R}^k\times\mathbb{R}^k)} \\
&= \int_{\mathbb{R}^n}\int_{\mathbb{R}^k}\int_{\mathbb{R}^k} |g_\varepsilon(t-s,x,z,v)\sigma^\hbar_\varepsilon(v)\rho^\hbar_{\varepsilon,j-1}(s,z,y,u)|\ dv\ du\ dz \\
&= \int_{\mathbb{R}^n}\int_{\mathbb{R}^k} |g_\varepsilon(t-s,x,z,v)\sigma^\hbar_\varepsilon(v)|\ \|\rho^\hbar_{\varepsilon,j-1}(s,z,y,\cdot)\|_{L^1(\mathbb{R}^k)}\ dv\ dz,
\end{aligned}$$

therefore

$$\|\rho^\hbar_{\varepsilon,j}(t,x,y,\cdot)\|_{L^1(\mathbb{R}^k)} \le \int_0^t \left(\int_{\mathbb{R}^n}\int_{\mathbb{R}^k} |g_\varepsilon(t-s,x,z,v)\sigma^\hbar_\varepsilon(v)|\ \|\rho^\hbar_{\varepsilon,j-1}(s,z,y,\cdot)\|_{L^1(\mathbb{R}^k)}\ dv\ dz \right) ds,$$

and iterating this inequality we obtain

$$\begin{aligned}
&\|\rho^\hbar_{\varepsilon,j}(t,x,y,\cdot)\|_{L^1(\mathbb{R}^k)} \\
&\le \int_{\Delta_j} \left(\int_{(\mathbb{R}^n)^{j+1}} \int_{(\mathbb{R}^k)^j} \prod_{k=1}^{j} |g_\varepsilon(t_{k-1}-t_k,x_k,x_{k+1},v_k)\sigma^\hbar_\varepsilon(v_k)|\ \|\rho^\hbar_{\varepsilon,0}(t_j,x_{j+1},y,\cdot)\|_{L^1(\mathbb{R}^k)} dv dx \right) dt,
\end{aligned}$$

where $dv = dv_1\cdots dv_j$, $dx = dx_1\cdots dx_{j+1}$, $dt = dt_1\cdots dt_j$, $\Delta_j = \{(t_1,\dots,t_j)\ :\ 0 \le t_j \le t_{j-1} \le \dots \le t_1 \le t\}$ is the $j-$dimensional simplex and with the agreeing that $x_0 = x$ and $t_0 = t$. Now, by definition of $\rho^\hbar_{\varepsilon,0}$, by (4.10) applied in a similar way of (4.18) we obtain

$$\sup_{x_j\in\mathbb{R}^n} \int_{\mathbb{R}^n}\int_{\mathbb{R}^k} |g_\varepsilon(t_{j-1}-t_j,x_j,x_{j+1},v_j)\sigma^\hbar_\varepsilon(v_j)|\ \|\rho^\hbar_{\varepsilon,0}(t_j,x_{j+1},y,\cdot)\|_{L^1(\mathbb{R}^k)}\ dx_{j+1}\ dv_j \le K^\hbar_\varepsilon$$

where the constant $K^\hbar_\varepsilon$ depend (as shown) from ε and $\hbar$ but also from t, that we consider fixed. In order to conclude we observe that iterating the previous estimate we get:

$$\|\rho^\hbar_{\varepsilon,j}(t,x,y,\cdot)\|_{L^1(\mathbb{R}^k)} \le K^\hbar_{\varepsilon,j}\int_{\Delta_j} dt = K^\hbar_{\varepsilon,j}\frac{t^j}{j!},$$

and now the conclusion follows easily. □

Now we consider the previuos result about integral representations of the regularized Propagator $U_\varepsilon(t)$, together with the result, Th. (4.1), on the covergence to the exact Propagator $U(t)$ as $\varepsilon \to 0$.

