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Abstract

This work deal with the subject of asymptotic expansions for both finite and infinite dimensional integrals. We first discuss a long standing problem related to the formation of crystals at zero temperature. The majority of the techniques used in this part come from the classical theory of *Laplace Integrals* in many dimensions and from the theory of *Cluster Expansions* in Probability Theory. We then move to the *Quantum scenario* in order to study the Caldeira-Legget model by the rigorous definition of the *Influence Functional* introduced by Feynman and Vernon. We make use of the theory of *Feynman Path Integrals*, providing the possibility to exploit the infinite dimensional generalization of the *Stationary Phase method* to study the asymptotics of the integrals characterizing the Caldeira-Legget model. An analogous study is made for a problem related to the semiclassical limit for the *stochastic Schrödinger equation* introduced by Belavkin (white noise given by a Brownian motion). Moreover we give an overview of the results related to the asymptotic expansions of integrals spanning from the unidimensional, real case, to the infinite dimensional environment and including *Stokes phenomena, detailed multidimensional expansions, uniform asymptotics* and *asymptotics for coalescing saddle points*.

Zusammenfassung

Diese Arbeit befasst sich mit asymptotischen Erweiterungen für endlich und unendlich dimensionale Integrale. Als Erstes betrachten wir ein seit lange ungelöstes Problem, daß eng mit der Bildung von Kristallen bei Nulltemperatur verbunden ist. Die meisten Methoden, die in diesem Teil angewandt werden, kommen aus der klassischen Theorie der mehrdimensionalen Laplace-Integrale und aus der Wahscheinlichkeitstheorie (Cluster-Entwicklungen). Wir gehen danach zur Quantenmechanik über, um das Caldeira-Leggett Modell mit Hilfe des von Feynman und Vernon eingeführtes Einflussfunktionals zu untersuchen. Wir benutzen die Theorie der Feynmanschen Pfadintegrale, um die unendlich-dimensionale Verallgemeinerung der Methode der stationären Phase für das Studium der Asymptoten, die das Caldeira-Leggett Modell beschreiben, einzusetzen. Eine analoge Betrachtung ist an einem Problem, das mit dem semiklassischen Grenzwert der bei Belavkin eingeführten stochastischen Schrödinger-Gleichung, mit einem so genannten weissen Rauschen einer Brownsche Bewegung, verbunden ist, angewandt. Ausserdem geben wir einen Überblick über Resultate betreffend der asymptotischen Erweiterung von Integralen, vom eindimensionalen reellen Fall bis zu unendlich-dimensionalen Problemstellungen, einschließlich von Stokes Phänomenen, detaillierten mehrdimensionalen Erweiterungen, gleichmäßigen und verbundenen Sattelpunkt-Asymptoten.

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Introduction

We would like to start the presentation of this work with some of the major criticisms to the subject of Asymptotic Expansions. The first was written by the mathematician Niels Hendrik Abel in 1828:

Divergent series are the invention of the Devil, and it is shameful to base on them any dimostration whatsoever

More than 150 years do not change completely this kind of toughts since, in 1992, Richard E. Meyer, see [Mey92], wrote

I was led to contemplate a heretical question: are higher approximation than the first justifiable ? My experience indicates yes, but rarely.[...] Solutions as an end in themselves are pure mathematics; do we really need to know them to eight significant decimals ?

It is also possible to find doubtful attitudes couched by scientists who actively work on this subject, e.g. by N.G. de Bruijn in [dB81]:

What is asymptotics? This question is about as difficult to answer as the question: what is mathematics?

or by J.P. Boyd in [Boy99]:

I no more understood the reason why some series diverge than why my son is lefthanded

The radical scepticism of Meyer is justified since a wide range of applied mathematicians, engineers or experimental physicists might say that they have no need of anything else than the first term of an asymptotic expansion and/or that the exponentially small terms would be destroyed by the action of natural perturbations. Hence a fundamental question, see [Boy99], arises: Is this trip necessary ?

The answer is definitively yes since the above points of view easily lead to inconsistencies. The key point is that some features of physical systems are related to the behaviour of exponentially small terms, say , in expressions of the type $\exp(-\frac{\lambda}{\epsilon})$, $\lambda > 0$, $\epsilon > 0$ small, which cannot be approximated as a power series in $\epsilon > 0$, actually all their derivatives are zero at $\epsilon = 0$. Such exponentially small effects are invisible in terms of power series expansions, nevertheless there are a multitude of cases where one has to take into account such apparently insignificant terms. For example, as showed by J.R. Oppenheimer in [Opp28] in the study of the quantum Stark model, in the presence of an external field of strength ϵ , hydrogen atoms disassociate. This phenomenon happens on a timescale which is inversely proportional to the imaginary part of an eigenvalue of the Schödinger equation, which is exponentially small in ϵ , then this tiny imaginary value completely controls the lifetime of the molecule. Closely related to this work is the independent discovery of Quantum Tunneling by Gamow, Condon and Gurney (1928), see e.g. [Raz03].

Other examples come from the theory Hele-Shaw cells where a viscous fluid is injected between two closely-spaced plates and a fingershaped flow may develop. In a model of this type nomerous exponentially small terms arise from the singular perturbation expansions of the Kruskal-Segur equation, see e.g. [KS85, SJK98], and they are stable under the action of physical contaminations as expressed by an inhomogeneous nonlinear term, since this only affects them by prefactors: here the exponentially small terms are a fundamental property of the asymptotic solution.

Another example in quantum mechanics is the double-well model where the eigenvalues of the Schrödinger equation come in pairs and the difference between each pair is exponentially small in the ϵ -size of the internuclear separation.

Another type of problems show how exponential smallness is the corner stone for the very existence (or non existence) of solutions. This happens, for example, when a melt interface between a solid and a liquid is unstable, breaking up into dendritic fingers. Experiments show that the fingers not only have a parabolic shape, as expected from the theory, but also have a definite width which cannot be described by a power series in the surface tension, see e.g. [Hut97, Pri00].

In their work Kruskal and Segur showed that the complex-plane matched asymptotics method of Pokrovskii and Khalatnikov, see [PK61], could be used in order to study a simple model of crystal growth furnishing one of the triggers for the resurgence in exponential asymptotics.

Other examples can be found in [SJK98] where solutions of certain problems under quantisation conditions lead to a determination of the position of singularities in the complex plane. In these cases the existence of exponentially small terms selects the principal solution. As Boyd write in [Boy99]:

Such beyond-all-orders features are like mathematical stealth aircraft, flying unseen by the radar of the conventional asymptotics

Subtler phenomena appear whenever the singularity of a model under study may vary in its position. In fact exponentially small terms which initially might be discarded can grow to dominate the solution as described, for example, in the work of Boasman and Keating in [PJ95] on perturbed Anosov maps of Quantum Chaos. In this scenario the perturbations imposed to the dynamical system gave rise to singularities in the complex plane, which contribute exponentially small terms to the semiclassical expansion of the trace of the spectral operator. The size of their contribution is determined by the physical perturbation parameter. As the parameter increases the singularities are able to approach, coalesce on and bifurcate along the real axis where they dominate the eigenvalue statistics. The use of asymptotic methods is not confined to finite dimensional problems, as proved by Albeverio et al. in several works related to the theory of Feynman path integrals, in relation to quantum theory and optics, see e.g. [AHK77, Alb86, AB93, Alb97, AHK76].

Last but not least a full comprehension of the Stokes phenomenon, (the presence of one exponential times a power series in ϵ regions of the ϵ -complex plane but two exponentials in other regions), can only be achieved by looking at the exponential small terms.

With previous ideas in mind it might not be surprising that in the past Asymptotic Analysis was considered more as an art than a discipline. This was undoubtedly due to the heterogeneity of the reaserchers and to their fields of work. Simply speaking, starting from the seminal works of Stirling, MacLaurin, Euler, Stieltjes and Poincaré, who gave the rigourous definition of asymptotic expansions, asymptotic methods have been applied in all branches of mathematics physics and natural sciences since they allow us to obtain a quantitative description of a phenomenon as well as its qualitative behaviour. Asymptotics is now perceived as a common thread in many different areas and next to classical books of Dingle, Copson, de Brujin, Erdélyi etc., see e.g. [Din73, Cop65, dB81, Erd56], one can also find contemporary books like the ones of Estrada and Kanwal [EK94], Fedoryuk [Fed89], Jones [Jon97], Ramis [RAM93], Stein [Ste93].

It is not just by chance that the past decade has seen a blossoming of interest on the subject. In particular we would like to mention the development of comprehensive theories of Borel Transforms, the concept of Resurgence Theory by Ecalle (which describes certain classes of asymptotic expansion in which the exponentially small terms associated with Stokes phenomena are related to the further terms of the expansion, i.e. to the analytic properties of a progenitor function); smoothing of Stokes Phenomenon; systematic expansions of better than exponential accuracy (Hyperasymptotics) [BH91, Boy90, Daa98]; study of the first realistic error bounds for saddlepoint methods; deeper knowledge of the universality in the form of the higher terms of both local and uniformly valid asymptotic expansions, understanding how local expansions

can be used to determine global properties of solutions; development of practical algebraic methods for resolving the Riemann sheet structure of multidimensional integrals and the calculation of the intersection numbers for curves of differing homologies.

Asymptotic analysis methods have also been successfully applied to situations as varied as the dendritic growth of crystals; the selection of flows in viscous fingering, phase formation in fluids, the coupling of multiple length scales in fluids flow; tip propagation in fracture mechanics and buckling; nonlinear mappings, Hamiltonian systems and chaotic motion; reaction diffusion equations; the calculation of non-trivial zeros of the Riemann zeta function and spectral determinants; quantum maps; semiclassical expansions of quantum spectral functions. See e.g. [Vor83, HS99, DDP97, BH94] and references therein.

Is it possible to investigate the above-mentioned huge amount of heterogeneous questions in a systematic way? This is exactly the core of our work. In fact our aim is to attack several kind of problems, which naturally arise in Asymptotic Analysis, by the use of their integral representation by combining classical methods of the asymptotic of finite dimensional integrals, see e.g. [dB81, BH86] and newer developments of the finite dimensional theory in connection with specific methods of asymptotics of infinite dimensional integrals and the theory of singularities, see e.g [Fed89, Arn91, Mas77, MF76, Dui74].

The embedding of finite dimensional problems into infinite dimensional ones has been already shown to be useful in connection with quantum theory, where Feynman path integral methods and their associated asymptotics lead to powerful results, see e.g. [AM04c]. We think that this approach will provide a more unified treatment of the subject.

The necessity to have accurate Integral Expansions naturally emerges from Statistical Mechanics problems, see e.g. [DS84, Ell85] or works like [APK06, AP06, Per], where the bond between the subject and Probability Theory becomes direct and clear. Lastly, as mentioned above, a generalization of the same techniques of Asymptotic Integral Expansions can be applied to the intriguing field of infinite dimensional oscillatory integrals providing a rigorous treatment of many problems of Quantum Theory, see e.g. [APM06b, ACPM06], in particular problems including those related to the rapidly expanding field of Quantum Computing.

Open Problems

The list of open problems which could be attacked from the point of view of the asymptotic expansion of integrals methods is a large as the set of bonds linking ideas developed in this work with the ongoing research, hence what follows cannot be an exhaustive inventory.

Since a unified treatment of asymptotic control of small exponential terms is still missing, our project is higly innovative being based on a systematic use of infinite dimensional asymptotic methods. Our research will provide a variety of interesting spin-off both theoretical and practical which will be used from a pure mathematical point of view as in engineering tasks.

An important part of the present study about dynamical systems, such as they appear e.g. in the KAM theory, have to deal with perturbations under the action of which integrable models become chaotic, but the chaos is confined to exponentially small regions. Through Arnold diffusion, dynamical system can move great distances on exponentially long time scales even in the case of weak contaminations.

Another area of interest is constituited by nonlinear coherent structures that would be immortal were it not for weak radiation from the core structure. The latter situation is linked to the theory of weakly nonlocal solitary waves that arises, for example, in fiber optics and hydrodynamics applications.

A third area of study is crystal formation and solidification, in which the work of Kruskal and Segur, see e.g. [KS85, SJK98], resolved a long-standing problem in the theory of dendritic fingers and touched off a great plume of activity.

Fluid mechanics is a fourth area in which ongoing research on the subject is very active, especially in order to study Kelvin wave instability in oceanography and atmospheric dynamics, or radiative decay of free oscillations bound to islands. In the quantum scattering field the work made by Meyer, see [Mey76, Mey80, Mey90] and references therein, supplies an up to date challenge since it led to further studies of exponential small terms in connection with the WKB theory and quantum tunneling phenomena. The above mentioned theory of Resurgence by Ecalle may be viewed as one of the more abstract fields of research directly linked to our ideas on Asymptotic Expansions of Integrals and, at the same time, it offers a connection with recent developments made by Pham, Ramis, Delabaere et al., see e.g. [SS96] and references therein for a detailed introduction.

A seventh line of active research falls in the long-standing questions related to Stokes phenomenon and it is of great interest both for physicists and applied mathematicians. A new boost to this task rises from a work by Berry in which the discontinuity in the numerical value of an asymptotic expansion at Stokes line could be smoothed, the effect of this impulse is far from its end. The use of infinite dimensional methods in Statistical Mechanics (e.g. low temperature expansions via multidimensional Laplace method, study of Large Deviations and Cluster Expansions in Probability theory, etc.), Quantum Mechanics (e.g. semiclassical expansions) and certain problems of low dimensional Topology (e.g. Chern-Simons integrals, Vassiliev knot invariants) has proven to be extremely useful and to have important connections with main problems of present Mathematics and Theoretical Physics.

Plan of the work

In this work we present two different type of generalizations of asymptotic expansions for integrals in the finite dimensional case as well as in the infinite dimensional one. In particular in Ch.(1) we discuss a long standing problem related to the formation of crystals at zero temperature. The majority of the techniques used in this part come from the classical theory of *Laplace Integrals* in many dimensions and from the theory of *Cluster Expansions* in Probability Theory.

In Ch.(2) we move to the Quantum scenario in order to study the important model of Caldeira and Legget by the rigorous definition of the Influence Functional introduced by Feynman and Vernon. We make use of the theory of Feynman Path Integrals providing the possibility to exploit the infinite dimensional generalization of the Stationary Phase method to study the asymptotics of the integrals characterizing the Caldeira-Legget model. An analogous study is done in Ch.(3) for a different problem related to the semiclassical limit for the stochastic Schrödinger equation introduced by Belavkin (white noise given by a Brownian motion). The original results described in Ch.(2) and Ch.(3) are obtained using the new developments for the asymptotic expansions for infinite dimensional oscillating integrals given in Sec.(7.2) of Ch.(7)

In Ch.(4,5,6,7) we give an overview of the results related to the asymptotic expansions of integrals spanning from the unidimensional, real case, to the infinite dimensional environment and including Stokes phenomena, detailed multidimensional expansions, uniform asymptotics, asymptotics for coalescing saddle points, mentioning also the theories of Hyperasymptotics, Resurgence and Distributional Approach.

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"El hombre tiene que forjar día a día su espíritu revolucionario."

Ernesto Guevara de la Serna

"We have to become the change that we want to see."

Mahatma Gandhi

CHAPTER 1

The Crystal Problem

1.1. Statement of the Problem

Do crystals really exist ? What are we talking about when we talk about crystals ? Simply speaking when we talk about crystals we have in mind a three-dimensional structure in which a single scheme is periodically repeated. Mathematically we can formulate the same rough definition without limiting the dimension of the structure, i.e. we can consider crystalline structures living in the d - dimensional euclidean space. Several physical experiences suggest that the nature of solids at low temperature is of the previous type, i.e. they present a periodic structure which is the result of many copies of the same ordered unit cell. These natural facts suggest the following intriguing question: Why crystals ? To be more precise and following Radin's thought, see e.g. [Rad87], we would like to rigorously formulate the Crystal Problem in a suitable mathematical form such that is could be possible to prove that, at low temperatures, Nature prefers ordered structures instead of developing amorphous ones.

The stated problem has a natural and well known translation in the language of mathematical physics. In particular let us consider a physical system composed by a finite number of interacting particles confined in a bounded region of the space, say a cube with edges of length N in \mathbb{R}^d . Assume that the interaction is given by a pair potential V which is a function of the distance between the selected couple of particles only. Then we can write down the partition function for the system at inverse temperature $T \equiv \frac{1}{\beta}$, $\beta > 0$, and we would like to know whether in the low temperature regime, the Gibbs states of the system, i.e. those corresponding to minimizing energy configurations, are periodic. The next step is to control whether the possibly crystalline structure, realized at low temperature in a bounded region, remains stable when we consider an infinite extension of the previous system, i.e. taking the limit $N \to \infty$. The picture we have in mind is well depicted in section 2 of [Rad87] and can be viewed as the Gibbs's state interpretation of the *Crystal Problem*. It is not difficult to reformulate the whole question in a pure mathematical language. In [Rad87] an extensive list of this reformulations is given. We think that, among this mathematical approaches, the most interesting one consists in an accurate use of the theory of asymptotic expansions of integrals. Before going on we refer the reader to Sec. 6 of [Rad87] in order to have a detailed survey of recent results on the subject. Moreover very interesting ideas related to the problem of the stability of symmetries for equilibrium configurations can be found in [KD82b, KD82a], while the approach that we will use in what follows is based on [AeKH⁺89, AGH⁺93]. More recently, in [The06], a proof of crystallization, at low temperature and in two dimensions, is given for a system of classical particles interacting by a pair potential, studing the asymptotic behaviour of the corresponding ground energy. Moreover in [Süt05] it is proved that, for a class of translational invariant pair interactions, there exist periodic ground states for classical particle systems in three dimensions and it is showed that there exist crystal structures which are stable against a certain class of perturbations. For a quantum mechanical analogue of the crystal problem one can see [LK86, Lie87].

We analyze the case of uniformly bounded fluctuations of a system of classical particles around a hypothetical crystalline ground state. Our analysis is based on [AeKH⁺89, AGH⁺93] and it starts with the study of the finite volume scenario, i.e. the case in which interacting particles are confined in a bounded box of size N in d-dimensional space. Then we generalize some of the obtained results to the infinite volume case. The studied fluctuations are described with respect to a certain class of well defined potentials which have to satisfy some general conditions. Our analysis will be developed in the *low temperature* regime making use of some asymptotic methods of expansions for the integral defining the quantities of interest. In particular we use the Laplace method in many dimensions in connection with some cluster expansions techniques.

1.2. The Finite Volume Case

We consider a system of n classical particles which has, for semplicity, mass equal to 1 and are enclosed in some bounded region of \mathbb{R}^d . Let thus N > 0 be a given integer, and consider the bounded volume:

$$\Lambda_N \equiv \left\{ x = (x^1, \dots, x^d) \in \mathbb{R}^d : \mid x^i \mid \le N, i = 1, \dots, d \right\}$$

A configuration of particles for our system is simply an n dimensional vector of positions in Λ_N , i.e. $x^{(n)} = (x_1, \ldots, x_n)$ such that $x_i \in \Lambda_N$, $\forall i = 1, \ldots, n$, the collection of such vectors will be indicated by $X^{(n)}$. The interactions between the particles are expressed in terms of a two body, central, translational invariant potential

$$V:\Lambda_N\times\Lambda_N\to\mathbb{R}$$

i.e. $V(x,y) \equiv \Phi(|x-y|)$ which Φ a lower bounded real valued function of compact support on \mathbb{R}^+ and sufficiently smooth.

Moreover each particle *i* of position $x_i \in \Lambda_N$, possesses its momentum $p_i \in \mathbb{R}^d$, i = 1, ..., n, hence the phase space of the system is described by:

$$(p,x) \equiv ((p_1,x_1),\dots,(p_n,x_n))$$
 (1.1)

The *Hamiltonian* of our system of particles reads:

$$H^{(n)}((p,x)) \equiv \sum_{i=1}^{n} \frac{p_i^2}{2} + \frac{1}{2} \sum_{i \neq j=1}^{n} \Phi(|x_i - x_j|)$$
(1.2)

where:

$$|x_i^j| \le N$$
 and $p_i \in \mathbb{R}^d$ $\forall i = 1, \dots, n, j = 1, \dots, d$

Then the *Maxwell-Boltzmann* ensemble partition function, for the inverse temperature parameter $\beta = \frac{1}{T} > 0$, is as follows:

$$Z_N^{(n)}(\beta) \equiv \int_{\left(\mathbb{R}^d \times \Lambda_N\right)^n} e^{-\beta H^{(n)}(p,x)} dp_1 \cdots dp_n dx_1 \cdots dx_n$$
(1.3)

Performing the integral in (1.3) with respect to the momentum variables we get:

$$Z_N^{(n)}(\beta) = \left(\frac{2\pi}{\beta}\right)^{\frac{dn}{2}} \int_{\Lambda_N^n} e^{-\beta H^{(n)}(x)} dx_1 \cdots dx_n$$
(1.4)

where:

$$H^{(n)}(x) \equiv \frac{1}{2} \sum_{i \neq j=1}^{n} \Phi(|x_i - x_j|)$$

and we made use of the well known n- dimensional Gaussian integral:

$$\left(\frac{\beta}{2\pi}\right)^{\frac{dn}{2}} \int_{\mathbb{R}^{dn}} e^{-\frac{\beta p^2}{2}} dp_1 \cdots dp_n = 1 \quad ; \quad p^2 \equiv \sum_{i=1}^n p_i^2$$

In order to study the asymptotic behaviour of (1.4) as the temperature converges to zero, namely $\beta \uparrow +\infty$, we will use the Laplace method¹ for the asymptotics of integrals. For this we need to control the Hessian of the Hamiltonian $H^{(n)}$ evaluated at the minima of $H^{(n)}$. If the minima X_1, \ldots, X_m of $H^{(n)}$ are *well separated* then, applying the Laplace method of asymptotics to (1.4), we have the following asymptotic formula for $\beta \to \infty$:

$$Z_N^{(n)}(\beta) \asymp \sum_{j=1}^m e^{-\beta H(X_j)} \int\limits_{\Lambda_N^n} e^{-\frac{\beta}{2} \langle (x-X_j), \mathscr{H}|_{X_j}(x-X_j) \rangle} dx_1 \cdots dx_n$$
(1.5)

¹See e.g. Ch.4 of [dB81] or Ch.4 of this thesis.

where if $a(\beta)$ and $b(\beta)$ are two real function of the parameter β then $a(\beta) \simeq b(\beta)$ stands for $\lim_{\beta \to \infty} \frac{a(\beta)}{b(\beta)} = const$. Moreover $\mathscr{H} \mid_{X_j}$ denotes the dn-square Hessian matrix of the Hamiltonian $H^{(n)}$ evaluated at the minimum point X_j and the error made is controlled by :

$$\int_{\Delta_N^n} e^{-\beta \mathscr{R}(X_j;x)} dx_1 \cdots dx_n$$

where $\mathscr{R}(X_j; x)$ equals the tail of the expansion of H around the *jth* minimum point as shown² in Ch.(4) Sec.(4.2).

Remark 1.2.1. We refer the reader to Sec.(1.2.1) for a more detailed and precise statement of the asymptotics given in (1.5).