Theorem 4.8. *Let $H = -\frac{\hbar^2}{2m}\Delta + V(x)$ where $V \in C^2(\mathbb{R}^n)$ with compact support, and $\psi(t) := e^{-\frac{i}{\hbar}tH}\varphi$, $\varphi \in H^2(\mathbb{R}^n)$. Choose a generating function S weakly quadratic at infinity for the submanifold Λ_t.*
Then, for any $\varepsilon > 0$ there exists $\rho^\hbar_\varepsilon(t,x,y,u)$ such that:

$$\psi(t) \overset{L^2(\mathbb{R}^n)}{=} \lim_{\varepsilon\to 0^+}\psi_\varepsilon(t), \quad \psi_\varepsilon(t,x) = \int_{\mathbb{R}^n}\left(\int_{\mathbb{R}^k} e^{\frac{i}{(1+\varepsilon^2)\hbar}S(t,x,y,u)}\rho^\hbar_\varepsilon(t,x,y,u)du \right)\varphi(y)dy. \tag{4.25}$$

Proof. In the Theorem (4.1) we proved

$$e^{-\frac{i}{\hbar}tH}\varphi = \lim_{\varepsilon\to 0^+} e^{-\frac{i+\varepsilon}{\hbar}tH_\varepsilon}\varphi.$$

Now, applying Theorem (4.7) we obtain immediatly the representation 4.25. □

4.4 Path Integral representation

In this last section we apply the results previously obtained, in order to realize a Path Integral representation of the Propagator. More precisely we consider Thereom 4.8, where now we make a particular choice of generating function, namely the generating function of Theorem 2.10 involving the Action functional. We are now ready to prove the following:

Theorem 4.9. *Take the operator* $H = -\frac{\hbar^2}{2m}\Delta_x + V(x)$ *where* $V \in C^2(\mathbb{R}^n)$ *with compact support. Then the solution of the Schrödinger equation*

$$\begin{cases} i\hbar\partial_t\psi(t,x) = \left(-\frac{\hbar^2}{2m}\Delta_x + V(x)\right)\psi(t,x), \\ \\ \psi(0,x) = \varphi(x) \in H^2(\mathbb{R}^n), \end{cases} \tag{4.26}$$

admits the path integral representation:

$$\psi(t,\cdot) \overset{L^2(\mathbb{R}^n)}{=} \lim_{\varepsilon\to 0^+} \psi_\varepsilon(t,\cdot), \tag{4.27}$$

$$\psi_\varepsilon(t,x) = \int_{\mathbb{R}^n} U_\varepsilon(t,x,y)\varphi(y)\ dy, \quad U_\varepsilon(t,x,y) = \int_{\Gamma(t,x,y)} e^{\frac{i}{(1+\varepsilon^2)\hbar}A[\gamma]}\, P_\varepsilon^\hbar(d\gamma), \tag{4.28}$$

where $\gamma \in \Gamma(t,x,y) \subset H^1([0,t];\mathbb{R}^{2n})$, *and* $\Gamma(t,x,y)$ *it is a finite dimensional manifold.*

Proof. As corollary of previous result we choose the global generating function described in Theorem (2.10), where

$$S(t,x,y,u) = A[\gamma^x(t,x,y,u)] = \int_0^t \frac{1}{2}m|\dot\gamma^x(s)|^2 - V(\gamma^x(s))\,ds. \tag{4.29}$$

The action functional $A[\cdot]$ is evaluated on a suitable set of curves γ^x with parameters $(t,x,y,u) \in [0,T]\times\mathbb{R}^n\times\mathbb{R}^n\times\mathbb{R}^k$. The curves $\gamma^x(t,x,y,u)(\cdot) \in H^1([0,t];\mathbb{R}^{2n})$ are constructed as follows:

$$\gamma^x(t,x,y,u)(s) := y + \frac{x-y}{t}s + \int_0^s \phi^x(r)dr - \frac{s}{t}\int_0^t \phi^x(r)dr\,, \quad \phi^x(s) := u^x(s) + f^x(t,x,y,u)(s). \tag{4.30}$$

For construction $u^x(\cdot) \in \mathbb{P}_N L^2([0,t];\mathbb{R}^n)$ while the functions $f^x(\cdot) \in \mathbb{Q}_N L^2([0,t];\mathbb{R}^n)$ are defined in [7].

The space of curves $\Gamma(t,x,y) := \{\gamma(t,x,y,u)(\cdot) | u \in \mathbb{R}^k\} \simeq \mathbb{R}^k$ has a structure of finite dimensional manifold as we have seen in the Remark 2.11, and of course it has also the structure of measurable space.

Thus we can apply the generalized theorem of change of variables from the domain $\mathbb{R}^k$ to $\Gamma(t,x,y)$ in this way:

$$\begin{aligned} U^\varepsilon(t)\,\varphi &= \int_{\mathbb{R}^n}\int_{\mathbb{R}^k} e^{\frac{i}{(1+\varepsilon^2)\hbar}S(t,x,y,u)}\rho_\varepsilon^\hbar(t,x,y,u)\ du\ \varphi(y)\ dy \\ &= \int_{\mathbb{R}^n}\int_{\mathbb{R}^k} e^{\frac{i}{(1+\varepsilon^2)\hbar}A[\gamma(t,x,y,u)]}\rho_\varepsilon^\hbar(t,x,y,u)\ du\ \varphi(y)\ dy \\ &= \int_{\mathbb{R}^n}\int_{\Gamma(t,x,y)} e^{\frac{i}{(1+\varepsilon^2)\hbar}A[\gamma]}\,P_\varepsilon^\hbar(d\gamma)\ \varphi(y)\ dy. \end{aligned}$$

We conclude that the kernel admids the representation:

$$U_\varepsilon(t,x,y) = \int_{\Gamma(t,x,y)} e^{\frac{i}{(1+\varepsilon^2)\hbar}A[\gamma]}\ P_\varepsilon^\hbar(d\gamma),$$

where we have defined $P_\varepsilon^\hbar(d\gamma) := \gamma_\star[\rho_\varepsilon^\hbar(u)du]$, as the complex image measure of the map $\gamma : \mathbb{R}^k \to \Gamma(t,x,y)$ on the complex measure $\rho_\varepsilon^\hbar(t,x,y,u)du$. $\square$

Appendix

In this appendix we prove some properties about generating functions that are necessary to prove Theorem 2.8.

We define the Hamiltonian function $H(x,p) := \frac{p^2}{2m} + V(x)$ where $V \in C^2(\mathbb{R}^n)$ has compact support, and denote ϕ_H^t as the group of canonical transformations definined on $T^\star\mathbb{R}^n$ that solves the related Hamilton's equations; $(x,p)(t) := \phi_H^t(y,\xi)$ solves:

$$\begin{cases} \dot{x} = \nabla_p H(x,p) \\ \\ \dot{p} = -\nabla_x H(x,p). \end{cases} \tag{4.31}$$

Let us consider the family of Lagrangian submanifolds

$$\Lambda_t := \big\{(y,\xi;x,p) \in T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n : (x,p) = \phi_H^t(y,\xi)\big\}. \tag{4.32}$$

Suppose that $S(t,x,y,u) : [0,T] \times \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^k \to \mathbb{R}$ is a global generating function:

$$\Lambda_t = \{(y,\xi;x,p) \in T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n : p = \nabla_x S, \quad \xi = -\nabla_y S, \quad 0 = \nabla_u S\}. \tag{4.33}$$

Now we define the symplectic transformation:

$$h : T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n \longrightarrow T^\star(\mathbb{R}^n \times \mathbb{R}^n)$$

$$(y,\xi;x,p) \longmapsto \Big(\hat{X}_1, \hat{X}_2; \hat{P}_1, \hat{P}_2\Big) := \Big(\frac{x+y}{2}, \frac{\xi+p}{2}; p-\xi, y-x\Big)$$

The set $\hat{\Lambda}_t := h(\Lambda_t)$, for every t fixed, is a Lagrangian submanifold because it is defined as the image of a Lagrangian submanifold Λ_t through a symplectic transformation h. We state that a related generating function is:

$$\hat{S}(t,\hat{X}_1,\hat{X}_2,\omega) := S(t,\alpha,\beta,u) + (\alpha+\beta-2\hat{X}_1)\gamma + \hat{X}_2(\beta-\alpha) \quad \omega := (\alpha,\beta,\gamma,u). \tag{4.34}$$

More precisely:

$$\hat{\Lambda}_t = \Big\{\Big(\hat{X}_1, \hat{X}_2; \hat{P}_1, \hat{P}_2\Big) \in T^\star(\mathbb{R}^n \times \mathbb{R}^n) \ : \ \hat{P}_1 = \nabla_{\hat{X}_1} S \quad \hat{P}_2 = \nabla_{\hat{X}_2} S \quad 0 = \nabla_\omega S\Big\}.$$