Remark 1.2.2. The problem of finding whether the Hamiltonian $H^{(n)}$ has a minimum at an almost regular configuration actually constitutes the Crystal Problem. Taking into account the surface effects we do not expect that the ground states of our systems in a bounded volume give rise to absolutely regular configurations. Only in the Thermodynamic Limit, namely taking $N \uparrow \infty$ and $n \uparrow \infty$ keeping the particle density $\rho \equiv \frac{n}{(2N)^d}$ fixed, we can expect this effect, for ρ larger than a certain value ρ_{cr} .

In order to deal with the crystalline structures let us introduce the following definition:

Definition 1.2.1. Let $\{v_1, \ldots, v_d : \forall v_i \in \mathbb{R}^d, \forall i = 1, \ldots, d\}$ be a set of d independent vectors in \mathbb{R}^d . An infinite Bravais lattice, with generators v_1, \ldots, v_d , is defined as:

$$\Omega_{\infty} \equiv \{\sum_{k=1}^{d} \alpha_k v_k : \alpha_k \in \mathbb{Z}, k = 1, \dots, d\}$$

We denote the restriction of a Bravais lattice Ω_{∞} to a bounded set $B \subsetneq \mathbb{R}^d$ by Ω_B , i.e. $\Omega_B \equiv \Omega_{\infty} \cap B$. According $\Omega_{\Lambda_N} \equiv \Omega_N$ will denote the restriction of Ω_{∞} to the *d*-dimensional hypercube of 2N-length edge. As seen before to the *jth* particle in the box Λ_N there is associated a *d*-dimensional vector x_j which specifies its spatial position, therefore to the whole set of particles in Λ_N there is associated a vector $x = (x_1, \ldots, x_n)$, i.e. an element of the previously defined space of configurations $X^{(n)}$. Using the vectors v_1, \ldots, v_d which span the space Ω_{∞} we can introduce the following equivalence relation in \mathbb{R}^d :

$$\forall (w_1, w_2) \in \mathbb{R}^d \times \mathbb{R}^d \Rightarrow w_1 \stackrel{\Omega}{\sim} w_2 \leftrightarrow \exists z \in \mathbb{Z}^d : w_1 + z = w_2$$

Let us define $\stackrel{\Omega_N}{\sim}$ to be the restriction of the equivalence relation $\stackrel{\Omega}{\sim}$ to Ω_N . If a particle λ in Λ_N is spatially identified by the vector x_{λ} , then using the equivalence relation $\stackrel{\Omega_N}{\sim}$, we can think of it as being embedded in the convex envelope of:

$$S \equiv \left\{ \sum_{k=1}^{d} \alpha_i v_i : \alpha_i \in \{0, 1\}, i = 1, \dots, d \right\}$$

²See also e.g. Ch.(8) of [BH86] or Ch.(1) Sec.(2) of [Fed89]

Thus we identify the d-dimensional position x_{λ} of the particle $\lambda \in \Lambda_N$ by its representative in S under the action of $\stackrel{\Omega_N}{\sim}$.

Remark 1.2.3. ³ In what follows we will assume that the number $|\Omega_N|$ of crystalline points equals the number n of particles $\{\gamma_i : i = 1, ..., n\}$ in the bounded box Λ_N .

Using the previous equivalence relation $\stackrel{\Omega_N}{\sim}$ we can define the displacement of a particle $\lambda \in \Lambda_N$, of position x_{λ} , with respect to the grid designed by Ω_N , by a vector $y_{\mu(\lambda)} \equiv x_{\lambda} - \mu(\lambda)$, where $\mu(\lambda)$ is a selected point of the lattice Ω_N .

It follows that for each set of n particles $(\lambda_1 \dots, \lambda_n) \in \Lambda_N$, i.e. for each configuration $x = (x_1, \dots, x_n) \in X^{(n)}$, there is associated a *displacement configuration* $y(x) \equiv (y_1, \dots, y_n)$ where, in order to semplify our notation, we denote by y_j the displacement of the particle λ_j from Ω_N , i.e. according to previous definition:

$$y_j \equiv y_{\mu(\lambda_j)} \tag{1.6}$$

with $|y_i| \leq N$ for all i = 1, ..., n. By Remark (1.2.3) we have that the previous correspondence, via displacement coordinates, between particles $\lambda \in \Lambda_N$ and lattice points $\mu \in \Omega_N$ can be realized in a *one-to-one* manner.

Hence we can write the *energy function* of the original systems of *n*-particles $(\lambda_1, \ldots, \lambda_n)$ of coordinates (x_1, \ldots, x_n) as follows:

$$\mathfrak{E}(x) = \frac{1}{2} \sum_{\substack{\mu_i, \mu_j \in \Omega_N \\ \mu_i \neq \mu_j}} V\left((\mu_i + y_i) - (\mu_j + y_j)\right)$$
(1.7)

where we have set $x_i = \mu_i + y_i$, for all i = 1, ..., n.

Let us define the *Crystalline Energy Function* as:

$$\mathfrak{E}^{cr}(\Omega_N) \equiv \frac{1}{2} \sum_{\substack{\mu_i, \mu_j \in \Omega_N \\ \mu_i \neq \mu_j}} V(\mu_i - \mu_j)$$
(1.8)

Then, for a fixed n-particle configuration $x = (x_1, \ldots, x_n) \in X^{(n)}$ and making use of the above definition for the *displacement configuration* $y(x) = (y_1, \ldots, y_n)$ such that $x_i = y_i + \mu_i$ for all $i = 1, \ldots, n$, we can express the *Deviation Energy Function* as:

$$\mathfrak{E}^{dev}(\Omega_N \mid \{y_\lambda\}_{\lambda \in \Omega_N}) \equiv \mathfrak{E}(x) - \mathfrak{E}^{cr}(\Omega_N) = = \frac{1}{2} \sum_{\substack{\mu_i, \mu_j \in \Omega_N \\ \mu_i \neq \mu_j}} V\left((\mu_i + y_i) - (\mu_j - y_j)\right) - \frac{1}{2} \sum_{\substack{\mu_i, \mu_j \in \Omega_N \\ \mu_i \neq \mu_j}} V(\mu_i - \mu_j)$$
(1.9)

We point out that $\mathfrak{E}^{dev}(\Omega_N \mid \{y_\lambda\}_{\lambda \in \Omega_N})$ expresses the energy deviation of the real configuration x from the crystalline energy $\mathfrak{E}^{cr}(\Omega_N)$ associated to the configuration Ω_N .

³This is a standard and natural assumption in *condensed matter* theory, see e.g. [Zim72].

1.2 The Finite Volume Case

We note that due to the periodicity of the Bravais lattice, the crystalline energy function $\mathfrak{E}^{cr}(\Omega_N)$, which is a function of $d \mid \Omega_N \mid$ variables, actually depends only on the choice of the set $v \equiv (v_1, \ldots, v_d)$ of d linear independent vectors which span Ω_{∞} , i.e. on the following set of cordinates:

$$\xi_1 \equiv v_1^1, \xi_2 \equiv v_1^2, \dots \xi_d = v_1^d, \dots, \xi_{d^2 - (d-1)} \equiv v_d^1, \xi_{d^2 - (d-2)} \equiv v_d^2, \dots, \xi_{d^2} \equiv v_d^d$$

We shall then also write $\mathfrak{E}^{cr}(\Omega_N)(v)$ for $\mathfrak{E}^{cr}(\Omega_N)$. A crystalline configuration is a (local) stationary minimum point for $\mathfrak{E}^{cr}(\Omega_N)$ if and only if the following conditions are fulfilled:

$$\begin{cases}
\partial \xi_1 \mathfrak{E}^{(cr)} \left(v_1^1, \dots, v_d^d \right) = 0 \\
\partial \xi_2 \mathfrak{E}^{(cr)} \left(v_1^1, \dots, v_d^d \right) = 0 \\
\vdots \\
\partial \xi_{d^2} \mathfrak{E}^{(cr)} \left(v_1^1, \dots, v_d^d \right) = 0
\end{cases}$$
(1.10)

and the *Hessian* matrix:

$$\left(\mathscr{H}\mathfrak{E}^{cr}\right)(v) = \left(\frac{\partial^2 \mathfrak{E}^{(cr)}(v)}{\partial \xi_i \partial \xi_j}\right)_{i,j=1,\dots,d^2}$$
(1.11)

evaluated at the point $\{v_i^1, \ldots, v_i^d : i = 1, \ldots, d\}$ is positive definite.

Let us state the following Hypothesis:

- (H1a) There exists a positive density value ρ_{cr} such that for $\rho \geq \rho_{cr}$ there exists a set of d linear independent vectors $\mathbf{v} = (v_1, \dots, v_d)$ such that conditions (1.10) and (1.11) are fulfilled, i.e. there exists a *Bravais lattice solution* of the minimizing problem for $\mathfrak{E}^{cr}(\Omega_N)$. Moreover there exists N_0 s.t. this holds uniformly for all $N > N_0$.
- (H1b) The deviation energy $\mathfrak{E}^{dev}\left(\Omega_N, \{y_i\}_{\mu_i \in \Omega_N}\right)$ has a local minimum in: $\{y_i = 0, i = 1, \dots, n, \lambda \in \Omega_N\}$

Remark 1.2.4. From (1.9) we have that
$$\{y_i = 0, i = 1, ..., n, \lambda \in \Omega_N\}$$
 is a local minimum for \mathfrak{E} . Condition (H1b) can be derived from the following condition for the displacement configua-
tion $\{y_i\}_{\mu_i \in \Omega_N}$:

$$\frac{1}{2} \sum_{\substack{\mu_i, \mu_j \in \Omega_N \\ \mu_i \neq \mu_j}} \left((y_i - y_j), (\mathscr{H}\Phi) \left(\mu_i - \mu_j \right) \cdot (y_i - y_j) \right) > 0$$
(1.12)

where $(\mathscr{H}\Phi)(\lambda)$ is the Hessian of Φ evaluated at the lattice point λ .

Remark 1.2.5. The discussion of the fullfillment of the Hypothesis is quite involved. For d = 1 we refer to [Rad87]. For d = 2, 3, ... we refer to [Süt05, The06], see also [AeKH⁺89]. Here we shall proceed by deducing consequences of this hypothesis.

1.2 The Finite Volume Case

Condition (1.12) can be used to deduce the existence of a functional integral representation of the quantities of interest. For this reason let us define the following matrix:

$$A_N(\mu_i, \mu_j) \equiv \begin{cases} 2\sum_{\mu_k \in \Omega_N, \mu_k \neq \mu_i} \left(\mathscr{H}\Phi\right) \left(\mu_i - \mu_k\right) & \text{if } \mu_i = \mu_j \\ -\mathscr{H}\Phi(\mu_i - \mu_j) & \text{if } \mu_i \neq \mu_j \end{cases}$$
(1.13)

Since the potential V only depends on the distance then for all $\mu_i, \mu_j \in \Omega_N$ we have that $\Phi(\mu_i - \mu_j) = \Phi(\mu_j - \mu_i)$ and the following equality holds:

$$\frac{1}{2} \sum_{\mu_i, \mu_j \in \Omega_N} \langle y_{\mu_i} - y_{\mu_j}, [\mathscr{H}\Phi(\mu_i - \mu_j)] \cdot (y_{\mu_i} - y_{\mu_j}) \rangle = \sum_{\lambda, \mu \in \Omega_N} \langle y_{\mu_i}, A_N(\lambda, \mu) \cdot y_{\mu_j} \rangle$$
(1.14)

Condition (1.12) implies that the matrix A_N is strictly positive definite on the space \mathbb{R}^{dn} , where $n \equiv |\Omega_N|$. Therefore it is possible to define the following zero-mean Gaussian measure on the Borel σ -algebra of the subsets of \mathbb{R}^{dn} , absolutely continuous with respect to the Lebesgue measure dx on \mathbb{R}^{dn} :

$$\mu_N^0(dx) \equiv z_N^{(n)} e^{-\frac{1}{2}\langle x, C_N^{-1}x \rangle} dx$$
(1.15)

where the elements the covariance matrix C_N are defined as follows:

$$(C_N(\mu_i, \mu_j))_{ij} \equiv (A_N(\mu_i, \mu_j))_{ij}^{-1}$$
(1.16)

 $|C_N|$ is the determinant of C_N and for $x = (x_1, \ldots, x_n)$ we have defined:

$$z_N^{(n)} \equiv \sqrt{\frac{|C_N|^{-1}}{(2\pi)^{dn}}}$$
(1.17)

and:

$$\langle x, C_N^{-1} x \rangle \equiv \sum_{i=1}^n \langle x_i, \sum_{j=1}^n C_N^{-1}(\mu_i, \mu_j) x_j \rangle$$

In what follows we shall also denote the element $(C_N(\mu_i, \mu_j)_{i,j})$ of the covariance matrix C_N by $C_N(\mu_i - \mu_j)$, for i, j = 1, ..., n

For all $\alpha = (\alpha_1, \ldots, \alpha_n) \in \mathbb{R}^{dn}$, we have the following characteristic function associated to μ_0^N :

$$\hat{\mu}_N^0(\alpha) = \int_{\mathbb{R}^{dn}} e^{i\sum_{k=1}^n \langle \alpha_k, y_k \rangle} d\mu_N^0(y_1, \dots, y_n) = e^{-\frac{1}{2}\langle C_N \alpha, \alpha \rangle}$$
(1.18)

Now let Γ_N be the restriction to the Λ_N of the dual lattice associated to the definition (1.2.1), namely $\Gamma_N \equiv \Gamma \cap \Lambda_N$. Then:

$$\Gamma \equiv \left\{ \sum_{i=1}^{d} \beta_i w_i : \beta_i \in \mathbb{Z}, i = 1, \dots, d \right\}$$
(1.19)

in such a way that:

$$\langle v_i, w_j \rangle = \delta_{ij} ; i, j = 1, \dots, d$$

Remark 1.2.6. For d = 3 the set Γ is generated by:

$$w_1 \equiv \frac{v_2 \times v_3}{\langle v_1, v_2 \times v_3 \rangle} w_2 \equiv \frac{v_3 \times v_1}{\langle v_1, v_2 \times v_3 \rangle} w_3 \equiv \frac{v_1 \times v_2}{\langle v_1, v_2 \times v_3 \rangle}$$

From the form of Γ given in (1.19), it follows that the dual group, i.e. the Brillouin zone, associated to the Bravais lattice defined in Def.(1.2.1) reads:

$$\hat{\Omega} \equiv \mathbb{R}^d / \Gamma = \left\{ \sum_{i=1}^d \gamma_i w_i : \gamma_i \in \left[-\frac{1}{2}, \frac{1}{2} \right] \right\}$$
(1.20)

Hence (1.14) can be rewritten as:

$$\sum_{\substack{p \in \hat{\Omega}_N \\ p \neq 0}} \overline{\hat{y}_N(p)} \left(\hat{A}_N(0) - \hat{A}_N(p) \right) \hat{y}_N(p) = \sum_{\substack{\mu_i, \mu_j \in \Omega_N \\ \mu_i \neq \mu_j}} \langle y_{\mu_i}, A_N(\mu_i, \mu_j) y_{\mu_j} \rangle$$
(1.21)

where we have defined the quantities:

$$\hat{A}_N(p) \equiv \sum_{k=1}^n \left(\mathscr{H}\Phi \right)(\mu_k) e^{ip \cdot \mu_k} \quad ; \quad \hat{y}_N(p) \equiv \sum_{k=1}^n y_k e^{ip \cdot y_k} \tag{1.22}$$

Using (1.22) we can state the following:

Proposition 1.2.1. Let $\{y_i = 0 : i = 1, ..., n\}$ be the null displacement configuration with respect to the points $\{\mu_i : i = 1, ..., n\}$ of the lattice Ω_N and suppose that it is a stationary point for the deviation energy $\mathfrak{E}_{\Omega_N}^{cr}$. Then it is a local minimum iff $\hat{A}_N(0) - \hat{A}_N(p)$ is a strictly positive definite matrix for all $p \in \Omega_N$.

Proof 1.2.1. The proposition follows from the Fourier representation of the left hand side quantity in (1.14) made above in (1.21) and recalling that the condition (H1b) stated before can be derived using (1.12).

As we have done in (1.16) it is possible to write the following representation for the inverse matrices $(A_N(\mu_i, \mu_j))^{-1}$ in terms of those defined in (1.22). For all $\mu_i, \mu_j \in \Omega_N$ we have from (1.16), (1.21) and (1.22) that:

$$C_N(\mu_i - \mu_j) \equiv (A_N)^{-1} (\mu_i, \mu_j) = \sum_{\substack{p \in \hat{\Omega}_N \\ p \neq 0}} e^{ip \cdot (\mu_i - \mu_j)} \left(\hat{A}_N(0) - \hat{A}_N(p) \right)^{-1}$$
(1.23)

Now it is possible to rewrite the Gaussian measure μ_N^0 defined in (1.15) as follows:

$$\mu_N^0(dy) = z_N^{(n)} \, e^{-\frac{1}{2}\langle y, A_N y \rangle} dy \tag{1.24}$$

where, as before, $y = (y_1, \ldots, y_n)$, $\langle y, A_N y \rangle = \sum_{i,j=1}^n \langle y_i, A_N(\mu_i, \mu_j) y_j \rangle$ and $|A_N|$ denotes the determinant of A_N .

Theorem 1.2.1. Let V be a pair-particle potential depending only on the distance between the two particles and fulfilling the Hypotheses (H1). Then the canonical partition function $Z_N^n(\beta)$ of a configuration-particles $x = (x_1, \ldots, x_n) \in \Lambda_N$ at inverse temperature β with respect to the minimum given by Ω_N for $\mathfrak{E}(x)$, reads as follows:

$$Z_N^n(\beta) = \left(\frac{2\pi}{\beta}\right)^{\frac{dn}{2}} Z_N^{cr} \cdot z_N^{(n)} \cdot Z_N^{dev}(\beta)$$
(1.25)

where we made use of the following definitions for the crystalline partition function:

$$Z_N^{cr} \equiv e^{-\beta \mathfrak{E}_N^{cr}(\Omega_N)} \tag{1.26}$$

and for the deviation partition function:

$$Z_N^{dev}(\beta) \equiv \int_{\mathbb{R}^{dn}} \chi_N(y) e^{-\beta \mathscr{R}\left(\Omega_N | \left\{\frac{y_i}{\sqrt{\beta}}\right\}_{i=1,\dots,n}\right)} d\mu_N^0(y)$$
(1.27)

Here χ_N is the indicator function of the measurable set $\Lambda_N \equiv \{y \in \mathbb{R}^{dn} \mid y_i \mid \leq N\}$ and:

$$\mathscr{R}\left(\Omega_N \mid \{y_i\}_{\mu_i \in \Omega_N}\right) \equiv \mathfrak{E}_N(x) - \frac{1}{2} \sum_{i,j=1}^n (y_i - y_j) \mathscr{H}\Phi(\mu_i - \mu_j) \cdot (y_i - y_j)) - \mathfrak{E}_N^{cr}(\Omega_N)$$

the remainder of the Taylor expansions of the total energy of the configuration of particles x around the local minimum Ω_N .

Proof 1.2.2. By the Taylor expansion of $Z_N^{(n)}(\beta)$ given by (1.4) around the minimizing configuration given by the Bravais lattice defined in Def.(1.2.1) up to the second order, we have:

$$Z_N^n(\beta) = \left(\frac{2\pi}{\beta}\right)^{\frac{dn}{2}} \int\limits_{\Lambda_N^n} e^{-\beta \mathfrak{E}^{(cr)}(\Omega_N)} e^{-\frac{\beta}{2}\sum_{i,j=1}^n (y_i - y_j) \mathscr{H}\Phi(\mu_i - \mu_j) \cdot (y_i - y_j))} e^{-\beta \mathscr{R}\left(\Omega_N | \{y_i\}_{\mu_i \in \Omega_N}\right)} dy_1 \cdots dy_n$$

We use (1.14) in order to write $Z_N^n(\beta)$ in terms of (1.24) and then we perform the integration with respect to the Gaussian measure, making also the following change of variables: $y_i \mapsto \frac{y_i}{\sqrt{\beta}}$ for all i = 1, ..., n in order to gain a β factor in front of the remainder.

Let us define the free energy density of our confined system, see e.g. [Rue99]:

$$P_N(\beta) \equiv \frac{1}{\beta \mid \Lambda_N \mid} \ln Z_N^n(\beta)$$
(1.28)

Using the result of theorem (1.2.1) we have:

$$\beta P_N(\beta) = \frac{dn}{2} \ln 2\pi - dn \ln \beta + \beta P_N^{cr}(\Omega_N \mid \beta) + \beta \tilde{z}_N + \beta p_N(\beta)$$
(1.29)

where we have defined the crystalline free energy density:

$$P_N^{cr}\left(\Omega_N \mid \beta\right) = \frac{1}{\beta \mid \Lambda_N \mid} \ln\left[e^{-\beta \mathfrak{E}^{cr}\left(\Omega_N\right)}\right] = -\frac{\mathfrak{E}^{cr}\left(\Omega_N\right)}{\mid \Lambda_N \mid}$$
(1.30)

and we have introduced the free energy density of non Gaussian fluctuations around Ω_N as follows:

$$p_N(\beta) \equiv \frac{1}{\beta \mid \Lambda_N \mid} \ln \int_{\mathbb{R}^{dn}} \chi_N(y) e^{-\beta \mathscr{R} \left(\Omega_N \mid \left\{\frac{y_i}{\sqrt{\beta}}\right\}_{\mu_i \in \Omega_N}\right)} d\mu_N^0(y)$$
(1.31)

We have also set:

$$\tilde{z}_N \equiv \frac{1}{2\beta} \frac{1}{|\Lambda_N|} \ln z_N^{(n)} \tag{1.32}$$

1.2.1. Detailed Laplace Method in the Finite Volume Case

Here we shall apply the results obtained below in Ch.(4) Sec.(4.2.1) to analyze the problem introduced in Sec.(1.2) and give a more detailed version of the Laplace Method used to study the behaviour, in the limit $\beta \to \infty$, of the partition function (1.4). This allows us, in particular, to find the asymptotic formula (1.5). We shall thus consider the asymptotics of the following integral:

$$I_N^{(n)}(\beta) \equiv \int_{\Lambda_N^n} e^{-\beta H^{(n)}(x)} dx_1 \cdots dx_n$$
(1.33)

where, as in Sec.(1.2),

$$H^{(n)}(x) = \frac{1}{2} \sum_{i \neq j}^{n} \Phi\left(\mid x_i - x_j \mid \right)$$
(1.34)

when $\beta \to \infty$. The Crystal hypothesis implies that the absolute minimum of (1.34) is reached at the point:

$$X_0 \equiv (x_1, \dots, x_n) = (\mu_1, \dots, \mu_n)$$

i.e. when the particles $(\lambda_1, \ldots, \lambda_n)$ sit on the vertices of Ω_N . Since the point (μ_1, \ldots, μ_n) is in the interior of the domain Λ_N^n we can apply the method of Ch.(4) Sec. (4.2.1), below. Then the leading term of (1.33) when $\beta \to \infty$ is given by:

$$\frac{e^{-\beta H^{(n)}(X_0)}}{\sqrt{\left|\mathscr{H}\right|_{x=X_0}}} \left(\frac{2\pi}{\beta}\right)^{\frac{dn}{2}}$$
(1.35)

where $\mathscr{H}|_{x=X_0}$ denotes the $dn \times dn$ -dimensional square Hessian matrix of the Hamiltonian $H^{(n)}$ evaluated at the point X_0 , and $|\mathscr{H}|_{X_0}|$ its determinant.

Let us now assume that $\Phi \in C_0^{\infty}$, then it is possible to write the complete asymptotic expansion of $I_N^{(n)}(\beta)$ in inverse powers of β . Since \mathscr{H} is strictly positive definite in a neighbourhood of X_0 there exists a $dn \times dn$ orthogonal matrix Q such that:

$$Q^T \mathscr{H} Q = (\alpha_1, \dots, \alpha_{dn}) \cdot I_{dn}$$

where $\alpha_1, \ldots, \alpha_{dn}$ are the strictly positive eigenvalues of \mathscr{H} and I_{dn} is the unit matrix in \mathbb{R}^{dn} . Now define the following change of coordinates:

$$(x - X_0) = \langle Q \cdot \left(\left(\sqrt{\alpha_1}, \dots, \sqrt{\alpha_{dn}} \right) \cdot I_{dn} \right)^t, z \rangle$$
(1.36)

where $(\alpha_1, \ldots, \alpha_{dn})$ is dn - dimensional vector given by the eigenvalues α_i , $i = 1, \ldots, dn$. Equation (1.36) implies that, near z = 0, we have:

$$f(z) \equiv H^{(n)}(X_0) - H^{(n)}(x(z)) \sim \frac{z^2}{2}$$
(1.37)

If we take $\xi_i = h_i(z)$ $\forall i = 1, ..., dn$ such that:

$$h_i = z_i + o(|z|)$$
 for $|z| \rightarrow 0$ and $i = 1, \dots, dn$

with:

$$\sum_{i=1}^{dn} h_i^2(z) = 2f(z)$$

then (1.37) holds throughout Λ_N and since $\nabla H^{(n)} = 0$ only at X_0 then the Jacobian:

$$J(\xi) = \frac{\partial(x_1, \dots, x_{dn})}{\partial(\xi_1, \dots, \xi_{dn})}$$
(1.38)

is negative and finite throughout Λ_N .

Let us define $G_0(\xi) \equiv J(\xi)$, on the basis of Sec.(4.2.1) of Ch.(4), with the notations explained there we have the following:

Theorem 1.2.2. The partition function integral (1.33) has the following asymptotic expansion for $\beta \to +\infty$:

$$I_{N}^{(n)}(\beta) \asymp e^{-\beta H^{(n)}(X_{0})} \left(\frac{2\pi}{\beta}\right)^{\frac{dn}{2}} \sum_{j \ge 0} \frac{\Delta_{\xi}^{j} G_{0}|_{\xi=0}}{\left((j!)2\beta\right)^{j}}$$
(1.39)

Here we have $\triangle_{\xi}^{0}G_{0} \mid \xi = 0 \equiv \left(|\mathscr{H}|_{x=X_{0}} \right)^{-\frac{1}{2}}$. In particular:

$$I_{N}^{(n)}(\beta) = \left(\frac{2\pi}{\beta}\right)^{\frac{dn}{2}} \frac{e^{-\beta H^{(n)}(X_{0})}}{\sqrt{|\mathscr{H}|_{x=X_{0}}|}} + \left(\frac{2\pi}{\beta}\right)^{\frac{dn}{2}} \left(\frac{1}{2}\right) (|\mathscr{H}|_{x=X_{0}}|)^{-\frac{1}{2}} \left[-\sum_{p,q,r,s=1}^{dn} \frac{\partial^{3d} H^{(n)}}{\partial x_{s} \partial x_{r} \partial x_{q}} B_{sq}\right]_{x=X_{0}} + O\left(|x - X_{0}|^{3}\right)$$
(1.40)

where the matrix $B = (B_{ij})_{l,m=1,\dots,dn}$ is defined in such a way that:

$$B_{ij}\left(\mathscr{H}_{ij}\mid_{x=X_0}\right)=\delta_{im}$$

Remark 1.2.7. The result stated by (1.39) can be written in a more explicit manner expressing the quantities $\Delta_{\xi}^{j}G_{0}|_{\xi=0}$ in terms of the Hamiltonian function $H^{(n)}$ and G_{0} . Nevertheless, in the general case, it is not simple to explicitly determine the function $G_{0}(\xi)$.

1.3. Finite Volume Cluster Expansion

In what follows we shall develop the rigorous *Cluster Expansion* for the partition function defined in Sec. (1.2), analyze its behaviour in the low temperature regime and state some remarks on the thermodynamic limit of the studied system.

In Sec. (1.2) we reduced the study of $Z_N^{(n)}(\beta)$ to the analysis of the partition function $Z_N^{dev}(\beta)$ which can be viewed as the partition function of a gas of dipoles sitting on the lattice Ω_N and interacting with each other via a potential determined by:

$$\mathscr{R}\left(\Omega_N \mid \left\{\frac{y_i}{\sqrt{\beta}}\right\}_{\mu_i \in \Omega_N}\right) = \sum_{\mu_i, \mu_j \in \Omega_N} \mathscr{R}_{\Omega_N}\left(\mu_i - \mu_j \mid \frac{y_i - y_j}{\sqrt{\beta}}\right)$$
(1.41)

where:

$$\mathscr{R}_{\Omega_N}\left(\mu_i - \mu_j \mid \frac{y_i - y_j}{\sqrt{\beta}}\right) \equiv V\left(\mu_i + \frac{1}{\sqrt{\beta}}y_i - \mu_j - \frac{1}{\sqrt{\beta}}y_j\right) + V(\mu_i - \mu_j) - \frac{1}{2}\left(\frac{y_i - y_j}{\sqrt{\beta}}\left[(\mathscr{H}\Phi)(\mu_i - \mu_j)\right]\frac{y_i - y_j}{\sqrt{\beta}}\right)$$
(1.42)

In order to study $Z_N^{dev}(\beta)$ we shall make the following hypothesis for the Taylor remainders appearing in (1.42):

Hypotesis 1.3.1. There exists a family of complex measures $\left(d\lambda_{\mu_i}^{(N)}\right)_{\mu\in\Omega_N}$ in \mathbb{R}^d such that for all $\mu_i - \mu_j$, whit $(\mu_i, \mu_j) \in \Omega_N \times \Omega_N$, one has:

$$\mathscr{R}_{\Omega_N}(\mu_i - \mu_j \ x) = \int_{\mathbb{R}^d} e^{i\alpha x} d\lambda^{(N)}_{\mu_i - \mu_j} \quad , \quad x \in K$$
(1.43)

where:

- K is a compact subser of \mathbb{R}^d containing the ball of center 0 and radius $R_0 \in \mathbb{R}^+$, where Φ , as a function of the distance, has support in $[0, R_0]$
- $\bar{\lambda}^{(N)}_{\mu}(\alpha) = d\lambda^{(N)}_{\mu}(-\alpha)$, in order for $\mathscr{R}_{\Omega_N}(\mu_i \mu_j \mid x)$ to be a real quantity.

Remark 1.3.1. The measures $\lambda_{\mu_i}^{(N)}$ appearing in hypothesis (1.3.1) depend on the size of the box Λ_N . In using (1.41) and (1.43), we have to observe that the variables $\left\{\frac{y_i}{\sqrt{\beta}}\right\}_{\mu_i \in \Omega_N}$ belong to a compact set. This can be achieved for all $\beta > \beta_0^{(N)}$, for some suitable $\beta_0^{(N)} > 0$.

Remark 1.3.2. Assumption (1.3.1) is working one as first step. For a future study of the thermodynamic limit it should be relaxed, e.g. by allowing λ to become general functions in order to preserve the regularity and stability necessary for the existence of the thermodynamic limit, see [Rue99].

For all vectors $(\lambda_i, \lambda_j, \mu_i, \mu_j, \alpha_i, \alpha_j) \in (\Omega_N)^4 \times \mathbb{R}^2$, let us define the following quantities:

$$V_N(\alpha_i\lambda_i\mu_i \mid \alpha_j\lambda_j\mu_j) \equiv \alpha_i \left(C_N(\lambda_i - \lambda_j) + C_N(\mu_i - \mu_j) - C_N(\lambda_i - \mu_j) - C_N(\mu_j - \lambda_i)\right)\alpha_j$$
(1.44)

The following holds:

Proposition 1.3.1. For the partition function $Z_N^{dev}(\beta)$ defined in (1.27) the following absolutely convergent expansion in powers of β holds:

$$Z_N^d(\beta) = \sum_{n \ge 0} \frac{(-\beta)^n}{n!} \sum_{\mu_i, \mu_j \in \Omega_N} \int e^{-\frac{1}{\beta} \sum_{1 \le i < j \le n} V_N(\alpha_i \lambda_i \mu_i | \alpha_j \lambda_j \mu_j)} \otimes_{l=1}^n d\lambda_{\mu_i - \mu_j}^{(N)}(\alpha_l)$$
(1.45)

Proof 1.3.1. By (1.22), (1.23) and the definition of V_N , we have the following formula:

$$\int_{\Lambda_N} \prod_{j=1}^n \left(e^{\frac{i}{\sqrt{\beta}}\alpha_j y_{\lambda_j}} \cdot e^{-\frac{i}{\sqrt{\beta}}\alpha_j y_{\mu_j}} \right) \mu_0^N(dy) = e^{-\frac{1}{\beta}\sum_{1 \le i < j \le n} V_N(\alpha_i \lambda_i \mu_i | \alpha_j \lambda_j \mu_j)}$$
(1.46)

On the other hand, by the assumption made in (1.3.1), we have an integral representation for the remainders $\mathscr{R}\left(\lambda - \mu \mid \frac{y_i - y_j}{\sqrt{\beta}}\right)$ as characteristic functions associated to the measures $d\lambda_{\mu_i - \mu_j}^{(N)}$ for all the crystalline points $\mu_i, \mu_j \in \Omega_N$ and we obtain the desired expansion. Moreover from the simple inequality:

$$\left|\mu_N^0\left(e^{i\sum_{\mu\in\Omega_N}\alpha_\mu y_\mu}\right)\right| \le 1 \tag{1.47}$$

we obtain the following estimate:

$$Z_N^{dev}(\beta) \le e^{\beta \mu_N^* D_N} \tag{1.48}$$

where we have defined: $\mu_N^* \equiv \max_{\mu \in \Omega_N} \left\{ \int_{\mathbb{R}^3} d \mid \lambda_{\mu}^{(N)} \mid \right\}$, and D_N is the cardinality of the set $\{\mu_i, \mu_j \in \Omega_N : \mid \mu_i - \mu_j \mid < R_0\}$.

Using Prop.(1.3.1) we also obtain an upper bound for the *dipole free energy density* for all $\beta > \beta_0^{(N)}$:

$$p_N^d(\beta) \equiv D_N^{-1} \ln Z_N^{dev} \le \beta \mu_N^* \tag{1.49}$$

1.3.1. Bounded Dipole Length Gas

From the estimate (1.49) it follows that if we want to control the free energy density in (1.31) for large but finite N, we must control the following ratio:

$$\frac{\ln Z_N^{dev}}{|\Lambda_N|}$$

Remark 1.3.3. Since our potential Φ has, by assumption, a compact support we can choose a positive constant $\beta_1^{(N)}$, i.e. a sufficiently small temperature T depending on N, such that if $\beta > \beta_1^{(N)}$ and $|\mu_i - \mu_j|$ is greater than a fixed positive constant R then:

$$\mathscr{R}_{\Omega_N}\left(\mu_i - \mu_j \mid \frac{y_i - y_j}{\sqrt{\beta}}\right) = 0$$

for all i, j = 1, ..., n.

In what follows we always take $\beta = \beta(N) \ge \max\left\{\beta_0^{(N)}, \beta_0^{(N)}\right\}$ in order to satisfy the conditions stated in Rem.(1.3.1) and Rem.(1.3.3).

By previous remark we restrict the admissible *length of the dipoles* by R and define the following bounded partition function:

$$Z_N^{bd}(\beta) \equiv \int_{\mathbb{R}^{dn}} e^{\mathscr{R}_N^{\mu} \left(\Omega_N | \left\{\frac{y_{\mu}}{\sqrt{\beta}}\right\}_{\mu \in \Omega_N}\right)} \mu_N^0(dy)$$
(1.50)

where the restricted Taylor remainder \mathscr{R}^{μ}_{N} is defined as follows:

$$\mathscr{R}_{N}^{\mu}\left(\Omega_{N} \mid \left\{\frac{y_{\mu}}{\sqrt{\beta}}\right\}_{\mu \in \Omega_{N}}\right) \equiv \sum_{\substack{\mu_{i}, \mu_{j} \in \Omega_{N} \\ |\mu_{i} - \mu_{j}| \leq R}} \mathscr{R}_{N}\left(\mu_{i} - \mu_{j} \mid \left\{\frac{\mu_{i} - \mu_{j}}{\sqrt{\beta}}\right\}\right)$$
(1.51)

Now we would like to obtain the analogue of the result in proposition (1.3.1) for large but finite N for the quantity Z_N^{bd} (which can be viewed as a grand canonical partition function of a system of dipoles of length bounded by R, defined on the lattice Ω_N and in termal equilibrium at the temperature $T = \beta^{-1}$).

Let us define the following quantities:

$$D_N^R(K) \equiv D_N^R(1) \times \dots \times D_N^R(K) =$$

= {(\alpha_1, \lambda_1, \mu_1), \ldots (\alpha_K, \lambda_K, \mu_K) | \lambda_i, \mu_i \in \Omega_N, | \mu_i - \lambda_i | < R, \alpha_i \in \mathbb{R}^3} (1.52)

For $\omega \in D_N^R(K)$ we define:

$$\omega = ((\alpha_1, \lambda_1, \mu_1), \dots, (\alpha_n, \lambda_n, \mu_n)) \equiv (\alpha, \lambda, \mu)_n \quad and \quad (\alpha_i, \lambda_i, \mu_i) \equiv d(i) \forall (\alpha_i, \lambda_i, \mu_i) \in D_N^R(i)$$
(1.53)

We will also use the following notations:

$$\int d_N^R(i) \equiv \sum_{\substack{\lambda_i, \mu_i \in \Omega_N \\ |\lambda_i - \mu_i| < R}} \int d\lambda_{\lambda_i - \mu_i}^{(N)}(\alpha_i) \quad \text{and} \quad \int d_N^R(1, \dots, n) \equiv \int d_N^R(n) \cdots \int d_N^R(1) \quad (1.54)$$

Moreover we define:

$$\mathscr{E}_N\left((\alpha,\lambda,\mu)_n\right) \equiv \sum_{1 \le i < j \le n} V_N(\alpha_i,\lambda_i,\mu_i \mid \alpha_j\lambda_j\mu_j)$$
(1.55)

and:

$$\mathscr{E}_{N}\left((\alpha,\lambda,\mu)_{n}\mid(\alpha',\lambda',\mu')_{m}\right)\equiv \mathscr{E}_{N}\left((\alpha,\lambda,\mu)_{n}\cup(\alpha',\lambda',\mu')_{m}\right)-\mathscr{E}_{N}\left((\alpha,\lambda,\mu)_{n}\right)-\mathscr{E}_{N}\left((\alpha',\lambda',\mu')_{m}\right)$$
(1.56)

Using previous notations we can rewrite (1.50) as follows:

$$Z_N^{bd} = \sum_{n \ge 0} \frac{(-\beta)^n}{n!} \int d_N^R(1, \dots, n) e^{-\frac{1}{\beta} \mathscr{E}_N(d(1), \dots, d(n))}$$
(1.57)

1.3.2. Cluster Expansion

In this section we will follow [AeK73] in order to apply the method of the linked cluster expansion for the free energy density for large but finite volume. Let us to define the set \mathscr{G}_n^N of all n – linear graphs that can be built on the set $D_N^R(n)$ defined before. Let $\Gamma \in \mathscr{G}_n^N$, Γ be characterized by a set of vertices $\mathscr{V} = \mathscr{V}(\Gamma)$ and by a set of arcs $\mathscr{A} = \mathscr{A}(\Gamma)$. For every point $(\alpha_i, \lambda_i, \mu_i)$ of Γ define the following vertex function:

$$V_N(i) \equiv e^{-\frac{1}{\beta}\alpha_i^2(C_N(0) - C_N(\lambda_i - \mu_i))}$$
(1.58)

From the positive defineteness of the covariance matrix C_N it follows that $C_N(0) - C_N(\mu) \ge 0$ for all $\mu \in \Omega_N$. From this and (1.58) we have the following estimate for the vertex contribution:

$$\left\|\prod_{i\in\mathscr{V}(\Gamma)}V_N(i)\right\| \le 1 \tag{1.59}$$

Let Γ be an element of \mathscr{G}_n^N and let $l \in \mathscr{A}(\Gamma)$, l linking a starting point $l_s = (\alpha_{l_s}, \lambda_{l_s}, \mu_{l_s})$ to an ending point $l_e = (\alpha_{l_e}, \lambda_{l_e}, \mu_{l_e})$. Let us define the following arc function:

$$V_N(l) \equiv V_N(l_s \mid l_e) \tag{1.60}$$

Using definitions (1.58) and (1.60) we can compute the weight of a graph $\Gamma \in \mathscr{G}_n^N$ as follows:

$$w_N^n(\Gamma) = \frac{1}{D_N^R} \int d_N^R(1) \cdot \int d_N^R(n) \prod_{l \in \mathscr{A}(\Gamma)} \left(e^{-\frac{1}{\beta}V_N(l) - 1} \right) \prod_{i \in \mathscr{V}(\Gamma)} V_N(i)$$
(1.61)

while the weight of the entire set \mathscr{G}_n^N is:

$$w(\mathscr{G}_n^N) = \sum_{\Gamma \in \mathscr{G}_n^N} w_N^n(\Gamma)$$
(1.62)

Using previous definitions one can state the following result:

Proposition 1.3.2. For the bounded partition function Z_N^{bd} defined by (1.50), the following cluster expansion holds:

$$Z_N^{bd} = e^{\sum_{n=1}^{\infty} (-\beta)^n \cdot w_N^n}$$

where the series is absolute convergent.

Proof 1.3.2. Given an element $\Gamma \in \mathscr{G}_n^N$ we define:

$$\mathscr{M}(\mathscr{V}(\Gamma)) \equiv \prod_{i,j\in\mathscr{V}(\Gamma)} \left[e^{-\frac{1}{\beta}V_N(d(i)|d(j))} - 1 \right]$$
(1.63)

then, see [Rue99, AeK73], we have:

$$e^{-\frac{1}{\beta}\mathscr{E}_{N}(d(1),\dots,d(n))} = \prod_{i=1}^{n} V_{N}(i) \prod_{1 \le i \ne j \le n} e^{-\frac{1}{\beta}V_{N}(d(i)|d(j))} =$$
$$= \prod_{i=1}^{n} V_{N}(i) \prod_{1 \le i \ne j \le n} \left(\left[e^{-\frac{1}{\beta}V_{N}(d(i)|d(j))} - 1 \right] + 1 \right) =$$
$$= \prod_{i=1}^{n} V_{N}(i) \sum_{\Gamma \subset \{1,\dots,n\}} \mathscr{M}(d(i \in \Gamma))$$

Since by:

$$Z_N^{bd} = \sum_{n \ge 0} \frac{(-\beta)^n}{n!} \int d_N^R(1, \dots, n) e^{-\frac{1}{\beta} \mathscr{E}_N(d(1), \dots, d(n))}$$

we have then:

$$Z_N^{bd} = \sum_{n \ge 0} \frac{(-\beta)^n}{n!} \int d_N^R(1, \dots, n) \prod_{i=1}^n V_N(i) \sum_{\Gamma \subset \{1, \dots, n\}} \mathscr{M}(d(i \in \Gamma))$$

and computing the sum we obtain the result.

Now we are in a position to state the following result concerning the finiteness of the *dipole* free energy density for large but finite N:

Theorem 1.3.1. Let $n \in \mathbb{N}$, $\Gamma \in \mathscr{G}_n^N$ and $\beta \in \mathbb{R} - \{0\}$, then:

$$\mid w_N^n(\Gamma) \mid < \infty \tag{1.64}$$

Proof 1.3.3. Let us firt recall some facts from Graph Theory. We are studying particular graphs $\Gamma \in \mathscr{G}_n^N$ which are undirected and simple trees, this means that given $\Gamma \in \mathscr{G}_n^N$ for any two vertices of Γ , they are connected by exactly one undirected simple, i.e. with no loop allowed, path, moreover Γ is connected. We adopt the following definition of a spanning tree $\mathscr{S}(\Gamma)$ of the graph Γ as the tree composed of all the vertices $i \in \mathscr{V}(\Gamma)$ and of a, not necessarily proper, subset of arcs of $\mathscr{A}(\Gamma)$. Hence we can construct $\mathscr{S}(\Gamma)$ selecting some edges of Γ in such a a way that they form a sub-tree spanning every vertex of the original tree Γ . This means that, for connected graphs $\Gamma \in \mathscr{G}_N^n$, a spanning tree can be defined as a minimal set of edges that connect all vertices. If a tree is a connected graph then it admits a spanning tree, moreover the Cayley's formula tells us the number of these trees. Let $\Gamma \in \mathscr{G}_N^n$ and \mathscr{S} be one of its spanning tree, then we define:

$$|\mathscr{A}'| = |\mathscr{A}'(\Gamma)| \equiv k + s$$

where $k \equiv |\mathscr{A}(\mathscr{S})|$ is the number of elements in $\mathscr{A}(\mathscr{S})$ and $s = |\mathscr{A}'| - k$ (which equals the number of edges in the subgraph $\Gamma - \mathscr{S}$). Then we can estimate the contribution to the total weight $w_N^n(\Gamma)$ coming from the arcs $l \notin \mathscr{S}$ as follows:

$$\sup_{l} \left\| e^{\frac{1}{\beta}V_{N}(l)} - 1 \right\| \le c \cdot \frac{C_{1}}{\beta} \mid \alpha_{l_{s}} - \alpha_{l_{e}} \mid e^{\frac{c \cdot C_{2}\alpha_{l_{s}}\alpha_{l_{e}}}{\beta}}$$
(1.65)

where the c = c(d) is a positive constant and the quantities C_1 and C_2 are defined as follows:

$$C_1 \equiv \sup_N \left(\sup_{\mu \in \Omega_N} \|C_N(\mu)\| \right)$$

$$C_2 \equiv \sup_{\mu \in B_R(0)} \sup \left\{ \mid \alpha \mid : \alpha \in supp(d\lambda_{\mu}^{(N)}) \right\}$$

From this it follows:

$$|w_n^N(\Gamma)| \le C_3 b_N^n \left(\mathscr{S}(\Gamma)\right) \tag{1.66}$$

where

$$C_3 = C_3(\beta) \equiv \frac{c}{\beta} C_1 \cdot C_2^2 e^{\frac{c \cdot C_1 C_2^2}{\beta}}$$

Let us set $\hat{C}_3 \equiv e^{\frac{c \cdot C_1 C_2^2}{\beta}}$, then, recalling (1.61), we have:

$$w_N^n(\mathscr{S}(\Gamma)) \le \frac{\hat{C}_3^{n-1}}{\mid D_N^R(1) \mid} \int \mid d_N^R(1, \dots, n) \mid \prod_{i=1}^{n-1} \|V_N(d(i) \mid d(i+1)\|$$
(1.67)

Let $\rho \in \Omega_N$ then the following holds

$$V_N((\alpha_i, \lambda_i + \rho, \mu_i + \rho) \mid (\alpha_j, \lambda_j + \rho, \mu_j + \rho) =$$

= $\alpha_i (C_N((\lambda_i + \rho) - (\lambda_j + \rho)) + C_N((\mu_i + \rho) - (\mu_j + \rho)) +$
- $C_N((\lambda_i + \rho) - (\mu_j + \rho)) - C_N((\mu_j + \rho) - (\lambda_i + \rho)))\alpha_j =$
= $V_N(\alpha_i \lambda_i \mu_i \mid \alpha_j \lambda_j \mu_j)$

Hence for a fixed size N the quantity on the right hand side of (1.67) is bounded by:

$$c(\beta^{-1}) \sum_{\lambda_{1} \in B_{R}(0)} \sum_{\substack{\lambda_{2}, \mu_{2} \in \Omega_{N} \\ |\lambda_{2} - \mu_{2}| \leq R}} \cdots \sum_{\substack{\lambda_{n}, \mu_{n} \in \Omega_{N} \\ |\lambda_{n} - \mu_{n}| \leq R}} \int d \mid \lambda_{\lambda_{j} - \mu_{j}} \mid (\alpha_{j}) \cdots \int d \mid \lambda_{\lambda_{n} - \mu_{n}} \mid (\alpha_{n}) \times \prod_{\substack{\lambda_{n} \in B_{R}(0) \\ |\lambda_{2} - \mu_{2}| \leq R}} \|V_{N}(\alpha_{j}, \lambda_{j}, \mu_{j} \mid \alpha_{j+1}\lambda_{j+1}\mu_{j+1})\| \leq d \leq \hat{c}(\beta^{-1}) \sum_{\substack{\lambda_{1} \in B_{R}(0) \\ |\lambda_{2} - \mu_{2}| \leq R}} \sum_{\substack{\lambda_{2}, \mu_{2} \in \Omega_{N} \\ |\lambda_{2} - \mu_{2}| \leq R}} (I_{N}(\alpha_{1}, \lambda_{1}, 0, \alpha_{2}, \lambda_{2}, \mu_{2}))^{n-1}$$

where $c(\beta^{-1})$, $\hat{c}(\beta^{-1})$ are constants depending on β^{-1} and possibly on R,

$$I_N(\alpha_1,\lambda_1,\mu_1,\alpha_2,\lambda_2,\mu_2) \equiv \int V_N(\alpha_1,\lambda_1,\mu_1 \mid \alpha_2,\lambda_2,\mu_2) d \mid \lambda_{\lambda_1}^{(N)} \mid (\alpha_1) d \mid \lambda_{\lambda_2-\mu_2} \mid (\alpha_2) d \mid \lambda_{\lambda_2-\mu_2} \mid (\alpha_2) d \mid \lambda_{\lambda_1} \mid (\alpha_1) d \mid \lambda_{\lambda_2-\mu_2} \mid (\alpha_2) d \mid \lambda_{\lambda_1} \mid (\alpha_2) d \mid \lambda_{\lambda_2} \mid (\alpha_2) d \mid \lambda_{\lambda_2} \mid (\alpha_2) d \mid \lambda_{\lambda_2} \mid (\alpha_2) d \mid \lambda_{\lambda_1} \mid (\alpha_2) d \mid \lambda_{\lambda_2} \mid (\alpha_2) d$$

and the statement of the theorem follows.