The sistems of equations read exactly:

$$\begin{aligned}\hat{P}_1 &= \nabla_{\hat{X}_1} S = -2\gamma \\ \hat{P}_2 &= \nabla_{\hat{X}_2} S = \beta - \alpha \\ 0 &= \nabla_\alpha \hat{S} = \nabla_\alpha S + \gamma - \hat{X}_2 \\ 0 &= \nabla_\beta \hat{S} = \nabla_\beta S + \gamma + \hat{X}_2 \\ 0 &= \nabla_\gamma \hat{S} = \alpha + \beta - 2\hat{X}_1 \\ 0 &= \nabla_u \hat{S} = \nabla_u S \end{aligned} \tag{4.35}$$

We remember that, from tha initial hypotesis, S generates Λ_t, so we obtain:

$$\begin{aligned}\gamma &= -\frac{(\nabla_\alpha S + \nabla_\beta S)}{2} \\ \hat{P}_1 &= -2\gamma = \nabla_\alpha S + \nabla_\beta S = p - \xi \\ \hat{P}_2 &= \beta - \alpha = y - x \\ \hat{X}_1 &= \frac{(\alpha+\beta)}{2} = \frac{(x+y)}{2} \\ \hat{X}_2 &= \frac{(\nabla_\alpha S - \nabla_\beta S)}{2} = \frac{p+\xi}{2} \\ 0 &= \nabla_u S \end{aligned} \tag{4.36}$$

these relations correspond exactly to the Lagrangian submanifold $\hat{\Lambda}_t$.
Now we consider the inverse transformation h^{-1}:

$$h^{-1} : T^\star(\mathbb{R}^n \times \mathbb{R}^n) \longrightarrow T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n$$

$$(\hat{X}_1, \hat{X}_2; \hat{P}_1, \hat{P}_2) \longmapsto (y, \xi; x, p) := \Big(\hat{X}_1 + \frac{1}{2}\hat{P}_2, \hat{X}_2 - \frac{1}{2}\hat{P}_1; \hat{X}_1 - \frac{1}{2}\hat{P}_2, \hat{X}_2 + \frac{1}{2}\hat{P}_1\Big)$$

and a generating function $\hat{S}$ of $\hat{\Lambda}_t$. We prove that a generating function S for Λ_t can be constructed as:

$$S(t,x,y,\chi) = \hat{S}(t,\delta,\rho,\omega) - y\Big(\rho - \frac{1}{2}\mu\Big) + x\Big(\rho + \frac{1}{2}\mu\Big) - \mu\delta \quad \chi = (\delta,\rho,\mu,\omega) \tag{4.37}$$

Indeed we prove that the function S so contructed generates Λ_t:

$$\Lambda_t = \{(y,\xi;x,p) \in T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n : p = \nabla_x S, \quad \xi = -\nabla_y S, \quad 0 = \nabla_\chi S\} \tag{4.38}$$

The sistems of related equations reads:

$$\begin{aligned} p &= \nabla_x S = \rho + \frac{\mu}{2} \\ \xi &= -\nabla_y S = \rho - \frac{\mu}{2} \\ 0 &= \nabla_\delta S = \nabla_\delta \hat{S} - \mu \\ 0 &= \nabla_\rho S = \nabla_\rho \hat{S} + x - y \\ 0 &= \nabla_\mu S = \frac{(x+y)}{2} - \delta \\ 0 &= \nabla_\omega S = \nabla_\omega \hat{S} \end{aligned} \tag{4.39}$$

By using the fact that $\hat{S}$ generates $\hat{\Lambda}_t$, we obtain:

$$\begin{aligned}
\mu &= \nabla_\delta \hat{S} = \hat{P}_1 \\
p &= \rho + \frac{\mu}{2} = \hat{X}_2 + \frac{\hat{P}_1}{2} \\
\xi &= \rho - \frac{\mu}{2} = \hat{X}_2 - \frac{\hat{P}_1}{2} \\
0 &= \nabla_\rho S + x - y = \hat{P}_2 + x - y \\
0 &= \frac{(x+y)}{2} - \delta = \frac{(x+y)}{2} - \hat{X}_1 \\
0 &= \nabla_u S
\end{aligned} \tag{4.40}$$