1.3.3. Towards Zero Temperature in the Finite Volume

In what follows we will use the result obtained in theorem (1.3.1) in order to study the behaviour of the weights $w_N^n(\Gamma)$, i.e. the virial coefficients, when the temperature approaches zero, i.e. in the limit $\beta \to \infty$.

Theorem 1.3.2. Under the hypothesis of theorem (1.3.1) we have:

$$\lim_{\beta \to \infty} w_N^n(\beta) = 0 \quad and \quad \lim_{\beta \to \infty} \frac{d^k w_N^n(\beta)}{d^k \left(-\frac{1}{\beta}\right)} = 0$$

Proof 1.3.4. From theorem (1.3.1) and exploiting the translational invariance property of the potential we can assume that the graphs Γ always have at least one of their vertices located at some point $(0, \lambda) \equiv (0, 0, \lambda)$ providing $\lambda \in B_R(0)$, hence:

$$w_N^n(\Gamma) = \sum_{\mu_1 \in B_R(0), (0,\mu_1) \in \mathscr{V}(\Gamma)} \int d\lambda_{\mu_1}^{(N)}(\alpha_1) \cdots \prod_{l \in \mathscr{L}(\Gamma)} \left[e^{-\frac{1}{\beta}V_N(l)} - 1 \right] \cdot \prod_{i \in \mathscr{V}(\Gamma)} V(i)$$
(1.68)

From this it follows that, for a given graph Γ , $w_N^n(\Gamma)$ is an analytic function of the temperature $T = \frac{1}{\beta}$ for $\beta \neq 0$ and that $\lim_{\beta \to \infty} w_N^n(\Gamma) = 0$. Hence, for every graph Γ , we can perform the

following Taylor expansion:

$$\frac{d^{k}w_{N}^{n}(\Gamma)}{d\left(-\frac{1}{\beta}\right)^{k}} = \sum_{\substack{k_{1},\dots,k_{\mid\mathcal{L}(\Gamma)\mid}\ r_{j},\dots,r_{\mid\mathcal{V}(\Gamma)\mid}\\ \sum_{i=1}^{\mid\mathcal{L}(\Gamma)\mid}\ k_{i}+\sum_{j=1}^{\mid\mathcal{L}(\Gamma)\mid}\ r_{j}=k}} \sum_{\substack{\left(-\frac{1}{\beta}\right)^{\sum_{i=1}^{\mid\mathcal{L}(\Gamma)\mid}\ k_{i}+\sum_{j=1}^{\mid\mathcal{L}(\Gamma)\mid}\ r_{j}=1}\\ = \sum_{\substack{\mu_{1}\in B_{R}(0)\\(0,\mu_{1})\in\mathcal{L}(\Gamma)}} \int d\lambda_{\mu_{1}}^{(N)}\cdots \prod_{l=1}^{\mid\mathcal{L}(\Gamma)\mid}\ V_{N}(l)^{k_{i}}\prod_{j=1}^{\mid\mathcal{V}(\Gamma)\mid}\ V_{N}(j)^{r_{j}}\times \\ \times \prod_{l\in\mathcal{L}(\Gamma)} e^{-\frac{1}{\beta}V_{N}(l)-(1-\theta(k_{l}))}\prod_{i\in\mathcal{V}(\Gamma)}V(i)$$
(1.69)

Since the number of restricted graphs that we are considering is finite we have then:

$$\lim_{\beta \to \infty} \frac{d^k w_N^n(\Gamma)}{d\left(-\frac{1}{\beta}\right)^k} = 0 \tag{1.70}$$

Now we would like to study the *cluster expansion* for the free energy density of non Gaussian fluctuations around the crystalline structure for large but finite N. We have to control the behaviour of the cluster expansion of the quantity $p_N(\beta)$ defined by (1.31):

For any given couple of points $(\alpha_i, \lambda_i, \mu_i), (\alpha_j, \lambda_j, \mu_j)$ we have that for a given n - linear graph $\Gamma = (\alpha, \lambda, \mu)_n$ the energy $\mathscr{E}_N((\alpha, \lambda, \mu)_n)$ defined by Eq. (1.55) can be written as follows:

$$\mathscr{E}_N((\alpha,\lambda,\mu)_n) = \sum_{1 \le i \ne j \le n} \alpha_i (C_{\mathbb{N}}(\lambda_i - \lambda_j) + C_N(\mu_i - \mu_j) + C_N(\lambda_i - \mu_j) - C_N(\mu_j - \lambda_i))\alpha_j$$

for every sets $(\alpha, \lambda, \mu)_n, (\alpha', \lambda', \mu')_m$

Now consider a vector $\gamma \in [0,1]^{n-1}$ and let us recursively define the following sequence of energies:

$$\mathscr{E}_{N}^{0}((\alpha,\lambda,\mu)_{n}) \equiv \mathscr{E}_{N}((\alpha,\lambda,\mu)_{n})$$
$$\mathscr{E}_{N}^{i}((\alpha,\lambda,\mu)_{n}) \equiv (1-s_{i})\mathscr{E}_{N}((\alpha,\lambda,\mu)_{n} \mid (\alpha_{i},\lambda_{i},\mu_{i})) + s_{i}\mathscr{E}_{N}^{i-1}((\alpha,\lambda,\mu)_{n}) \qquad (1.71)$$
$$\mathscr{E}_{N}^{n-1}((\alpha,\lambda,\mu)_{n}) \equiv \mathscr{E}_{N}^{n}((s)_{n-1})$$

Then the following theorem holds:

Theorem 1.3.3. By (1.3.1) the free energy density $p_N(\beta)$ has a convergent expansion in terms of the weights $w_N^n(\beta)$.
Proof 1.3.5. Let us consider the following set of functions:

$$\mathscr{F}_n \equiv \{\eta : \{1, \dots, n\} \to \{1, \dots, n\} : \eta(i) \le i, \ \forall i = 1, \dots, n\}$$
 (1.72)

For any couple: $(\eta, (s)_{n-1}) \in \mathscr{F}_n \times [0, 1]^{n-1}$ and any $n \ge 1$ let us define the function:

$$f(\eta, (s)_{n-1}) = \prod_{i=2}^{n-1} s_{i-1} s_{i-2} \cdots s_{\eta(i)}$$
(1.73)

with $f(\eta, s_1) \equiv 1$. Then the virial coefficient $w_N^n = w_N^n(\beta)$ can be rewritten as follows:

$$w_N^n(\beta) = \frac{1}{(-\beta)^{n-1}} \sum_{\eta \in \mathscr{F}_n} \int d(s)_{n-1} \int d_N^R(\alpha, \lambda, \mu)_n f(\eta, (s)_{n-1} \times \prod_{i=1}^{n-1} (d(i+1) \mid d(\eta(i))) e^{-\frac{1}{\beta} \mathscr{E}_N^n((s)_{n-1})}$$

where we have defined:

$$\int d_N^R(\alpha,\lambda,\mu)_n = \sum_{\mu_1 \in B_R(0)} \int d\lambda_{\mu_1}^{(N)}(\alpha_1) \sum_{\substack{\lambda_2,\mu_2 \in \Omega_N \\ |\lambda_2 - \mu_2| < R}} \int d\lambda_{\lambda_2 - \mu_1}^{(N)}$$

The definition (1.71) leads to a convex sums of energies, hence, at every step of the induction, we have an energy function which is positive definite and then also the final one maintains this property. From, e.g. [BF78] one can deduce:

$$\sum_{\eta \in \mathscr{F}_n} \int d(s)_{n-1} f(\eta, (s)_{n-1}) \le e^{n-1}$$

Using this and Th. (1.3.3) we obtain the following bound on the coefficient $w_N^n(\beta)$:

$$|w_{N}^{n}(\beta)| \leq \frac{\cdot e^{n-1}}{n\beta^{n-1}} \times \left\| \sup_{\substack{\mu \in B_{R}(0)}} \left(\int d \mid \lambda_{\mu}(\alpha) \mid \mid \alpha \mid \right) \sum_{\substack{\lambda', \mu' \in \Omega_{N} \\ \mid \lambda' - \mu' \mid < R}} \int d \mid \lambda_{\lambda' - \mu'}(\alpha') \mid \alpha' \mid \left\| \hat{V}_{N}(0, \lambda \mid \lambda', \mu') \right\| \right\|^{n-1}$$

where we used the notation in (1.44). Recalling the definition in (1.71), we have obtained the desired expansion of the free energy density $p_N(\beta)$ which can be rewritten as follows:

$$p_N(\beta) = (-\beta) \sum_{n \ge 1} \frac{1}{n} \sum_{\eta \in \mathscr{F}} \int d(s)_{n-1} \int d_N^R(\alpha, \lambda, \mu)_n f(\eta, (s)_{n-1}) \times \prod_{i=1}^{n-1} \mathscr{E}_N\left(d(i+1) \mid d(\eta(i)) e^{-\frac{1}{\beta} \mathscr{E}_N^n[(s)_{n-1}]}\right)$$
(1.74)

as an absolutely convergent series for any $\beta > 0$

 \Box .

Remark 1.3.4. We would like to underline that it is possible to control the limit for $N \to +\infty$ of \tilde{z}_N .

Let us start recalling the definition of the infinitely extended lattice. Let $\{v_1, v_2, v_3 : v_i \in \mathbb{R}^d\}$ be a set of d independent vectors in \mathbb{R}^d , then an infinite Bravais lattice is defined as:

$$\Omega_{\infty} \equiv \{\sum_{k=1}^{d} \alpha_k v_k : \alpha_k \in \mathbb{Z}, k = 1, \dots, d\}$$

then we define the infinite dual lattice Γ_{∞} and the associated Brillouin zones $\hat{\Omega}_{\infty} \equiv \mathbb{R}^d / \Gamma_{\infty}$. Let us set for all $p \in \hat{\Omega}_{\infty}$:

$$\hat{A}_{\infty}(p) \equiv \sum_{\mu \in \Omega_{\infty}, \mu \neq 0} [\mathscr{H}\Phi](\mu) e^{ip \cdot \mu}$$
(1.75)

Since $\mathscr{H}\Phi(\cdot)$ has compact support, then $\hat{A}_{\infty}(p)$ is a well defined quantity, in fact it is the limit of $\hat{A}_N(p)$ when $N \to +\infty$. We can then go to the limit for $N \to +\infty$ in the formula (1.21) and get

$$\frac{1}{2}\sum_{\substack{\mu_i,\mu_j\in\Omega_{\infty}\\\mu_i\neq\mu_j}} (y_i - y_j, [\mathscr{H}\Phi(\mu_i - \mu_j)](y_i - y_j)) = \int_{\hat{\Omega}_{\infty}} \overline{\hat{y}(p)} \left(\hat{A}_{\infty}(0) - \hat{A}_{\infty}(p)\right) \hat{y}(p) dp \qquad (1.76)$$

where $\hat{y}_N(p) \equiv \sum_{\mu \in \Omega_\infty} y_\mu e^{ip \cdot \mu}$ which is well defined for all $L^2(\Omega_\infty)$ functions y of compact support.

Since:

$$\tilde{z}_N = \frac{1}{2\beta \mid \Lambda_N \mid} \ln \left| \frac{1}{2\pi} A_N(\mu_i, \mu_j)_{\mu_i, \mu_j \in \Omega_N} \right| = \frac{1}{2\beta \mid \Lambda_N \mid} \sum_{p \in \hat{\Omega}_N} tr \ln \left(\hat{A}_N(0) - \hat{A}_N(p) \right)$$

then if:

.

$$\lim_{N \to +\infty} \sum_{p \in \hat{\Omega}_N} tr \ln \left(\hat{A}_N(0) - \hat{A}_N(p) \right)$$
(1.77)

exists then it would be given by:

$$\int_{\mathbb{R}^d} tr ln \left[\hat{A}_{\infty} - \hat{A}_{\infty}(p) \right] dp \tag{1.78}$$

and we would have the formula:

$$\tilde{z}_N \xrightarrow{N \to \infty} \frac{1}{2\beta \mid \Lambda_N \mid} \int_{\hat{\Lambda}} tr ln \left[\hat{A}_{\infty} - \hat{A}_{\infty}(p) \right] dp$$
(1.79)

Remark 1.3.5. The limit (1.77) exists and is given by (1.78), and hence (1.79) holds, e.g. if $\hat{A}_N(0) - \hat{A}_N(p) \ge cp^2$ for all |p| sufficiently small, and some constant c independent of N. At least for any fixed N, this bound is easily seen to hold, on the basis of our assumption on Φ .

CHAPTER 2

The Feynman-Vernon influence functional

2.1. Introduction

In what follows we will give a rigorous representation of the Feynman-Vernon influence functional used to describe open quantum systems. It is based on the theory of infinite dimensional oscillatory integrals, see Ch. (7). This allows us to rigorously describe the density matrices characterizing the well known Caldeira-Leggett model of two quantum systems with a quadratic interaction. Once this rigorous description is achieved we can use, in principle, the techniques developed in Ch.(7) in order to obtain asymptotic expansion of the infinite dimensional integrals occurring in the Caldeira-Legget model.

2.1.1. Open Quantum Systems

One of the crucial problems of modern physics consists in understanding the behaviour of an *open quantum system*, i.e. of a quantum system coupled with a second system often called *reservoir* or *enviroment*. One is interested in the dynamics of the first system, taking into account the influence of the environment on it. A typical example is the study of a quantum particle submitted to the measurement of an observable. In fact, from a quantum mechanical point of view, the interaction with the measuring apparatus cannot be neglected and modifies the dynamics of the particle. On the other hand the evolution of the measuring instrument is not of primary interest.

A particularly intriguing approach to this problem was proposed in 1963 by Feynman and Vernon (see [FH65, FV63]) within the path integral formulation of quantum mechanics. In 1942 R.P. Feynman [Fey42], see also [Bro05], following a suggestion by Dirac (see [Dir33, Dir47], proposed an alternative (Lagrangian) formulation of quantum mechanics (published in [Fey48]), that is an heuristic, but very suggestive representation for the solution of the Schrödinger

2.1 Introduction

equation

$$\begin{cases} i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2M}\Delta\psi + V\psi\\ \psi(0,x) = \psi_0(x) \end{cases}$$
(2.1)

describing the time evolution of the state ψ of a d-dimensional quantum particle. The parameter \hbar is the reduced Planck constant, m > 0 is the mass of the particle and $F = -\nabla V$ is an external force. According to Feynman's proposal the wave function of the system at time t evaluated at the point $x \in \mathbb{R}^d$ is heuristically given as an "integral over histories", or as an integral over all possible paths γ in the configuration space of the system with finite energy passing in the point x at time t:

$$\psi(t,x) = \left(\int_{\{\gamma|\gamma(t)=x\}} e^{\frac{i}{\hbar}S_t^{\circ}(\gamma)} D\gamma \right)^{-1} \int_{\{\gamma|\gamma(t)=x\}} e^{\frac{i}{\hbar}S_t(\gamma)} \psi_0(\gamma(0)) D\gamma \quad (2.2)$$

where $S_t(\gamma)$ is the classical action of the system evaluated along the path γ , i.e. :

$$S_t(\gamma) \equiv S_t^{\circ}(\gamma) - \int_0^t V(\gamma(s))ds, \qquad (2.3)$$

$$S_t^{\circ}(\gamma) \equiv \frac{M}{2} \int_0^t |\dot{\gamma}(s)|^2 ds, \qquad (2.4)$$

 $D\gamma$ is an heuristic Lebesgue "flat" measure on the space of paths and:

$$\left(\int_{\{\gamma|\gamma(t)=x\}} e^{\frac{i}{\hbar}S_t^{\circ}(\gamma)}D\gamma\right)^{-1}$$

is a normalization constant.

Feynman and Vernon (see [FH65, FV63]) generalized this idea to the study of the time evolution of the reduced density operator of a system in interaction with an environment. Let denote ρ_A, ρ_B , respectively, the initial density matrices of the system and of the environment, S_A, S_B , respectively, the action functionals of the system and of the environment and S_I the contribution to the total action due to the interaction. Then the kernel of the reduced density operator of the system ρ_R (obtained by tracing over the environmental coordinates) is heuristically given by:

$$\rho_R(t, x, y) = \iint_{\substack{\gamma(t)=x\\\gamma'(t)=y}} e^{\frac{i}{\hbar}(S_A(\gamma) - S_A(\gamma'))} F(\gamma, \gamma') \rho_A(\gamma(0), \gamma'(0)) D\gamma D\gamma' \quad (2.5)$$

where F is the formal influence functional (IF):

$$F(\gamma, \gamma') = \iint_{\substack{\Gamma(t)=Q\\ \Gamma'(t)=Q}} e^{\frac{i}{\hbar}(S_B(\Gamma) - S_B(\Gamma'))} e^{\frac{i}{\hbar}(S_I(\Gamma, \gamma) - S_I(\Gamma', \gamma'))} \times$$

$$\times \rho_B(\Gamma(0), \Gamma'(0)) D\Gamma D\Gamma' dQ''$$
(2.6)

The number of spin-offs originated by the seminal work [FV63] is so large that it is nearly impossible to give here a complete list, and we limit ourselves to shortly mention some of them.

Probably the most influential contributions can be found in [CL83a, CL83b], where Caldeira and Leggett applied the heuristic IF method in order to study the quantum Brownian motion (QBM), i.e. the analogous of the *classical Brownian motion* but for a quantum particle, and the tunneling phenomenon in dissipative systems. Latter papers triggered a chain-reaction which is actually far from its end. In [Leg84] (see also [CL81, Cal83]) Leggett determined the imaginary-time functional which supplies the tunnelling rate form of a metastable state at zero temperature, in a formal WKB limit, in presence of an arbitrary linear dissipation mechanism. In [CL85] an explicit calculation of the time-dependent density matrix is given describing the damping on quantum interference between two Gaussian wave packets in a harmonic potential and the obtained results are in agreement with the quantum theory of measurement, see e.g. [Zur82].

In [HA85] the decoupled particle-bath initial condition previously used, was compared with the initial off-diagonal coherence of the reduced density matrix, constituting the *thermal initial condition*.

A wide-range use of the IF approach was given in [LCD⁺87] where the authors on the basis of their previous experiences managed to give a deep view to the dynamics of a two-state system coupled to a dissipative environment.

In [CH87] an application of the IF formalism was given in order to study the reduced density operator of a particle coupled with a fermionic environment. Similar applications may be found in [Sch82, Gui84, Che87, Zwe87, BSZ92], where the fluctuations in the motion of a heavy particle interacting with a free fermion gas are studied, providing various type of classical and semiclassical expansion either with and without weak-potential or linear response assumptions.

Chen's approach was extended in the case of a boson bath in [CLL89].

The heuristic IF approach was generalized in [SC87, SC90] to a nonfactorizable initial system-plus-reservoir density operator without specific symmetry assumptions.

Since heterogeneous problems related to macroscopic effects in quantum system require extensions to the QBM theory, following [CL83a] various attempts to derive a *master-equation* (ME) were made in order to include general initial conditions and nonlinear couplings. The ME for linear coupling and ohmic environment at high temperature found in [CL83a] was first extended to arbitrary temperature in [UZ89] and afterwards obtained for more general environments and nonlocal couplings, which produce colored noise and nonlocal dissipation, see [GSI88, HPZ92, Bru93, HPZ93, BG03] and references therein.

A complementary use of the IF approach to the description of Markovian open quantum systems can be found in [Str97], where the IF method is used in order to develop the ME of general Lindblad positive-semigroup (see [Lin76]) and the propagator in a formal stationary phase approximation is calculated.

The derivation of the ME for the reduced dynamics of quantum system have gained a lot of contributions by the use of mathematical respectively physical path integrals (PI) techniques (see e.g. [Exn85, JL02] respectively [Wei99, BP02, Kle04, GZ04] and references therein).

The IF formalism was also used in a *parametric random matrices approach* to the problem of dissipation in many-body systems, see e.g. [BDK95, BDK96, BDK97, BDK98] and references therein, where the derived form of the IF differs from the one in [CL83a] and recovers the latter as the first term of its formal Taylor expansion.

The emerging theory of Quantum Computation is another field of application of the IF method since the implementation of real quantum processors is often hampered by the quantum decoherence phenomenon, see e.g. [Deu89, Unr95, BDE95, DS98, PZ99, GJZ⁺03, SH04] and references therein.

Despite the broad range of its applications, a rigorous mathematical construction of the IF is still missing.

Our aim is to fill this gap following the ideas introduced in [AHK76, AHK77] in connection with the rigorous mathematical definition of Feynman path integrals (2.2) and in order to realize formulae (2.5) and (2.6) as well defined infinite dimensional oscillatory integrals on a suitable Hilbert space.

Before we go over to a short description of our present work we would like to outline that there are rigorous works on models of particles in interaction with heat bath not based on the IF approach, e.g. see [Dav73, CEFM00] and references therein.

In Sec. (2.2) we recall some known results, extend the definition of infinite dimensional oscillatory integrals and prove some important properties, for more details see Ch (7), [AGM03, AGM04, AM05b, AM05a, AM04b, AM04c, AM04a] and references therein.

In Sec. (2.3) the new functional integral is used in the study of the time evolution of two linearly interacting quantum systems. A mathematical formalization of the Feynman-Vernon's theory of the IF is given in Sec. (2.4). The main results in this section are Theorems (2.3.3)and (2.3.4) where a conseguence of the Rem.(2.4.1) is used in order to prove the integrability of certain function. The last part is devoted to the study of the Caldeira-Leggett model, see [CL83a], in the case of a finite dimensional heat bath.

2.2. Fresnel Integrals

In the following we shall denote by \mathcal{H} a (finite or infinite dimensional) real separable Hilbert space, whose elements will be denoted by $x, y \in \mathcal{H}$ and the scalar product with $\langle x, y \rangle$. The function $f : \mathcal{H} \to \mathbb{C}$ will be a function on \mathcal{H} and $L : D(L) \subseteq \mathcal{H} \to \mathcal{H}$ an invertible, densely defined and self-adjoint operator.

Let us denote by $\mathcal{M}(\mathcal{H})$ the Banach space of the complex bounded variation measures on \mathcal{H} , endowed with the total variation norm, that is:

$$\mu \in \mathcal{M}(\mathcal{H}), \qquad \|\mu\| = \sup \sum_{i} |\mu(E_i)|,$$

where the supremum is taken over all sequences $\{E_i\}$ of pairwise disjoint Borel subsets of \mathcal{H} , such that $\bigcup_i E_i = \mathcal{H}$. $\mathcal{M}(\mathcal{H})$ is a Banach algebra, where the product of two measures $\mu * \nu$ is by definition their convolution:

$$\mu * \nu(E) = \int_{\mathcal{H}} \mu(E - x)\nu(dx), \qquad \mu, \nu \in \mathcal{M}(\mathcal{H})$$

and the unit element is the vector δ_0 .

Let $\mathcal{F}(\mathcal{H})$ be the space of complex functions on \mathcal{H} which are Fourier transforms of measures belonging to $\mathcal{M}(\mathcal{H})$, that is:

$$f: \mathcal{H} \to \mathbb{C}$$
 $f(x) = \int_{\mathcal{H}} e^{i\langle x, \beta \rangle} \mu_f(d\beta) \equiv \hat{\mu}_f(x).$

 $\mathcal{F}(\mathcal{H})$ is a Banach algebra of functions, where the product is the pointwise one; the unit element is the function 1, i.e. $1(x) = 1 \ \forall x \in \mathcal{H}$ and the norm is given by $||f|| = ||\mu_f||$.

The study of oscillatory integrals on \mathbb{R}^n with quadratic phase functions, i.e. the "Fresnel integrals",

$$\int e^{\frac{i}{2\hbar}\langle x,x\rangle} f(x)dx, \qquad \hbar > 0, \tag{2.7}$$

is a largely developed topic, and has strong connections with several problems in mathematics, e.g. in the theory of Fourier integral operators, and physics, e.g. in optics. Following Hörmander, the integral in (2.7) can be defined even if $f(\mathcal{H})$ is not summable by exploiting the cancellations due to the oscillatory behavior of the integrand, by means of a limiting procedure. More precisely the Fresnel integrals can be defined as the limit of a sequence of regularized, hence absolutely convergent, Lebesgue integrals. **Definition 1.** A function $f : \mathbb{R}^n \to \mathbb{C}$ is Fresnel integrable if and only if for each $\phi \in \mathcal{S}(\mathbb{R}^n)$ such that $\phi(0) = 1$ the limit

$$\lim_{\epsilon \to 0} (2\pi i\hbar)^{-n/2} \int e^{\frac{i}{2\hbar} \langle x, x \rangle} f(x) \phi(\epsilon x) dx$$
(2.8)

exists and is independent of ϕ . In this case the limit is called the Fresnel integral of f and denoted by

$$\widetilde{\int} e^{\frac{i}{2\hbar}\langle x,x\rangle} f(x) dx \tag{2.9}$$

In [ET84] this definition was generalized to the case \mathbb{R}^n is replaced by an infinite dimensional real separable Hilbert space \mathcal{H} . In fact an infinite dimensional Fresnel integral can be defined as the limit of a sequence of finite dimensional approximations:

Definition 2. Let $(\mathcal{H}, \langle , \rangle)$ be a real separable (infinite dimensional) Hilbert space. A function $f : \mathcal{H} \to \mathbb{C}$ is Fresnel integrable if and only if for any sequence $\{P_n\}_{n \in \mathbb{N}}$ of projectors onto ndimensional subspaces of \mathcal{H} , such that $P_n \leq P_{n+1}$ and $P_n \to 1$ strongly as $n \to \infty$ (1 being the identity operator in \mathcal{H}), the finite dimensional approximations

$$(2\pi i\hbar)^{-n/2} \int\limits_{P_n\mathcal{H}} e^{\frac{i}{2\hbar} \langle P_n x, P_n x \rangle} f(P_n x) d(P_n x),$$

are well defined (in the sense of definition 1) and the limit

$$\lim_{n \to \infty} (2\pi i\hbar)^{-n/2} \int_{P_n \mathcal{H}} e^{\frac{i}{2\hbar} \langle P_n x, P_n x \rangle} f(P_n x) d(P_n x)$$
(2.10)

exists and is independent of the sequence $\{P_n\}$. In this case the limit is called the Fresnel integral of f and is denoted by:

$$\widetilde{\int} e^{\frac{i}{2\hbar} \langle x, x \rangle} f(x) dx$$

Let us recall the following theorem:

Theorem 2.2.1. (Parseval Identity) Let $L : \mathcal{H} \to \mathcal{H}$ be a self adjoint trace-class operator, such that (I - L) is invertible. Let $y \in \mathcal{H}$ and let $f : \mathcal{H} \to \mathbb{C}$ be the Fourier transform of a complex bounded variation measure μ_f on \mathcal{H} . Then the function $e^{-\frac{i}{2\hbar}\langle x, Lx \rangle}e^{i\langle x, y \rangle}f(x)$ is Fresnel integrable and the corresponding Fresnel integral can be explicitly computed in terms of a well defined absolutely convergent integral with respect to a σ -additive measure μ_f , by means of the following Parseval-type equality:

$$\widetilde{\int} e^{\frac{i}{2\hbar} \langle x, x \rangle} e^{-\frac{i}{2\hbar} \langle x, Lx \rangle} e^{i \langle x, y \rangle} f(x) dx =$$

$$= (\det(I - L))^{-1/2} \int_{\mathcal{H}} e^{-\frac{i\hbar}{2} \langle \alpha + y, (I - L)^{-1} (\alpha + y) \rangle} \mu_f(d\alpha)$$
(2.11)

where $\det(I-L) = |\det(I-L)|e^{-\pi i \operatorname{Ind}(I-L)}$ is the Fredholm determinant of the operator (I-L), $|\det(I-L)|$ its absolute value and $\operatorname{Ind}((I-L))$ is the number of negative eigenvalues of the operator (I-L), counted with their multiplicity.

Proof 2.2.1. The result follows directly by theorem 2.1 in [AB93], see also [ET84], which states that for $g \in \mathcal{F}(\mathcal{H})$

$$\widetilde{\int} e^{\frac{i}{2\hbar}\langle x,x\rangle} e^{-\frac{i}{2\hbar}\langle x,Lx\rangle} g(x) dx = \frac{1}{\sqrt{\det(I-L)}} \int_{\mathcal{H}} e^{-\frac{i\hbar}{2}\langle \alpha,(I-L)^{-1}(\alpha)\rangle} \mu_g(d\alpha)$$

By taking $\mu_g \equiv \delta_y * \mu_f$ the conclusion follows.

By expression (7.3) the following result follows easily:

Corollary 1. Under the assumptions of theorem 2.2.1, the functional

$$f \in \mathcal{F}(\mathcal{H}) \mapsto \widetilde{\int} e^{\frac{i}{2\hbar} \langle x, (I-L)x \rangle} e^{i \langle x, y \rangle} f(x) dx$$

is continuous in the $\mathcal{F}(\mathcal{H})$ -norm.

Let us introduce now a new type of infinite dimensional oscillatory integrals on the product space $\mathcal{H} \times \mathcal{H}$ that will be applied in the next section to the time evolution of open quantum systems.

Definition 3. Let $f : \mathcal{H} \times \mathcal{H} \to \mathbb{C}$. If for any sequence P_n of projectors onto n-dimensional subspaces of \mathcal{H} , such that $P_n \leq P_{n+1}$ and $P_n \to 1$ strongly as $n \to \infty$ (1 being the identity operator in \mathcal{H}), the finite dimensional oscillatory integrals

$$\frac{1}{(2\pi\hbar)^n} \int\limits_{P_n\mathcal{H}} \int\limits_{P_n\mathcal{H}} \int e^{\frac{i}{2\hbar} \langle P_n x, P_n x \rangle} e^{-\frac{i}{2\hbar} \langle P_n y, P_n y \rangle} f(P_n x, P_n y) d(P_n x) d(P_n y)$$

are well defined and the limit

$$\frac{1}{(2\pi\hbar)^n} \int\limits_{P_n\mathcal{H}} \int\limits_{P_n\mathcal{H}} \int\limits_{P_n\mathcal{H}} e^{\frac{i}{2\hbar} \langle P_n x, P_n x \rangle} e^{-\frac{i}{2\hbar} \langle P_n y, P_n y \rangle} f(P_n x, P_n y) d(P_n x) d(P_n y)$$
(2.12)

exists and is independent of the sequence $\{P_n\}$, then it is denoted by:

$$\widetilde{\int} \widetilde{\int} e^{\frac{i}{2\hbar} \langle x, x \rangle} e^{-\frac{i}{2\hbar} \langle y, y \rangle} f(x, y) dx dy.$$

It is possible to prove a result analogous to theorem 2.2.1

Theorem 2.2.2. Let $L : \mathcal{H} \to \mathcal{H}$ be a trace class operator, such that I - L is invertible. Let $f : \mathcal{H} \times \mathcal{H} \to \mathbb{C}$ be the Fourier transform of a complex bounded variation measure μ_f on $\mathcal{H} \times \mathcal{H}$. Then the integral

$$\widetilde{\int \int} e^{\frac{i}{2\hbar} \langle x, x \rangle} e^{-\frac{i}{2\hbar} \langle y, y \rangle} e^{-\frac{i}{2\hbar} \langle x-y, L(x+y) \rangle} f(x,y) dx dy$$

is well defined and is equal to:

$$\frac{1}{\det(I-L)} \int_{\mathcal{H}} \int_{\mathcal{H}} \int_{\mathcal{H}} e^{-\frac{i\hbar}{2} \langle \alpha + \beta, (I-L)^{-1}(\alpha - \beta) \rangle} d\mu_f(\alpha, \beta)$$
(2.13)

where det(I - L) is the Fredholm determinant of the operator (I - L)

Proof 2.2.2. By definition, taking a sequence P_n of projectors onto n-dimensional subspaces of \mathcal{H} , such that $P_n \leq P_{n+1}$ and $P_n \to 1$ strongly as $n \to \infty$

$$\widetilde{\int \int} e^{\frac{i}{2\hbar} \langle x, x \rangle} e^{-\frac{i}{2\hbar} \langle y, y \rangle} e^{-\frac{i}{2\hbar} \langle x-y, L(x+y) \rangle} f(x,y) dx dy = = \lim_{n \to \infty} \frac{1}{(2\pi\hbar)^n} \int_{P_n \mathcal{H}} \int_{P_n \mathcal{H}} e^{\frac{i}{2\hbar} \langle x_n - y_n, (I_n - L_n)(x_n + y_n) \rangle} f(x_n, y_n) dx_n dy_n$$

where $x_n \equiv P_n x$, $x \in \mathcal{H}$, $I_n - L_n \equiv I_{|P_n \mathcal{H}} - P_n L P_n$. On the other hand, the finite dimensional approximations are defined by the following sequence of regularized integrals:

$$\frac{1}{(2\pi\hbar)^n} \int_{P_n\mathcal{H}} \int_{P_n\mathcal{H}} \int_{P_n\mathcal{H}} e^{\frac{i}{2\hbar}\langle x_n - y_n, (I_n - L_n)(x_n + y_n) \rangle} f(x_n, y_n) dx_n dy_n =$$
$$= \lim_{\epsilon \to 0} \frac{1}{(2\pi\hbar)^n} \int_{P_n\mathcal{H}} \int_{P_n\mathcal{H}} \int_{P_n\mathcal{H}} e^{\frac{i}{2\hbar}\langle x_n - y_n, (I_n - L_n)(x_n + y_n) \rangle} \phi(\epsilon x, \epsilon y) f(x_n, y_n) dx_n dy_n$$

with $\phi \in \mathcal{S}(\mathbb{R}^n \times \mathbb{R}^n), \ \phi(0) = 1.$

By introducing the new variables $z_n \equiv x_n - y_n$, $w_n \equiv x_n + y_n$, by taking $n \ge \overline{n}$ and by Fubini theorem, the latter is equal to:

$$\lim_{\epsilon \to 0} \frac{1}{(4\pi\hbar)^n} \int_{P_n \mathcal{H}} \int_{P_n \mathcal{H}} \int_{P_n \mathcal{H}} \int_{P_n \mathcal{H}} \int_{P_n \mathcal{H}} e^{i\langle\alpha, \frac{z+w}{2}\rangle + i\langle\beta, \frac{w-z}{2}\rangle} \times e^{\frac{i}{2\hbar}\langle z_n, (I_n - L_n)w_n \rangle} \phi(\epsilon \frac{z+w}{2}, \epsilon \frac{w-z}{2}) dz_n dw_n) d\mu_n(\alpha, \beta) = \lim_{\epsilon \to 0} \frac{\det(I_n - L_n)^{-1}}{(2\pi)^{2n}} \times \int_{P_n \mathcal{H}} \int_{P_n \mathcal{H}} \int_{P_n \mathcal{H}} e^{\frac{-i\hbar}{2}\langle\alpha + \beta - 2\epsilon\gamma, (I_n - L_n)^{-1}(\alpha - \beta - 2\epsilon\delta)\rangle} \tilde{\phi}_T(\gamma_n, \delta_n) d\gamma_n d\delta_n d\mu_n(\alpha, \beta)$$

where $\mu_n \in \mathcal{F}(P_n \mathcal{H} \times P_n \mathcal{H})$ is defined by:

$$\int_{P_n\mathcal{H}} \phi(x_n, y_n) d\mu_n(x_n, y_n) \equiv \int_{\mathcal{H}} \chi_{P_n\mathcal{H}}(x, y) \phi(P_n x, P_n y) d\mu(x, y)$$

and $\phi_T \in \mathcal{S}(P_n \mathcal{H} \times P_n \mathcal{H})$ is defined by:

$$\phi_T(z_n, w_n) \equiv \phi\left(\frac{z_n + w_n}{2}, \frac{w_n - z_n}{2}\right)$$

In the above calculation we have used the fact that if (I-L) is invertible which implies that, for any sequence $\{P_n\}_{n\in\mathbb{N}}$ of projection operators on \mathcal{H} , there exist an \bar{n} such that for any $n \geq \bar{n}$ the operator $P_n(I-L)P_n$ is invertible. Therefore by taking n sufficiently large we have that $\det(I_n - L_n) \neq 0$. By applying Lebesgue's dominated convergence theorem, and by the equality

$$\int_{P_n\mathcal{H}} \int_{P_n\mathcal{H}} \tilde{\phi}_T(\gamma_n, \delta_n) d\gamma_n d\delta_n = (2\pi)^{2n} \phi_T(0, 0)$$

the latter is equal to:

$$\det(I_n - L_n)^{-1} \int_{P_n \mathcal{H}} \int_{P_n \mathcal{H}} e^{-\frac{i\hbar}{2} \langle \alpha + \beta, (I_n - L_n)^{-1} (\alpha - \beta) \rangle} d\mu_n(\alpha, \beta)$$

By taking the limit $n \to \infty$ and by the convergence of $\det(I_n - L_n)$ to $\det(I - L)$, we get the final result

By expression (2.13) the next result follows easily:

Corollary 2. Under the assumptions of theorem 2.2.2, the functional

$$f \in \mathcal{F}(\mathcal{H} \times \mathcal{H}) \mapsto \widetilde{\int \int} e^{\frac{i}{2\hbar} \langle x, x \rangle} e^{-\frac{i}{2\hbar} \langle y, y \rangle} e^{-i \langle x-y, L(x+y) \rangle} f(x, y) dx dy$$

is continuous in the $\mathcal{F}(\mathcal{H} \times \mathcal{H})$ -norm.

It is possible to prove the following Fubini type theorem on the change of order of integration between oscillatory integrals and Lebesgue integrals.

Let $\{\mu_{\alpha} : \alpha \in \mathbb{R}^d\}$ be a family in $\mathcal{M}(\mathcal{H})$. We shall let $\int_{\mathbb{R}^d} \mu_{\alpha} d\alpha$ denote the measure defined by

$$\phi \mapsto \int_{\mathbb{R}^d} \int_{\mathcal{H}} \phi(x) d\mu_\alpha(x) d\alpha$$

whenever it exists.

Theorem 2.2.3. Let $(\mathcal{H}, \langle \rangle)$ and $L : \mathcal{H} \to \mathcal{H}$ as in the assumptions of theorem 2.2.2. Let $\mu : \mathbb{R}^d \to \mathcal{M}(\mathcal{H} \times \mathcal{H}), \alpha \mapsto \mu_{\alpha}$, be a continuous map such that

$$\int\limits_{\mathbb{R}^d} |\mu_{\alpha}| d\alpha < \infty.$$

Let $f_{\alpha}(x,y) = \hat{\mu}_{\alpha}(x,y), (x,y) \in \mathcal{H} \times \mathcal{H}$. Then $\int_{\mathbb{R}^d} f_{\alpha} d\alpha \in \mathcal{F}(\mathcal{H} \times \mathcal{H})$ and

$$\int_{\mathbb{R}^{d}} \widetilde{\int_{\mathcal{H}}} \widetilde{\int_{\mathcal{H}}} e^{\frac{i}{2\hbar} \langle x, x \rangle} e^{-\frac{i}{2\hbar} \langle y, y \rangle} e^{-\frac{i}{2\hbar} \langle x-y, L(x+y) \rangle} f_{\alpha}(x, y) dx dy d\alpha$$

$$= \widetilde{\int_{\mathcal{H}}} \widetilde{\int_{\mathcal{H}}} e^{\frac{i}{2\hbar} \langle x, x \rangle} e^{-\frac{i}{2\hbar} \langle y, y \rangle} e^{-\frac{i}{2\hbar} \langle x-y, L(x+y) \rangle} \int_{\mathbb{R}^{d}} f_{\alpha}(x) d\alpha dx dy \quad (2.14)$$

Proof 2.2.3. By definition of f_{α}

$$\int_{\mathbb{R}^d} f_\alpha d\alpha = \int_{\mathbb{R}^d} \int_{\mathcal{H} \times \mathcal{H}} e^{i\langle k, x \rangle + i\langle h, y \rangle} d\mu_\alpha(k, h) d\alpha = \int_{\mathcal{H} \times \mathcal{H}} e^{i\langle k, x \rangle + i\langle h, y \rangle} \int_{\mathbb{R}^d} d\mu_\alpha(k, h) d\alpha$$

so that $\int_{\mathbb{R}^d} f_{\alpha} d\alpha \in \mathcal{F}(\mathcal{H})$. By applying theorem 2.2.2 to the l.h.s. of (2.14), we have:

$$\int_{\mathbb{R}^d} \widetilde{\int_{\mathcal{H}}} \widetilde{\int_{\mathcal{H}}} e^{\frac{i}{2\hbar} \langle x, x \rangle} e^{-\frac{i}{2\hbar} \langle y, y \rangle} e^{-\frac{i}{2\hbar} \langle x-y, L(x+y) \rangle} f_{\alpha}(x, y) dx dy d\alpha$$

= det(I - L)⁻¹ $\int_{\mathbb{R}^d} \int_{\mathcal{H}} \int_{\mathcal{H}} e^{-\frac{i\hbar}{2} \langle k+h, (I-L)^{-1}(k-h) \rangle} d\mu_{\alpha}(k, h) d\alpha$

By the usual Fubini theorem the latter is equal to:

$$\det(I-L)^{-1} \int_{\mathcal{H}} \int_{\mathcal{H}} e^{-\frac{i\hbar}{2}\langle k+h,(I-L)^{-1}(k-h)\rangle} \int_{\mathbb{R}^d} d\mu_{\alpha}(k,h) d\alpha$$

that, by theorem 2.2.2 is equal to the r.h.s of of (2.14).

2.3. The Feynman-Vernon influence functional

The infinite dimensional oscillatory integrals of definition 2 provide a rigorous mathematical realization of the heuristic Feynman path integral representation for the solution of the Schrödinger equation. The aim of the present subsection is the extension of these results to the Feynman path integral representation of the time evolution of an open quantum system.

Let U_t be the unitary evolution operator on $L^2(\mathbb{R}^d)$ whose generator is the self-adjoint extension of the operator defined on $S(\mathbb{R}^d)$ by $-\frac{\Delta}{2m} + \frac{1}{2}x\Omega^2 x + v(x)$, where m > 0, Ω is a positive symmetric constant $d \times d$ matrix with eigenvalues Ω_j , $j = 1 \dots d$, and $v \in \mathcal{F}(\mathbb{R}^d)$, $v(x) = \hat{\mu}_v(x)$.