More clearly, we obtain the transformation h^{-1} on $\hat{\Lambda}_t$, that it is exactly Λ_t:

$$\begin{aligned}
p &= \hat{X}_2 + \frac{\hat{P}_1}{2} \\
\xi &= \hat{X}_2 - \frac{\hat{P}_1}{2} \\
x &= \hat{X}_1 - \frac{\hat{P}_2}{2} \\
y &= \hat{X}_1 + \frac{\hat{P}_2}{2}
\end{aligned} \tag{4.41}$$

To conclude we verify that $\hat{\Lambda}_t = \phi^t_{\hat{H}}(\hat{\Lambda}_0)$, the image an Hamiltonian flow $\phi^t_{\hat{H}}$. We prove that the corresponding Hamiltonan is:

$$\begin{aligned}
\hat{H}(\hat{X}_1, \hat{X}_2; \hat{P}_1, \hat{P}_2) &:= H\Big(\hat{X}_1 - \frac{1}{2}\hat{P}_2, \hat{X}_2 + \frac{1}{2}\hat{P}_1\Big) \\
&= \frac{1}{2m}\Big(\hat{X}_2 + \frac{1}{2}\hat{P}_1\Big)^2 + V\Big(\hat{X}_1 - \frac{1}{2}\hat{P}_2\Big) \\
&= \hat{H}_0 + \hat{H}_1
\end{aligned} \tag{4.42}$$

Indeed we remember that $\hat{\Lambda}_t := h(\Lambda_t)$, where:

$$h : T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n \longrightarrow T^\star(\mathbb{R}^n \times \mathbb{R}^n)$$

$$(y, \xi; x, p) \longmapsto \Big(\hat{X}_1, \hat{X}_2; \hat{P}_1, \hat{P}_2\Big) := \Big(\frac{x+y}{2}, \frac{\xi+p}{2}; p - \xi, y - x\Big)$$

and Λ_t is defined by (4.32).

We easily observe that the relations between derivatives of the variables $\Big(\hat{X}_1, \hat{X}_2; \hat{P}_1, \hat{P}_2\Big)$ relative to $\hat{\Lambda}_t$ and the variables $(y, \xi; x, p)$ of Λ_t corresponds to:

$$\begin{aligned}
\dot{\hat{P}}_1 &= \dot{p} \\
\dot{\hat{P}}_2 &= -\dot{x} \\
\dot{\hat{X}}_1 &= \frac{\dot{x}}{2} \\
\dot{\hat{X}}_2 &= \frac{\dot{p}}{2}
\end{aligned} \tag{4.43}$$

But the Hamilton's equations written for $\hat{H}$ are:

$$\begin{aligned}
\dot{\hat{P}}_1 &= -\nabla_{\hat{X}_1}\hat{H} = -\nabla V\left(\hat{X}_1 - \frac{1}{2}\hat{P}_2\right) \\
\dot{\hat{P}}_2 &= -\nabla_{\hat{X}_2}\hat{H} = -\frac{1}{m}\cdot\left(\hat{X}_2 + \frac{1}{2}\hat{P}_1\right) \\
\dot{\hat{X}}_1 &= \nabla_{\hat{P}_1}\hat{H} = \frac{1}{m}\cdot\left(\hat{X}_2 + \frac{1}{2}\hat{P}_1\right) \\
\dot{\hat{X}}_2 &= \nabla_{\hat{P}_2}\hat{H} = -\frac{1}{2}\nabla V\left(\hat{X}_1 - \frac{1}{2}\hat{P}_2\right)
\end{aligned}$$

Using the inverse transformation h^{-1} and the Hamilton's equations for H, we obtain the same group of relations:

$$\begin{aligned}
\dot{\hat{P}}_1 &= -\nabla V(x) = \dot{p} \\
\dot{\hat{P}}_2 &= -\frac{p}{m} = -\dot{x} \\
\dot{\hat{X}}_1 &= \frac{p}{2m} = \frac{\dot{x}}{2} \\
\dot{\hat{X}}_2 &= -\frac{\nabla V(x)}{2} = \frac{\dot{p}}{2}
\end{aligned} \tag{4.44}$$

This means that the Lagrangian submanifold $\hat{\Lambda}_t$ corresponds exactly to the image of Hamiltonian flow gererated by $\hat{H}$, that is $\hat{\Lambda}_t = \phi^t_{\hat{H}}(\hat{\Lambda}_0)$. □

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