The heuristic path integral representation given by Feynman for the solution of the Schrödinger equation (2.1) is given by:

$$(U(t)\psi_0)(x) = \iint_{\gamma(t)=x} e^{\frac{i}{2\hbar}(m\int_0^t \dot{\gamma}(s)^2 ds - \int_0^t \gamma(s)\Omega^2 \gamma(s)ds)} e^{-\frac{i}{\hbar}\int_0^t v(\gamma(s))ds} \phi_0(\gamma(0))d\gamma''$$

Let us assume for notation simplicity that m = 1 (this condition will soon be relaxed) and let us introduce the Cameron-Martin space \mathcal{H}_t , i.e. the Hilbert space of absolutely continuous paths $\gamma : [0, t] \to \mathbb{R}$, such that $\gamma(t) = 0$, and square integrable weak derivative $\int_0^t |\dot{\gamma}(s)|^2 ds < \infty$ endowed with the inner product $\langle \gamma_1, \gamma_2 \rangle = \int_0^t \dot{\gamma}_1(s) \cdot \dot{\gamma}_2(s) ds$. Let $L : \mathcal{H}_t \to \mathcal{H}_t$ be the trace class symmetric operator on \mathcal{H}_t given by:

$$(L\gamma)(s) = \int_{s}^{t} ds' \int_{0}^{s'} \gamma(s'') ds'', \qquad \gamma \in \mathcal{H}_{t}.$$
(2.15)

Let $\mathcal{H}_t^d \equiv \bigoplus_{i=1}^d \mathcal{H}_t$ and let $L_{\Omega} : \mathcal{H}_t^d \to \mathcal{H}_t^d$ be the trace class symmetric operator on \mathcal{H}_t^d given by:

$$(L_{\Omega}\gamma)(s) = \int_{s}^{t} ds' \int_{0}^{s'} (\Omega^{2}\gamma)(s'') ds'', \qquad \gamma \in \mathcal{H}_{t}^{d}$$

One can easily verify that $\langle \gamma_1, L_\Omega \gamma_2 \rangle = \int_0^t \gamma_1(s) \Omega^2 \gamma_2(s) ds$. Moreover if $t \neq (n + 1/2) \pi / \Omega_j$, $n \in \mathbb{Z}$ and Ω_j any eigenvalue of Ω , $(I - L_\Omega)$ is invertible with:

$$(I - L_{\Omega})^{-1}\gamma(s) = \gamma(s) - \Omega \int_{s}^{t} \sin[\Omega(s' - s)]\gamma(s')ds' + \\ + \sin[\Omega(t - s)] \int_{0}^{t} [\cos\Omega t]^{-1}\Omega\cos(\Omega s')\gamma(s')ds', \quad (2.16)$$

and

$$\det(I - L_{\Omega}) = \det(\cos(\Omega t))$$

see [ET84]. Thanks to these results and under suitable assumptions it is possible to realize the heuristic Feynman path integral representation for the solution of the Schrödinger equation as a well defined infinite dimensional oscillatory integral on the Hilbert space \mathcal{H}_t^d .

Theorem 2.3.1. Let $\phi_0 \in \mathcal{F}(\mathbb{R}^d)$. $t \neq (n+1/2)\pi/\Omega_j$, $n \in \mathbb{Z}$. Then the vector $\phi(t) \equiv U_t \phi_0$ is given by $x \mapsto \phi(t)(x)$, with:

$$e^{-\frac{i}{2\hbar}x\Omega^{2}xt}\int_{\mathcal{H}_{t}^{d}}e^{\frac{i}{2\hbar}\langle\gamma,(I-L)\gamma\rangle}e^{-\frac{i}{\hbar}\int_{0}^{t}x\Omega^{2}\gamma(s)ds}e^{-\frac{i}{\hbar}\int_{0}^{t}v(\gamma(s)+x)ds}\phi_{0}(\gamma(0)+x)d\gamma$$
(2.17)

For a detailed proof see [ET84].

This result can be generalized to the Feynman path integral representation of the time evolution of a mixed state:

Theorem 2.3.2. Let ρ be a density matrix operator on $L^2(\mathbb{R}^d)$, such that ρ admits a regular kernel $\rho(x, y)$, $x, y \in \mathbb{R}^d$. Let us consider a basis $\{e_i\}_{i \in \mathbb{N}}$ of $L^2(\mathbb{R}^d)$ and assume that ρ admits a decomposition into pure states of the form $\rho(x, y) = \sum_i \lambda_i e_i(x) e_i^*(y)$, with $\lambda_i > 0$, $\sum_i \lambda_i = 1$, $\langle e_i, e_j \rangle_{L^2(\mathbb{R}^d)} = \delta_{ij}$, and $e_i(x) = \hat{\mu}_i(x)$, satisfying:

$$\sum_{i} \lambda_i |\mu_i|^2 < \infty. \tag{2.18}$$

Let $t \neq (n + 1/2)\pi/\Omega_j$, $n \in \mathbb{Z}$. Then the density matrix operator at time t admits a smooth kernel $\rho_t(x, y)$ which is given by the infinite dimensional oscillatory integral:

$$e^{-\frac{i}{2\hbar}(x\Omega^{2}x-y\Omega^{2}y)t}\int_{\mathcal{H}_{t}^{m,d}\mathcal{H}_{t}^{m,d}}\int_{t}^{e^{\frac{i}{2\hbar}\langle\gamma,(I-L)\gamma\rangle}}e^{-\frac{i}{2\hbar}\langle\gamma',(I-L)\gamma'\rangle}e$$

Proof 2.3.1. By decomposing ρ into pure states, by corollary 2 and condition (2.18) the integral (2.19) is equal to:

$$\sum_{i} \lambda_{i} \left(e^{-\frac{i}{2\hbar}x\Omega^{2}xt} \int\limits_{\mathcal{H}_{t}^{m,d}} e^{\frac{i}{2\hbar}\langle\gamma,(I-L)\gamma} e^{-\frac{i}{\hbar}\int_{0}^{t}x\Omega^{2}\gamma(s)ds} e^{-\frac{i}{\hbar}\int_{0}^{t}v(\gamma(s)+x)ds} e_{i}(\gamma(0)+x)d\gamma \right)$$

$$\left(e^{\frac{i}{2\hbar}y\Omega^{2}yt} \int\limits_{\mathcal{H}_{t}^{m,d}} e^{-\frac{i}{2\hbar}\langle\gamma',(I-L)\gamma'} e^{\frac{i}{\hbar}\int_{0}^{t}y\Omega^{2}\gamma'(s)ds} e^{\frac{i}{\hbar}\int_{0}^{t}v(\gamma'(s)+y)ds} e^{*}_{i}(\gamma(0)+y)d\gamma \right)$$

$$= \sum_{i} \lambda_{i} \left(e^{-\frac{i}{2\hbar}x\Omega^{2}xt} \int\limits_{\mathcal{H}_{t}^{m,d}} e^{\frac{i}{2\hbar}\langle\gamma,(I-L)\gamma} e^{-\frac{i}{\hbar}\int_{0}^{t}x\Omega^{2}\gamma(s)ds} e^{-\frac{i}{\hbar}\int_{0}^{t}v(\gamma(s)+x)ds} e_{i}(\gamma(0)+x)d\gamma \right)$$

$$\left(e^{-\frac{i}{2\hbar}y\Omega^{2}yt} \int\limits_{\mathcal{H}_{t}^{m,d}} e^{\frac{i}{2\hbar}\langle\gamma',(I-L)\gamma'} e^{-\frac{i}{\hbar}\int_{0}^{t}y\Omega^{2}\gamma'(s)ds} e^{-\frac{i}{\hbar}\int_{0}^{t}v(\gamma'(s)+y)ds} e_{i}(\gamma(0)+y)d\gamma \right)^{*} \quad (2.20)$$

By theorem 2.3.2 the latter line is equal to $\sum_i \lambda_i U_t e_i(x) (U_t e_i)^*(y) = \rho_t(x, y).$

Remark 2.3.1. Heuristically expression (2.19) can be written as

$$\widetilde{\int \int e^{\frac{i}{\hbar}(S_t(\gamma+x)-S_t(\gamma'+y))}\rho(\gamma(0)+x,\gamma'(0)+y)d\gamma d\gamma'$$

where $S_t(\gamma)$ is the classical action of the system evaluated along the path defined in (2.3).

Let us consider now the time evolution of a quantum system made of two linearly interacting subsystems A and B. Let us assume that the state space of the system A is $L^2(\mathbb{R}^d)$ while the state space of the system B is $L^2(\mathbb{R}^N)$. Let the total Hamiltonian of the compound systems be of the form $H_{AB} = H_A + H_B + H_{INT}$, with

$$H_A = -\frac{\Delta_{\mathbb{R}^d}}{2M} + \frac{1}{2}x\Omega_A^2 x + v_A(x) \quad , \quad x \in \mathbb{R}^d$$

$$H_B = -\frac{\Delta_{\mathbb{R}^N}}{2m} + \frac{1}{2}R\Omega_B^2 R + v_B(R) \quad , \quad R \in \mathbb{R}^N$$

and $H_{INT} = xCR$, with $C : \mathbb{R}^N \to \mathbb{R}^d$ is a linear operator and Ω_A , resp. Ω_B , is a symmetric positive $d \times d$ (resp. $N \times N$) matrix. Let us assume that the quadratic part of the total potential, i.e. the function $x, R \mapsto \frac{1}{2}x\Omega_A^2 x + \frac{1}{2}R\Omega_B^2 R + xCR$ is positive definite (so that the total Hamiltonian is bounded from below). Let us assume moreover that the density matrix of the compound system factorizes $\rho_{AB} = \rho_A \rho_B$ and has a smooth kernel:

$$\rho_{AB}(x, y, R, Q) = \rho_A(x, y)\rho_B(R, Q)$$

We want to prove an infinite dimensional oscillatory integral representation for the reduced density operator at time t, namely $\int (U_t \rho_{AB} U_t^+)(x, y, R, R) dR$ where the unitary operator $U_t \equiv \exp\left(-\frac{1}{\hbar}Ht\right)$, heuristically:

$$\int \widetilde{\int}_{\Gamma(t)=R} \widetilde{\int}_{\Gamma'(t)=R} e^{\frac{i}{\hbar}(S_A(\gamma)+S_B(\Gamma)+S_{INT}(\gamma,\Gamma)-S_A(\gamma')-S_B(\Gamma')-S_{INT}(\gamma',\Gamma')} \times \rho_A(\gamma(0),\gamma'(0))\rho_B(\Gamma(0),\Gamma'(0))d\gamma d\gamma' d\Gamma d\Gamma' dR$$
(2.21)

 γ and Γ represent the generic path in the configuration space of the system, respectively of the *reservoir*, and:

$$S_A(\gamma) + S_B(\Gamma) + S_{INT}(\gamma, \Gamma) \equiv \int_0^t (\frac{M}{2} \dot{\gamma}^2(s) - \frac{1}{2} \gamma(s) \Omega_A^2 \gamma(s) - v_A(\gamma(s)) ds$$

+
$$\int_0^t (\frac{m}{2} \dot{\Gamma}^2(s) - \frac{1}{2} \Gamma(s) \Omega_B^2 \Gamma(s) - v_B(\Gamma(s)) ds + \int_0^t \gamma(s) C \Gamma(s) ds$$
(2.22)

By the transformations in the path space, given by:

$$\gamma \to \gamma / \sqrt{M} \text{ and } \Gamma \to \Gamma / \sqrt{m}$$
 (2.23)

formula (2.21) becomes:

$$\int \int \int \int e^{\frac{i}{2\hbar} \int_{0}^{t} (\dot{\gamma}^{2}(s) - \gamma(s) \frac{\Omega_{A}^{2}}{M} \gamma(s) - v_{A}(\frac{\gamma(s)}{M}) ds} \times e^{\frac{i}{2\hbar} \int_{0}^{t} (\dot{\Gamma}^{2}(s) - \Gamma(s) \frac{\Omega_{B}^{2}}{m} \Gamma(s) - v_{B}(\frac{\Gamma(s)}{m}) ds} e^{-\frac{i}{\hbar} \int_{0}^{t} \gamma(s) \frac{C}{\sqrt{mM}} \Gamma(s) ds} \times e^{-\frac{i}{2\hbar} \int_{0}^{t} (\dot{\Gamma}^{\prime})^{2}(s) - \gamma^{\prime}(s) \frac{\Omega_{A}^{2}}{M} \gamma^{\prime}(s) - v_{A}(\frac{\gamma^{\prime}(s)}{M}) ds} e^{-\frac{i}{2\hbar} \int_{0}^{t} (\dot{\Gamma}^{\prime})^{2}(s) - \Gamma^{\prime}(s) \frac{\Omega_{B}^{2}}{m} \Gamma^{\prime}(s) - v_{B}(\frac{\Gamma^{\prime}(s)}{m}) ds} \times e^{\frac{i}{\hbar} \int_{0}^{t} \gamma^{\prime}(s) \frac{C}{\sqrt{mM}} \Gamma^{\prime}(s) ds} \rho_{A}\left(\frac{\gamma(0)}{\sqrt{M}}, \frac{\gamma^{\prime}(0)}{\sqrt{M}}\right) \rho_{B}\left(\frac{\Gamma(0)}{\sqrt{m}}, \frac{\Gamma^{\prime}(0)}{\sqrt{m}}\right) d\gamma d\gamma^{\prime} d\Gamma d\Gamma^{\prime} dR,$$
(2.24)

By transformations in (2.23) it is possible to take unit masses m and M to conform to the setting of theorems 2.3.1 and 2.3.2.

Let us consider the two Hilbert spaces:

$$\mathcal{H}_t^d \equiv \underbrace{\mathcal{H}_t \oplus \dots \oplus \mathcal{H}_t}_{d-times}$$
 and $\mathcal{H}_t^N \equiv \underbrace{\mathcal{H}_t \oplus \dots \oplus \mathcal{H}_t}_{N-times}$

We shall denote an element of \mathcal{H}_t^d , respectively of \mathcal{H}_t^N , by γ , respectively Γ . Let $L: \mathcal{H}_t \to \mathcal{H}_t$ be the symmetric bounded operator on \mathcal{H}_t , defined by: $L\gamma(s) \equiv \int_s^t ds' \int_0^{s'} \gamma(s'') ds''$. Let $L_A : \mathcal{H}_t^d \to \mathcal{H}_t^d$, $L_B : \mathcal{H}_t^N \to \mathcal{H}_t^N$ and $L_{AB} : \mathcal{H}_t^d \oplus \mathcal{H}_t^N \to \mathcal{H}_t^d \oplus \mathcal{H}_t^N$ be the self adjoint

operators defined by:

$$L_A \gamma \equiv L^d \Omega_A^2 M^{-1} \gamma \tag{2.25}$$

$$L_B \Gamma \equiv L^N \Omega_B^2 m^{-1} \Gamma \tag{2.26}$$

$$L_{AB}(\gamma,\Gamma) \equiv (L_A\gamma + \frac{1}{\sqrt{mM}}L^d C\Gamma, L_B\Gamma + \frac{1}{\sqrt{mM}}L^N C^T\gamma)$$
(2.27)

where, for all $k \in \mathbb{N}$, L^k denotes the operator on \mathcal{H}_t^k defined by:

$$L^k \equiv L^{(1)} \otimes L^{(2)} \otimes \dots \otimes L^{(k)}$$

and:

$$L^{(k)} \equiv \mathbf{1} \otimes \mathbf{1} \otimes \cdots \otimes \mathbf{1} \otimes \underbrace{L}_{k^{th}element} \otimes \mathbf{1} \cdots \otimes \mathbf{1}$$

Lemma 1. Let $\Psi_0 \in L^2(\mathbb{R}^{n+d}) \cap \mathcal{F}(\mathbb{R}^{n+d})$, $v_A \in \mathcal{F}(\mathbb{R}^d)$, $v_B \in \mathcal{F}(\mathbb{R}^N)$ and $t \neq (n+1/2)\pi/\lambda_j$, where $n \in \mathbb{Z}$ and λ_j^2 , $j = 1, \ldots d + N$, are the eigenvalues of the matrix:

$$\begin{pmatrix} \Omega_A^{\prime 2} & C' \\ C'^T & \Omega_B^{\prime 2} \end{pmatrix} \qquad \Omega_A^{\prime} \equiv \Omega_A / \sqrt{M}, \\ \Omega_B^{\prime} \equiv \Omega_B / \sqrt{m}, \\ C' \equiv C / \sqrt{Mm} \qquad (2.28)$$

Then the solution of the Schrödinger equation evaluated at time t:

$$\begin{cases} i\hbar\frac{\partial}{\partial t}\Psi = H_{AB}\psi\\ \Psi(0,x,R) = \Psi_0(x,R), \qquad (x,R) \in \mathbb{R}^d \times \mathbb{R}^N \end{cases}$$
(2.29)

2.3 The Feynman-Vernon influence functional

is a smooth function and is represented by the infinite dimensional oscillatory integral:

$$\widetilde{\int}_{\mathcal{H}_{t}^{d} \oplus \mathcal{H}_{t}^{N}} e^{\frac{i}{2\hbar} \langle (\gamma, \Gamma), (I_{d+N} - L_{AB})(\gamma, \Gamma) \rangle} G(\gamma, \Gamma, x, R) \Psi_{0}'(\gamma(0) + x, \Gamma(0) + R) d\gamma d\Gamma$$
(2.30)

where we have defined the functions:

$$\Psi'_0(x,R) \equiv \Psi_0(x/\sqrt{M},R/\sqrt{m})$$

and:

$$G(\gamma, \Gamma, x, R) \equiv e^{-\frac{it}{2\hbar}x\Omega_A'^2 x - \frac{it}{2\hbar}R\Omega_B'^2 R - \frac{i}{\hbar}xC'Rt} \times \\ \times e^{-\frac{i}{\hbar}\int_0^t x\Omega_A'^2 \gamma(s)ds - \frac{i}{\hbar}\int_0^t R\Omega_B'^2 \Gamma(s)ds - \frac{i}{\hbar}\int_0^t xC'\Gamma(s)ds - \frac{i}{\hbar}\int_0^t \gamma(s)C'Rds} \times$$

$$\times e^{-\frac{i}{\hbar}\int_0^t v_A'(\gamma(s)+x)ds - \frac{i}{\hbar}\int_0^t v_B'(\Gamma(s)+x)ds}$$

$$(2.31)$$

while v'_A and v'_B are defined as follows:

$$v'_A(x) \equiv v_A(x/\sqrt{M}); v'_B(R) \equiv v_B(R/\sqrt{m})$$

Proof 2.3.2. Let ξ_1, \ldots, ξ_{d+N} be a system of normal coordinates in \mathbb{R}^{d+N} , with:

$$(x, R) = U(\xi_1, \dots, \xi_{d+N})$$
 and $U^T = U^{-1}$

then the quadratic part of the action is diagonalized and it is possible to apply theorem 2.3.1. The result follows by the invariance of the infinite dimensional oscillatory integrals under unitary transformation on paths space [AHK76], and by the infinite dimensional oscillatory integral representation for the solution of the Schrödinger equation with a potential of the type " harmonic oscillator plus Fourier transform of measure" (see [ABHK82, ET84, AB93] for more details).

Lemma 2. Let $f \in \mathcal{F}(\mathcal{H}^d_t \oplus \mathcal{H}^N_t)$, $f = \hat{\mu}$. Let t satisfy the following inequalities

$$t \neq (n+1/2)\pi/\Omega_j^A, \qquad n \in \mathbb{Z}, \quad j = 1\dots d,$$
(2.32)

$$t \neq (n+1/2)\pi/\Omega_i^B, \qquad n \in \mathbb{Z}, \quad j = 1\dots N,$$
(2.33)

$$t \neq (n+1/2)\pi/\lambda_j, \qquad n \in \mathbb{Z}, \quad j = 1 \dots d + N, \tag{2.34}$$

where Ω_j^A , $j = 1 \dots d$, Ω_j^B , $j = 1 \dots N$, and λ_j , $j = 1 \dots d + N$ are respectively the eigenvalues of the matrices Ω'_A , Ω'_B and of the matrix given by (2.28). Let L_A , L_B , L_{AB} be defined respectively by (2.25), (2.26) and (2.27). Then the function:

$$\gamma \in \mathcal{H}_t^d \mapsto \widetilde{\int}_{\mathcal{H}_t^N} e^{\frac{i}{2\hbar} \langle \Gamma, (I_N - L_B) \Gamma \rangle} e^{-\frac{i}{\hbar} \langle \Gamma, L^N C'^T \gamma \rangle} f(\gamma, \Gamma) d\Gamma$$

is Fresnel integrable and:

$$\int_{\mathcal{H}_{t}^{d} \oplus \mathcal{H}_{t}^{N}} e^{\frac{i}{2\hbar} \langle (\gamma, \Gamma), (I_{d+N} - L_{AB})(\gamma, \Gamma) \rangle} f(\gamma, \Gamma) d\gamma d\Gamma =
= \int_{\mathcal{H}_{t}^{d}} e^{\frac{i}{2\hbar} \langle \gamma, (I_{d} - L_{A})\gamma \rangle} \Big(\int_{\mathcal{H}_{t}^{N}} e^{\frac{i}{2\hbar} \langle \Gamma, (I_{N} - L_{B})\Gamma \rangle} e^{-\frac{i}{\hbar} \langle \Gamma, L^{N}C'^{T}\gamma \rangle} f(\gamma, \Gamma) d\Gamma \Big) d\gamma$$
(2.35)

Proof 2.3.3. By condition (2.33) the operator $I_N - L_B$ is invertible and by theorem 2.2.1 we have:

$$\int_{\mathcal{H}_{t}^{N}} e^{\frac{i}{2\hbar} \langle \Gamma, (I_{N}-L_{B})\Gamma \rangle} e^{-\frac{i}{\hbar} \langle \Gamma, L^{N}C'^{T}\gamma \rangle} f(\gamma, \Gamma) d\Gamma
= \det(I_{N}-L_{B})^{-1/2} \int_{\mathcal{H}_{t}^{N}} e^{-\frac{i\hbar}{2} \langle \Gamma - \frac{L^{N}C'^{T}\gamma}{\hbar}, (I_{N}-L_{B})^{-1}\Gamma - \frac{L^{N}C'^{T}\gamma}{\hbar} \rangle} d\mu_{\gamma}(\Gamma)
= \det(I_{N}-L_{B})^{-1/2} e^{-\frac{i}{2\hbar} \langle \gamma, C'L^{N}(I_{N}-L_{B})^{-1}L^{N}C'^{T}\gamma \rangle}
\int_{\mathcal{H}_{t}^{N}} e^{-\frac{i\hbar}{2} \langle \Gamma, (I_{N}-L_{B})^{-1}\Gamma \rangle} e^{i\langle \gamma, C'L^{N}(I_{N}-L_{B})^{-1}\Gamma \rangle} d\mu_{\gamma}(\Gamma) \quad (2.36)$$

where μ_{γ} is the measure on \mathcal{H}_t^N defined by:

$$\int_{\mathcal{H}_t^N} g(\Gamma) d\mu_{\gamma}(\Gamma) \equiv \int_{\mathcal{H}_t^d \times \mathcal{H}_t^N} g(\Gamma) e^{i \langle \gamma, \gamma' \rangle} d\mu(\gamma', \Gamma).$$

One can also easily verify that the operator on \mathcal{H}^d_t defined by:

$$\gamma \mapsto (L_A + C'L^N(I_N - L_B)^{-1}L^NC'^T)\gamma$$

is trace class and, if conditions (2.32),(2.32) and (2.34) are satisfied, the operator defined by:

$$\gamma \mapsto (I_d - L_A + C'L^N(I_N - L_B)^{-1}L^NC'^T)\gamma$$

is invertible. Moreover the function defined by

$$\gamma \mapsto \int_{\mathcal{H}^N_t} e^{-\frac{i\hbar}{2} \langle \Gamma, (I_N - L_B)^{-1} \Gamma \rangle} e^{i \langle \gamma, C' L^N (I_N - L_B)^{-1} \Gamma \rangle} d\mu_{\gamma}(\Gamma)$$

is the Fourier transform of the bounded variation measure ν on \mathcal{H}_t defined by

$$\int_{\mathcal{H}_t^d} g(\gamma) d\nu(\gamma) \equiv \int_{\mathcal{H}_t^d \times \mathcal{H}_t^N} g(\gamma + C' L^N (I_N - L_B)^{-1} \Gamma) e^{-\frac{i\hbar}{2} \langle \Gamma, (I_N - L_B)^{-1} \Gamma \rangle} d\mu(\gamma, \Gamma)$$

By applying theorem 2.2.1 we have:

$$\widetilde{\int}_{\mathcal{H}_{t}^{d}} e^{\frac{i}{2\hbar} \langle \gamma, (I_{d}-L_{A})\gamma \rangle} \left(\widetilde{\int}_{\mathcal{H}_{t}^{N}} e^{\frac{i}{2\hbar} \langle \Gamma, (I_{N}-L_{B})\Gamma \rangle} e^{-\frac{i}{\hbar} \langle \Gamma, L^{N}C'^{T}\gamma \rangle} f(\gamma, \Gamma) d\Gamma \right) d\gamma$$

$$= \det(I_{d}-L_{A}-C'L^{N}(I_{N}-L_{B})^{-1}L^{N}C'^{T})^{-1/2} \det(I_{N}-L_{B})^{-1/2}$$

$$\int_{\mathcal{H}_{t}^{d} \oplus \mathcal{H}_{t}^{N}} e^{-\frac{i\hbar}{2} \langle \gamma+C'L^{N}(I_{N}-L_{B})^{-1}\Gamma, (I_{d}-L_{A}-C'L^{N}(I_{N}-L_{B})^{-1}L^{N}C'^{T})^{-1}(\gamma+C'L^{N}(I_{N}-L_{B})^{-1}\Gamma) \rangle}$$

$$e^{-\frac{i\hbar}{2} \langle \Gamma, (I_{N}-L_{B})^{-1}\Gamma \rangle} d\mu(\gamma, \Gamma) \quad (2.37)$$

On the other hand the oscillatory integral:

$$\widetilde{\int}_{\mathcal{H}_t^d \oplus \mathcal{H}_t^N} e^{\frac{i}{2\hbar} \langle (\gamma, \Gamma), (I_{d+N} - L_{AB})(\gamma, \Gamma) \rangle} f(\gamma, \Gamma) d\gamma d\Gamma$$

is equal, again by theorem 2.2.1, to:

$$\det(I - L_{AB})^{-1/2} \int_{\mathcal{H}^d_t \oplus \mathcal{H}^N_t} e^{-\frac{i\hbar}{2} \langle (\gamma, \Gamma), (I_{d+N} - L_{AB})^{-1}(\gamma, \Gamma) \rangle} d\mu(\gamma, \Gamma)$$
(2.38)

Where L_{AB} is defined by (2.27), so that an element $(\gamma', \Gamma') \in \mathcal{H}_t^d \oplus \mathcal{H}_t^N$ is equal to:

 $(I_{d+N} - L_{AB})^{-1}(\gamma, \Gamma) \quad , \quad (\gamma, \Gamma) \in \mathcal{H}_t^d \oplus \mathcal{H}_t^N$

if and only if

$$\begin{cases} (I_d - L_A)\gamma' - L^d C'\Gamma' = \gamma \\ (I_N - L_B)\Gamma' - L^N C'^T \gamma' = \Gamma \end{cases}$$
(2.39)

and one can easily verify that the solution is:

$$\gamma' = (I_d - L_A - C'L^N(I_N - L_B)^{-1}L^NC'^T)^{-1}\gamma + (I_d - L_A)^{-1}L^dC'(I_N - L_B - L^NC'(I_d - L_A)^{-1}L^dC')^{-1}\Gamma$$

$$\Gamma' = (I_N - L_B)^{-1} L_N C'^T (I_d - L_A - L^d C' (I_N - L_B)^{-1} L_N C'^T)^{-1} \gamma + (I_N - L_B - L^N C'^T (I_d - L_A)^{-1} L^d C')^{-1} \Gamma \quad (2.40)$$

As a consequence the exponent in the integral (2.38) is equal to:

$$\langle (\gamma, \Gamma), (I_{d+N} - L_{AB})^{-1} (\gamma, \Gamma) \rangle_{\mathcal{H}_{t}^{d} \oplus \mathcal{H}_{t}^{N}} = = \langle \gamma, (I_{d} - L_{A} - C'L^{N}(I_{N} - L_{B})^{-1}L^{N}C'^{T})^{-1}\gamma \rangle_{\mathcal{H}_{t}^{d}} + \langle \gamma, (I_{d} - L_{A})^{-1}L^{d}C'(I_{N} - L_{B} - L^{N}C'(I_{d} - L_{A})^{-1}L^{d}C')^{-1}\Gamma \rangle_{\mathcal{H}_{t}^{d}} + + \langle \Gamma, (I_{N} - L_{B} - L^{N}C'^{T}(I_{d} - L_{A})^{-1}L^{d}C')^{-1}\Gamma \rangle_{\mathcal{H}_{t}^{N}} + \langle \Gamma, (I_{N} - L_{B})^{-1}L_{N}C'^{T}(I_{d} - L_{A} - L^{d}C'(I_{N} - L_{B})^{-1}L_{N}C'^{T})^{-1}\gamma \rangle_{\mathcal{H}_{t}^{N}}$$
(2.41)

2.3 The Feynman-Vernon influence functional

One can easily verify that:

$$(I_N - L_B - L^N C'^T (I_d - L_A)^{-1} L^d C')^{-1} = (I_N - L_B)^{-1} + (I_N - L_B)^{-1} L^N C'^T (I - L_A - C' L^N (I_N - L_B)^{-1} L^N C'^T)^{-1} C' L^N (I - L_B)^{-1},$$

and analogously:

$$(I_d - L_A - C'L^N(I_N - L_B)^{-1}L^NC'^T)^{-1}C'L^N(I_N - L_B)^{-1}$$

= $(I_d - L_A)^{-1}L^dC'(I_N - L_B - L^NC'^T(I_d - L_A)^{-1}L^dC')^{-1},$

from which we conclude that the integral (2.38) is equal to the integral (2.37). Equality (3.5) follows by the following relation:

$$\det(I - L_{AB}) = \det(I_d - L_A - C'L^N(I_N - L_B)^{-1}L^NC'^T)\det(I_N - L_B),$$
(2.42)

that can be verified by writing the operator $I_{d+N} - L_{AB}$ in the following block form:

$$I_{d+N} - L_{AB} = \begin{pmatrix} I_N - L_B & L^N C'^T \\ L^d C' & I_d - L_A \end{pmatrix}$$

by taking the finite dimensional approximation of both sides of equation (2.42) and by the analogous equality valid for finite dimensional matrices.

Lemma 3. Let $\psi_0^A \in L^2(\mathbb{R}^d) \cap \mathcal{F}(\mathbb{R}^d)$, $\psi_0^B \in L^2(\mathbb{R}^N) \cap \mathcal{F}(\mathbb{R}^N)$. Let t satisfy assumptions (2.32),(2.33) and (2.34). Then the solution of the Schrödinger equation (2.1) is equal to:

$$\widetilde{\int}_{\mathcal{H}_{t}^{d}} e^{\frac{i}{2\hbar} \langle \gamma, (I_{d} - L_{A}) \gamma \rangle} \left(\widetilde{\int}_{\mathcal{H}_{t}^{N}} e^{\frac{i}{2\hbar} \langle \Gamma, (I_{N} - L_{B}) \Gamma \rangle} e^{-\frac{i}{\hbar} \langle \Gamma, L^{N} C'^{T} \gamma \rangle} \times \right. \\
\times G(\gamma, \Gamma, x, R) \psi_{0,A}'(\gamma(0) + x) \psi_{0,B}'(\Gamma(0) + R) d\Gamma \right) d\gamma$$
(2.43)

where $G(\gamma, \Gamma, x, R)$ is given by (2.31) and

$$\psi'_{0,A}(x) \equiv \psi^A_0(x/\sqrt{M}) \quad ; \quad \psi'_{0,B}(R) \equiv \psi^B_0(R/\sqrt{m})$$

Proof 2.3.4. The result follows by lemma 1 and lemma 2 with $\psi_0 = \psi_0^A \otimes \psi_0^B$.

Theorem 2.3.3. Let ρ_0^A and ρ_0^B be two density matrix operators on $L^2(\mathbb{R}^d)$ and $L^2(\mathbb{R}^N)$ respectively. Let us assume that they have smooth kernels, denoted by $\rho_0^A(x, x')$ and $\rho_0^B(R, R')$. Let us assume moreover that they decompose into sums of pure states

$$\rho_0^A = \sum_i w_i^A P_{\psi_i^A}, \qquad \rho_0^B = \sum_j w_j^B P_{\psi_j^B}, \qquad \psi_i^A = \hat{\mu}_i^A, \psi_j^B = \hat{\mu}_j^B, \tag{2.44}$$

with $\mu_i^A \in \mathcal{F}(\mathbb{R}^d)$, $\mu_j^B \in \mathcal{F}(\mathbb{R}^N)$, and:

$$\sum_{i,j} w_i^A w_j^B |\mu_i^A|^2 |\mu_j^B|^2 < +\infty.$$
(2.45)

Let t satisfy assumptions (2.32), (2.33), (2.34).

Then the kernel $\rho_t(x, x', R, R')$ of the density operator of the system evaluated at time t is given by the following infinite dimensional oscillatory integral (in the sense of definition 7.1.3):

$$\int_{\mathcal{H}_{t}^{d} \oplus \mathcal{H}_{t}^{N}} \int_{\mathcal{H}_{t}^{d} \oplus \mathcal{H}_{t}^{N}} e^{\frac{i}{2\hbar} \langle (\gamma, \Gamma), (I_{d+N} - L_{AB})(\gamma, \Gamma) \rangle} e^{-\frac{i}{2\hbar} \langle (\gamma', \Gamma'), (I_{d+N} - L_{AB})(\gamma', \Gamma') \rangle} \\
G(\gamma, \Gamma, x, R) \bar{G}(\gamma', \Gamma', x', R') \rho_{0,A}'(\gamma(0) + x, \gamma'(0) + x') \\
\rho_{0,B}'(\Gamma(0) + R, \Gamma'(0) + R') d\gamma d\Gamma d\gamma' d\Gamma' \quad (2.46)$$

where $G(\gamma, \Gamma, x, R)$ is given by (2.31). It is also equal to:

$$\widetilde{\int}_{\mathcal{H}_{t}^{d}} \widetilde{\int}_{\mathcal{H}_{t}^{d}} e^{\frac{i}{2\hbar} \langle \gamma, (I_{d}-L_{A})\gamma \rangle} e^{-\frac{i}{2\hbar} \langle \gamma', (I_{d}-L_{A})\gamma' \rangle} \left(\widetilde{\int}_{\mathcal{H}_{t}^{N}} \widetilde{\int}_{\mathcal{H}_{t}^{N}} e^{\frac{i}{2\hbar} \langle \Gamma, (I_{N}-L_{B})\Gamma \rangle} e^{\frac{i}{2\hbar} \langle \Gamma, (I_{N}-L_{B})\Gamma' \rangle} e^{\frac{i}{\hbar} \langle \Gamma', L^{N}C^{T}\gamma' \rangle} G(\gamma, \Gamma, x, R) \bar{G}(\gamma', \Gamma', x', R') e^{-\frac{i}{\hbar} \langle \Gamma, (I_{N}-L_{B})\Gamma' \rangle} e^{\frac{i}{\hbar} \langle \Gamma', L^{N}C^{T}\gamma' \rangle} G(\gamma, \Gamma, x, R) \bar{G}(\gamma', \Gamma', x', R') e^{-\frac{i}{2\hbar} \langle \Gamma, (I_{N}-L_{B})\Gamma' \rangle} e^{-\frac{i}{2\hbar} \langle \Gamma, (I_{N}-L_{B})\Gamma' \rangle} e^{\frac{i}{\hbar} \langle \Gamma', L^{N}C^{T}\gamma' \rangle} G(\gamma, \Gamma, x, R) \bar{G}(\gamma', \Gamma', x', R') e^{-\frac{i}{2\hbar} \langle \Gamma, (I_{N}-L_{B})\Gamma' \rangle} e^{-\frac{i}{2\hbar} \langle \Gamma, (I_{N}-L_{A})\Gamma' \rangle} e^{-\frac{i}{2} \langle \Gamma, (I_{N}-L$$

where $\rho'_{0,A}(x,y) \equiv \rho_0^A(x/\sqrt{M}, y/\sqrt{M})$ and $\rho'_{0,B}(R,Q) \equiv \rho_0^B(R/\sqrt{m}, Q/\sqrt{m}).$

Proof 2.3.5. If ρ_0^A and ρ_0^B are pure states, the result is a direct consequence of lemma 1 and lemma 3.

For general ρ_0^A and ρ_0^B satisfying assumptions (2.44) and (2.45) the result follows by the continuity of the infinite dimensional oscillatory integral as a functional of $\mathcal{F}(\mathbb{R}^{N+d})$ (corollary 2).

Theorem 2.3.4. Let ρ_0^A and ρ_0^B be two density matrix operators on $L^2(\mathbb{R}^d)$ and $L^2(\mathbb{R}^N)$ respectively. Let us assume that they have regular kernels as assumed in theorem 2.3.2, denoted by $\rho_0^A(x, x')$ and $\rho_0^B(R, R')$. Let $\rho_0^B \in S(\mathbb{R}^N \times \mathbb{R}^N)$. Let us assume that t satisfies assumptions (2.32), (2.33), (2.34) and that t is such that the determinant of the $d \times d$ left upper block of the $n \times n$ matrix $\cos(\Omega t)$, Ω^2 being the matrix (2.28), is non vanishing.

Then the kernel $\rho_R(t, x, y)$ of the reduced density operator of the system A evaluated at time t is given by:

$$\rho_{R}(t,x,y) = e^{-\frac{it}{2\hbar}x\Omega_{A}^{\prime2}x}e^{\frac{it}{2\hbar}y\Omega_{A}^{\prime2}y} \widetilde{\int}_{\mathcal{H}_{t}^{d}} \widetilde{\int}_{\mathcal{H}_{t}^{d}} e^{\frac{i}{2\hbar}\langle\gamma,(I_{d}-L_{A})\gamma\rangle}e^{-\frac{i}{2\hbar}\langle\gamma',(I_{d}-L_{A})\gamma'\rangle} \\
e^{-\frac{i}{\hbar}\int_{0}^{t}x\Omega_{A}^{\prime2}\gamma(s)ds}e^{\frac{i}{\hbar}\int_{0}^{t}y\Omega_{A}^{\prime2}\gamma'(s)ds}e^{-\frac{i}{\hbar}\int_{0}^{t}v_{A}^{\prime}(\gamma(s)+x)ds+\frac{i}{\hbar}\int_{0}^{t}v_{A}^{\prime}(\gamma'(s)+y)ds} \\
F(\gamma,\gamma',x,y)\rho_{0,A}^{\prime}(\gamma(0)+x,\gamma'(0)+y)d\gamma d\gamma' \quad (2.48)$$

where $F(\gamma, \gamma', x, y)$ is the influence functional is given by:

$$F(\gamma,\gamma',x,y) \equiv \int_{\mathbb{R}^{N}} e^{-\frac{it}{\hbar}xC'R} e^{+\frac{it}{\hbar}yC'R} e^{-\frac{i}{\hbar}\int_{0}^{t}(\gamma(s)-\gamma'(s))C'Rds}$$

$$\widetilde{\int}_{\mathcal{H}_{t}^{N}} \widetilde{\int}_{\mathcal{H}_{t}^{N}} e^{\frac{i}{2\hbar}\langle\Gamma,(I_{N}-L_{B})\Gamma\rangle} e^{-\frac{i}{2\hbar}\langle\Gamma',(I_{N}-L_{B})\Gamma'\rangle} e^{-\frac{i}{\hbar}\langle\Gamma,L^{N}C'^{T}\gamma\rangle} e^{\frac{i}{\hbar}\langle\Gamma',L^{N}C'^{T}\gamma'\rangle}$$

$$e^{-\frac{i}{\hbar}\int_{0}^{t}R\Omega_{B}^{2}(\Gamma(s)-\Gamma'(s))ds} e^{-\frac{i}{\hbar}\int_{0}^{t}(xC'\Gamma(s)+yC'\Gamma'(s))ds}$$

$$e^{-\frac{i}{\hbar}\int_{0}^{t}v'_{B}(\Gamma(s)+R)ds+\frac{i}{\hbar}\int_{0}^{t}v'_{B}(\Gamma'(s)+R)ds} \rho'_{0,B}(\Gamma(0)+R,\Gamma'(0)+R)d\Gamma d\Gamma' dR \quad (2.49)$$

Proof 2.3.6. Let us assume for notation simplicity that m = M = 1. The result in the general case can be obtained by replacing

$$\Omega_A, \Omega_B, C, v_A, v_B, \rho_0^A, \rho_0^B$$

by

$$\Omega'_A, \Omega'_B, C', v'_A, v'_B, \rho'_{0,A}, \rho'_{0,B}$$

<u>First step</u>: Let us prove first of all that the functional $(\gamma\gamma') \mapsto F(\gamma, \gamma', x, y)$ is well defined for any $\gamma, \gamma' \in \mathcal{H}_t^d$, $x, y \in \mathbb{R}^d$ and it is Fresnel integrable in the sense of definition 7.1.3. By decomposing the mixed state ρ_0^B into pure states according to the formula (2.44), the influence functional can be written as:

$$\int\limits_{\mathbb{R}^N} \sum_j w_j^B \psi_j^B(x,\gamma;R) \psi_j^B(y,\gamma';R) dR$$

where $\psi_j^B(x,\gamma)$ is the solution of the Schrödinger equation with initial datum ψ_j^B and Hamiltonian $H = -\frac{1}{2}\Delta_R + \frac{1}{2}R\Omega^2 BR + (x+\gamma(t))CR + v_B(R)$. In particular, by the unitarity of the evolution operator, $\|\psi_j^B(x,\gamma)\|_{L^2(\mathbb{R}^N)} = 1$ for any $x \in \mathbb{R}^d \ \gamma \in \mathcal{H}_t^d$. As, by Schwarz inequality:

$$\sum_{j} w_{j}^{B} \int_{\mathbb{R}^{N}} \psi_{j}^{B}(x,\gamma;R) \psi_{j}^{B}(y,\gamma';R) dR$$

$$\leq \sum_{j} w_{j}^{B} \|\psi_{j}^{B}(x,\gamma)\|_{L^{2}(\mathbb{R}^{N})} \|\psi_{j}^{B}(y,\gamma')\|_{L^{2}(\mathbb{R}^{N})} = 1$$

we can conclude that $F(\gamma, \gamma', x, y)$ is well defined for any $x, y \in \mathbb{R}^d \ \gamma, \gamma' \in \mathcal{H}_t^d$. Moreover, by Lebesgue's dominated convergence theorem, we have:

$$\begin{split} F(\gamma,\gamma',x,y) &= \lim_{\epsilon \to 0^+} \int e^{-\epsilon R^2} e^{-\frac{it}{\hbar}xCR} e^{+\frac{it}{\hbar}yCR} e^{-\frac{i}{\hbar}\int_0^t (\gamma(s) - \gamma'(s))CRds} \\ & \widetilde{\int}_{\mathcal{H}_t^N} \widetilde{\int}_{\mathcal{H}_t^N} e^{\frac{i}{2\hbar} \langle \Gamma, (I_N - L_B)\Gamma \rangle} e^{-\frac{i}{2\hbar} \langle \Gamma', (I_N - L_B)\Gamma' \rangle} e^{-\frac{i}{\hbar} \langle \Gamma, L^N C^T \gamma \rangle} e^{\frac{i}{\hbar} \langle \Gamma', L^N C^T \gamma' \rangle} \\ & e^{-\frac{i}{\hbar}\int_0^t R\Omega_B^2(\Gamma(s) - \Gamma'(s))ds} e^{-\frac{i}{\hbar}\int_0^t (xC\Gamma(s) + yC\Gamma'(s))ds} \\ & e^{-\frac{i}{\hbar}\int_0^t v_B(\Gamma(s) + R)ds + \frac{i}{\hbar}\int_0^t v_B(\Gamma'(s) + R)ds} \rho_0^B(\Gamma(0) + R, \Gamma'(0) + R)d\Gamma d\Gamma' dR \end{split}$$

By theorem 2.2.2 we have:

$$F(\gamma,\gamma',x,y) = |\det(I_N - L_B)|^{-1} \lim_{\epsilon \to 0^+} \int dR e^{-\epsilon R^2} e^{-\frac{it}{\hbar}xCR} e^{+\frac{it}{\hbar}yCR} e^{-\frac{i}{\hbar}\int_0^t (\gamma(s) - \gamma'(s))CRds} \sum_{n=0}^\infty \sum_{m=0}^\infty \frac{1}{n!} \frac{1}{m!} (\frac{-i}{\hbar})^n (\frac{i}{\hbar})^m \int_{0}^{t} \dots \int_{0}^t \prod_{i=1}^t ds_i \prod_{j=1}^m dr_j \int_{\mathbb{R}^N} \dots \int_{\mathbb{R}^N} \prod_{k=0}^n \prod_{i=1}^n d\mu_v(k_i) \prod_{j=1}^m d\mu_v(h_j) \int_{\mathbb{R}^N} \int_{\mathbb{R}^N} dk_0 dh_0 \tilde{\rho}_b(k_0, h_0) e^{iR(k_0 - h_0 + \sum_{i=1}^n k_i + \sum_{j=1}^m h_j)} e^{-\frac{i\hbar}{2} \langle (-\frac{L^N C^T \gamma}{\hbar} - \frac{v\Omega_{B,R}}{\hbar} - \frac{vC_x}{\hbar} + k_0 G_0 + \sum_{i=1}^n k_i G_{s_i}), (I_N - L_B)^{-1} (-\frac{L^N C^T \gamma}{\hbar} - \frac{v\Omega_{B,R}}{\hbar} - \frac{vC_y}{\hbar} + h_0 G_0 - \sum_{j=1}^m h_j G_{r_j}), (I_N - L_B)^{-1} (-\frac{L^N C^T \gamma'}{\hbar} - \frac{v\Omega_B, R}{\hbar} - \frac{vC_y}{\hbar} + h_0 G_0 - \sum_{j=1}^m h_j G_{r_j}), (I_N - L_B)^{-1} (-\frac{L^N C^T \gamma'}{\hbar} - \frac{v\Omega_B, R}{\hbar} - \frac{vC_y}{\hbar} + h_0 G_0 - \sum_{j=1}^m h_j G_{r_j}), (I_N - L_B)^{-1} (-\frac{L^N C^T \gamma'}{\hbar} - \frac{v\Omega_B, R}{\hbar} - \frac{vC_y}{\hbar} + h_0 G_0 - \sum_{j=1}^m h_j G_{r_j}), (I_N - L_B)^{-1} (-\frac{L^N C^T \gamma'}{\hbar} - \frac{v\Omega_B, R}{\hbar} - \frac{vC_y}{\hbar} + h_0 G_0 - \sum_{j=1}^m h_j G_{r_j}), (I_N - L_B)^{-1} (-\frac{L^N C^T \gamma'}{\hbar} - \frac{v\Omega_B, R}{\hbar} - \frac{vC_y}{\hbar} + h_0 G_0 - \sum_{j=1}^m h_j G_{r_j}), (I_N - L_B)^{-1} (-\frac{L^N C^T \gamma'}{\hbar} - \frac{v\Omega_B, R}{\hbar} - \frac{vC_y}{\hbar} + h_0 G_0 - \sum_{j=1}^m h_j G_{r_j}), (I_N - L_B)^{-1} (-\frac{L^N C^T \gamma'}{\hbar} - \frac{v\Omega_B, R}{\hbar} - \frac{vC_y}{\hbar} + h_0 G_0 - \sum_{j=1}^m h_j G_{r_j}), (I_N - L_B)^{-1} (-\frac{L^N C^T \gamma'}{\hbar} - \frac{v\Omega_B, R}{\hbar} - \frac{vC_y}{\hbar} + h_0 G_0 - \sum_{j=1}^m h_j G_{r_j}), (I_N - L_B)^{-1} (-\frac{L^N C^T \gamma'}{\hbar} - \frac{v\Omega_B, R}{\hbar} - \frac{vC_y}{\hbar} + h_0 G_0 - \sum_{j=1}^m h_j G_{r_j}), (I_N - L_B)^{-1} (-\frac{L^N C^T \gamma'}{\hbar} - \frac{v\Omega_B, R}{\hbar} - \frac{vC_y}{\hbar} + h_0 G_0 - \sum_{j=1}^m h_j G_{r_j}), (I_N - L_B)^{-1} (-\frac{L^N C^T \gamma'}{\hbar} - \frac{v\Omega_B, R}{\hbar} - \frac{vC_y}{\hbar} + h_0 G_0 - \sum_{j=1}^m h_j G_{r_j}), (I_N - L_B)^{-1} (-\frac{L^N C^T \gamma'}{\hbar} - \frac{v\Omega_B, R}{\hbar} - \frac{vC_y}{\hbar} - \frac{U}{\hbar} - \frac{U}{\hbar}$$

where $v_B(R) = \int_{\mathbb{R}^N} e^{ikR} d\mu_v(R)$, $\rho_B(R,Q) = \int_{\mathbb{R}^N} \int_{\mathbb{R}^N} e^{ik_0R - ih_0Q} \tilde{\rho}_B(k_0,h_0) dk_0 dh_0$ and: $v_{\Omega_B,R}, v_{Cx}, G_s \in \mathcal{H}_t^N$, $s \in [0,t]$

are defined by

$$\begin{split} \langle v_{\Omega_B,R}, \Gamma \rangle &= \int_0^t R \Omega_B^2 \Gamma(s) ds, \\ \langle v_{CX}, \Gamma \rangle &= \int_0^t x C \Gamma(s) ds, \\ \langle G_s, \Gamma \rangle &= \Gamma(s). \end{split}$$

By Fubini theorem we have:

$$F(\gamma, \gamma', x, y) = |\det(I_N - L_B)|^{-1} \lim_{\epsilon \to 0^+} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{1}{n!} \frac{1}{m!} (\frac{-i}{\hbar})^n (\frac{i}{\hbar})^m$$

$$\int_{0}^{t} \dots \int_{0}^{t} \int_{0}^{t} \dots \int_{0}^{t} \prod_{i=1}^{n} ds_i \prod_{j=1}^{m} dr_j \int_{\mathbb{R}^N} \dots \int_{\mathbb{R}^N} \prod_{k=1}^{n} \dots \int_{\mathbb{R}^N} \prod_{i=1}^{n} d\mu_v(k_i) \prod_{j=1}^{m} d\mu_v(h_j)$$

$$\int_{\mathbb{R}^N} \int_{\mathbb{R}^N} dk_0 dh_0 \tilde{\rho}_b(k_0, h_0) g_1(\gamma') \bar{g}_1(\gamma) g_2(\gamma', h_0, -\mathbf{h}, \mathbf{r}, y) \bar{g}_2(\gamma, k_0, \mathbf{k}, \mathbf{s}, x) \qquad (2.50)$$

$$\int_{\mathbb{R}^N} dR e^{-\epsilon R^2} e^{-\frac{i}{\hbar} \int_{0}^{t} (\gamma(s) + x - \gamma'(s) - y) CR ds} e^{iR(k_0 - h_0 + \sum_{i=1}^{n} k_i + \sum_{j=1}^{m} h_j)}$$

$$e^{-\frac{i}{\hbar} R \int_{0}^{t} \Omega_B^2 (I - L_B)^{-1} (-\frac{vC_s x}{\hbar} + \frac{vC_s y}{\hbar} + (k_0 - h_0) G_0 + \sum_{i=1}^{n} k_i G_{s_i} + \sum_{j=1}^{m} h_j G_{r_j})}$$

where, for every paths $\gamma, \gamma', x \in \mathbb{R}^n, v_0 \in \mathbb{R}$ and vectors $\mathbf{v} = (v_1, \dots, v_n), \mathbf{w} = (w_1, \dots, w_n)$ we have defined the functions:

$$g_1(\gamma) \equiv e^{+\frac{i}{2\hbar} \langle L^N C^T \gamma, (I_N - L_B)^{-1} L^N C^T \gamma \rangle}$$
(2.51)

and

$$g_2(\gamma, v_0, \mathbf{v}, \mathbf{w}, x) \equiv e^{+\frac{i\hbar}{2} \langle v_0 G_0 + \sum_{i=1}^n v_i G_{w_i} - \frac{v_{C,x}}{\hbar}, (I_N - L_B)^{-1} (v_0 G_0 + \sum_{i=1}^n v_i G_{w_i} - \frac{v_{C,x}}{\hbar}) \rangle} \times e^{-i \langle L^N C^t \gamma, (I_N - L_B)^{-1} (v_0 G_0 + \sum_{i=1}^n v_i G_{w_i} - \frac{v_{C,x}}{\hbar}) \rangle}$$

$$(2.52)$$

By integrating with respect to R in (2.50) we have that the latter is equal to:

$$|\det(I_N - L_B)|^{-1} \lim_{\epsilon \to 0^+} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{1}{n!} \frac{1}{m!} \left(\frac{-i}{\hbar}\right)^n \left(\frac{i}{\hbar}\right)^m$$

$$\int_0^t \dots \int_0^t \int_0^t \dots \int_0^t \prod_{i=1}^n ds_i \prod_{j=1}^m dr_j \int_{\mathbb{R}^N} \dots \int_{\mathbb{R}^N} \prod_{k=1}^n d\mu_v(k_i) \prod_{j=1}^m d\mu_v(h_j) \qquad (2.53)$$

$$\int_{\mathbb{R}^N} \int_{\mathbb{R}^N} \left(\frac{\pi}{\epsilon}\right)^{N/2} \left(e^{-\frac{\omega^2}{4\epsilon}}\right) \tilde{\rho}_b(k_0, h_0) g_1(\gamma') \bar{g}_1(\gamma) g_2(\gamma', h_0, -\mathbf{h}, \mathbf{r}, y) \bar{g}_2(\gamma, k_0, \mathbf{k}, \mathbf{s}, x) dk_0 dh_0$$

where:

$$\omega \equiv \left| -\frac{1}{\hbar} \int_{0}^{t} (I - L_B)^{-1} C^T(\gamma(s) - \gamma'(s)) ds - \frac{1}{\hbar} (\Omega_B \cos \Omega_B t)^{-1} \sin(\Omega_B t) C^T(x - y) + (\cos \Omega_B t)^{-1} (k_0 - h_0 + \sum_{i=1}^{n} \cos(\Omega_B s_i) k_i + \sum_{j=1}^{m} \cos(\Omega_B r_j) h_j) \right|^2$$
(2.54)

By introducing the new integration variables:

$$k'_0 \equiv \frac{1}{\sqrt{\epsilon}}(k_0 - h_0 + a), \qquad h'_0 \equiv h_0 - \frac{1}{2}a$$

with:

$$a \equiv \sum_{i=1}^{n} \cos(\Omega_B s_i) k_i + \sum_{j=1}^{m} \cos(\Omega_B r_j) h_j - \cos(\Omega_B t) \frac{1}{\hbar} \int_0^t (I - L_B)^{-1} C^T(\gamma(s) + -\gamma'(s)) ds) - \frac{1}{\hbar} (\Omega_B)^{-1} \sin(\Omega_B t) C^T(x - y))$$

where:

$$\int_{0}^{t} (I - L_B)^{-1} C^T(\gamma(s) - \gamma'(s)) ds = \cos^{-1}(\Omega_B t) \int_{0}^{t} \cos(\Omega_B s) C^T(\gamma(s) - \gamma'(s)) ds$$

the integral in (2.53), with $k_0 = \sqrt{\epsilon}k'_0 + h'_0 - \frac{a}{2}$ and $h_0 = h'_0 + \frac{a}{2}$, can be written as:

$$\pi^{N/2} |\det(I_N - L_B)|^{-1} \lim_{\epsilon \to 0^+} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{1}{n!} \frac{1}{m!} \left(\frac{-i}{\hbar}\right)^n \left(\frac{i}{\hbar}\right)^m$$

$$\int_{0}^{t} \dots \int_{0}^{t} \int_{0}^{t} \dots \int_{0}^{t} \prod_{i=1}^{n} ds_i \prod_{j=1}^{m} dr_j \int_{\mathbb{R}^N} \dots \int_{\mathbb{R}^N} \prod_{k=1}^{n} \frac{1}{k} d\mu_v(k_i) \prod_{j=1}^{m} d\mu_v(h_j)$$

$$\int_{\mathbb{R}^N} \int_{\mathbb{R}^N} dk'_0 dh'_0 \tilde{\rho}_b (\sqrt{\epsilon}k'_0 + h'_0 - \frac{1}{2}a, h'_0 + \frac{1}{2}a) g_1(\gamma') \bar{g}_1(\gamma)$$

$$g_2(\gamma', h'_0 + \frac{a}{2}, -\mathbf{h}, \mathbf{r}, y) \bar{g}_2(\gamma, \sqrt{\epsilon}k'_0 + h'_0 - \frac{a}{2}, \mathbf{k}, \mathbf{s}, x) e^{-\frac{1}{4} |(\cos \Omega_B t)^{-1}k'_0|^2}$$

By letting $\epsilon \to 0$ and using dominated convergence, the integral reduces to the following form:

$$\begin{split} F(\gamma,\gamma',x,y) &= K(x,y,t)e^{-\frac{i}{2\hbar}\langle(\gamma-\gamma'),A(\gamma+\gamma')\rangle}e^{-\frac{i}{\hbar}\langle\gamma,CL^{N}(I_{N}-L_{B})^{-1}v_{C,y}\rangle} e^{\frac{i}{2\hbar}\langle\gamma',CL^{N}(I_{N}-L_{B})^{-1}v_{C,y}\rangle}e^{\frac{i}{2\hbar}C^{T}(x-y)\int_{0}^{t}\frac{\sin(\Omega_{B}t)\sin(\Omega_{B}(t-s))}{\Omega_{B}^{2}\cos(\Omega_{B}t)}C^{T}(\gamma(s)+\gamma'(s))ds} \\ &\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\frac{1}{n!}\frac{1}{m!}(\frac{-i}{\hbar})^{n}(\frac{i}{\hbar})^{m}\int_{0}^{t}\dots\int_{0}^{t}\int_{0}^{t}\dots\int_{0}^{t}\prod_{i=1}^{n}ds_{i}\prod_{j=1}^{m}dr_{j}\int\dots\int_{\mathbb{R}^{N}}\dots\int_{\mathbb{R}^{N}} \\ &\int_{\mathbb{R}^{N}}\dots\int_{\mathbb{R}^{N}}\prod_{i=1}^{n}d\mu_{v}(k_{i})\prod_{j=1}^{m}d\mu_{v}(h_{j})\int_{\mathbb{R}^{N}}dh'_{0}\tilde{\rho}_{b}(h'_{0}-\frac{1}{2}a,h'_{0}+\frac{1}{2}a) \\ &e^{-\frac{i\hbar}{2}\sum_{i,j=1}^{n}k_{i}\frac{\sin(\Omega_{B}(t-s_{i}\vee s_{j}))\cos(\Omega_{B}(s_{i}\wedge s_{j}))}{\Omega_{B}\cos(\Omega_{B}t)}}k_{j}e^{\frac{i\hbar}{2}\sum_{i,j=1}^{m}h_{i}\frac{\sin(\Omega_{B}(t-r_{i}\vee r_{j}))\cos(\Omega_{B}(r_{i}\wedge r_{j}))}{\Omega_{B}\cos(\Omega_{B}t)}}h_{j} \\ &e^{i\sum_{i=1}^{n}k_{i}\frac{\cos(\Omega_{B}s_{i})-\cos(\Omega_{B}t)}{\Omega_{B}^{2}\cos(\Omega_{B}t)}C^{T}x}e^{-i(h_{0}+\frac{a}{2})\frac{1-\cos(\Omega_{B}t)}{\Omega_{B}^{2}\cos(\Omega_{B}t)}}C^{T}y} \\ &e^{i(h_{0}-\frac{a}{2})\frac{1-\cos(\Omega_{B}t)}{\Omega_{B}^{2}\cos(\Omega_{B}t)}C^{T}}(\gamma(s)+\gamma'(s))ds(\sum_{i=1}^{n}\cos(\Omega_{B}s_{i})k_{i}+\sum_{j=1}^{m}\cos(\Omega_{B}r_{j})h_{j})} \\ &e^{ihh'_{0}\frac{\sin\Omega_{B}t}{\Omega_{B}\cos\Omega_{B}t}}a}e^{-ih(h'_{0}-a/2)\sum_{i=1}^{n}\frac{\sin(\Omega_{B}(t-s_{i}))}{\Omega_{B}\cos(\Omega_{B}t)}k_{i}}e^{-ih(h'_{0}+a/2)\sum_{j=1}^{m}\frac{\sin(\Omega_{B}(t-r_{j}))}{\Omega_{B}\cos(\Omega_{B}t)}h_{j}} \\ &e^{i(\gamma,\sum_{i=1}^{n}CL^{N}(I_{N}-L_{B})^{-1}k_{i}G_{s_{i}}}e^{i(\gamma',\sum_{j=1}^{m}CL^{N}(I_{N}-L_{B})^{-1}h_{j}G_{r_{j}}}e^{i(\gamma-\gamma',CL^{N}(I_{N}-L_{B})^{-1}h'_{0}G_{0}}} (2.55) \end{split}$$

where we have defined:

$$K(x,y,t) \equiv \pi^N 2^N e^{-\frac{i}{2\hbar}C^T(x-y)\left(\frac{t}{\Omega_B^2} - \frac{\sin(\Omega_B t)}{\Omega_B^3\cos(\Omega_B t)}\right)C^T(x-y)}$$

and

$$e^{-\frac{i}{2\hbar}\langle(\gamma-\gamma'),A(\gamma+\gamma')\rangle}e^{-\frac{i}{2\hbar}\langle C^{T}(\gamma-\gamma'),L^{N}(I_{N}-L_{B})^{-1}L^{N}C^{T}(\gamma+\gamma')\rangle}\times$$

$$\times e^{+\frac{i}{2\hbar}\cos(\Omega_{B}t)\langle C^{T}(\gamma(s)-\gamma'(s)),(I_{N}-L_{B})^{-1}v\rangle\langle L^{N}(I_{N}-L_{B})^{-1}G_{0},C^{T}(\gamma(s)+\gamma'(s))\rangle} = (2.56)$$

$$= e^{\frac{i}{2\hbar}\int_{0}^{t}C^{T}(\gamma-\gamma')(s)\Omega^{-1}\int_{0}^{s}\sin(\Omega_{B}(s-r))C^{T}(\gamma+\gamma')(r)drds}$$

with $v(s)_i \equiv \frac{t^2 - s^2}{2}, \ i = 1 \dots N, \ s \in [0, t].$

As we have assumed that the determinant of the $d \times d$ left upper block of the $n \times n$ matrix $\cos(\Omega t)$ (Ω^2 being the matrix (2.28)) is non vanishing, it is possible to prove, see Rem.(2.4.1), that the operator $I - L_A - A$ is invertible.

As $F(\gamma, \gamma', x, y)$ is of the form $F(\gamma, \gamma') = e^{-\frac{i}{2\hbar} \langle (\gamma - \gamma'), A(\gamma + \gamma') \rangle} f(\gamma, \gamma')$, with $f \in \mathcal{F}(\mathcal{H}_t^d \oplus \mathcal{H}_t^d)$, we can conclude that the influence functional is a Fresnel integrable function.

<u>Second step</u>: Let us prove that the reduced density operator $\rho_R(t, x, y)$ is given by the infinite dimensional oscillatory integral (2.48).

Let $\rho(t, x, y, R, Q)$ be the (smooth) kernel of the density operator of the compound system evaluated at time t. Then the integral giving the kernel of reduced density operator

$$\rho_R(t, x, y) \equiv \int \rho(t, x, y, R, R) dR$$

is absolutely convergent and by Lebesgue's dominated convergence theorem we have:

$$\rho_R(t, x, y) = \lim_{\epsilon \to 0} \int \rho(t, x, y, R, R) e^{-\epsilon R^2} dR$$

On the other hand the influence functional can be written as:

$$F(\gamma,\gamma') = e^{-\frac{i}{2\hbar} \langle (\gamma - \gamma'), A(\gamma + \gamma') \rangle} f(\gamma,\gamma')$$

with:

$$f: \mathcal{H}_t^d \oplus \mathcal{H}_t^d \to \mathbb{C}$$
 defined as follows $f = \lim_{\epsilon \to 0} f_\epsilon$, (2.57)

and where:

$$f_{\epsilon}(\gamma,\gamma') \equiv \pi^{N/2} |\det(I_N - L_B)|^{-1} \lim_{\epsilon \to 0^+} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{1}{n!} \frac{1}{m!} (\frac{-i}{\hbar})^n (\frac{i}{\hbar})^m$$
$$\int_{0}^{t} \dots \int_{0}^{t} \int_{0}^{t} \dots \int_{0}^{t} \prod_{i=1}^{n} ds_i \prod_{j=1}^{m} dr_j \int_{\mathbb{R}^N} \dots \int_{\mathbb{R}^N} \prod_{k=1}^{n} \prod_{i=1}^{n} d\mu_v(k_i) \prod_{j=1}^{m} d\mu_v(h_j)$$
$$\int_{\mathbb{R}^N} \int_{\mathbb{R}^N} dk'_0 dh'_0 \tilde{\rho}_b (\sqrt{\epsilon}k'_0 + h'_0 - \frac{1}{2}a, h'_0 + \frac{1}{2}a)$$
$$g_2(\gamma', h'_0 + \frac{a}{2}, -\mathbf{h}, \mathbf{r}, y) \bar{g}_2(\gamma, \sqrt{\epsilon}k'_0 + h'_0 - \frac{a}{2}, \mathbf{k}, \mathbf{s}, x) e^{-\frac{1}{4}|(\cos\Omega_B t)^{-1}k'_0|^2}$$

with $a' \equiv a + \cos(\Omega_B t) \frac{1}{\hbar} \int_0^t (I - L_B)^{-1} C^T(\gamma(s) - \gamma'(s)) ds$ and the limit (2.57) is meant in the $\mathcal{F}(\mathcal{H}^d_t \oplus \mathcal{H}^d_t)$ sense.

By the continuity of the infinite dimensional oscillatory integral as a functional on $\mathcal{F}(\mathcal{H}_t^d \oplus \mathcal{H}_t^d)$

(see corollary 2) we have that the r.h.s of equation (2.48) is equal to:

$$e^{-\frac{it}{2\hbar}x\Omega_{A}^{2}x}e^{\frac{it}{2\hbar}y\Omega_{A}^{2}y}\lim_{\epsilon \to 0} \widetilde{\int}_{\mathcal{H}_{t}^{d}} \widetilde{\int}_{\mathcal{H}_{t}^{d}} e^{\frac{i}{2\hbar}\langle\gamma,(I_{d}-L_{A})\gamma\rangle}e^{-\frac{i}{2\hbar}\langle\gamma',(I_{d}-L_{A})\gamma'\rangle}$$

$$e^{-\frac{i}{\hbar}\int_{0}^{t}x\Omega_{A}^{2}\gamma(s)ds}e^{\frac{i}{\hbar}\int_{0}^{t}y\Omega_{A}^{2}\gamma'(s)ds}e^{-\frac{i}{\hbar}\int_{0}^{t}v_{A}(\gamma(s)+x)ds+\frac{i}{\hbar}\int_{0}^{t}v_{A}(\gamma'(s)+y)ds}$$

$$e^{-\frac{i}{2\hbar}\langle(\gamma-\gamma'),A(\gamma+\gamma')\rangle}f_{\epsilon}(\gamma,\gamma')\rho_{0}^{A}(\gamma(0)+x,\gamma'(0)+y)d\gamma d\gamma' \quad (2.58)$$

On the other hand the latter is equal to:

$$\begin{split} e^{-\frac{it}{2\hbar}x\Omega_A^2x} e^{\frac{it}{2\hbar}y\Omega_A^2y} \lim_{\epsilon \to 0} \widetilde{\int}_{\mathcal{H}_t^d} \widetilde{\int}_{\mathcal{H}_t^d} e^{\frac{i}{2\hbar}\langle\gamma,(I_d-L_A)\gamma\rangle} e^{-\frac{i}{2\hbar}\langle\gamma',(I_d-L_A)\gamma'\rangle} \\ e^{-\frac{i}{\hbar}\int_0^t x\Omega_A^2\gamma(s)ds} e^{\frac{i}{\hbar}\int_0^t y\Omega_A^2\gamma'(s)ds} e^{-\frac{i}{\hbar}\int_0^t v_A(\gamma(s)+x)ds+\frac{i}{\hbar}\int_0^t v_A(\gamma'(s)+y)ds} \\ & (\int_{\mathbb{R}^N} dRe^{-\epsilon R^2}e^{-\frac{it}{\hbar}xCR}e^{+\frac{it}{\hbar}yCR}e^{-\frac{i}{\hbar}\int_0^t(\gamma(s)-\gamma'(s))CRds} \\ & \widetilde{\int}_{\mathcal{H}_t^N} \widetilde{\int}_{\mathcal{H}_t^N} e^{\frac{i}{2\hbar}\langle\Gamma,(I_N-L_B)\Gamma\rangle}e^{-\frac{i}{2\hbar}\langle\Gamma',(I_N-L_B)\Gamma'\rangle}e^{-\frac{i}{\hbar}\langle\Gamma,L^NC^T\gamma\rangle}e^{\frac{i}{\hbar}\langle\Gamma',L^NC^T\gamma'\rangle} \\ & e^{-\frac{i}{\hbar}\int_0^t R\Omega_B^2(\Gamma(s)-\Gamma'(s))ds}e^{-\frac{i}{\hbar}\int_0^t(xC\Gamma(s)+yC\Gamma'(s))ds} \end{split}$$

 $e^{-\frac{i}{\hbar}\int_0^t v_B(\Gamma(s)+R)ds+\frac{i}{\hbar}\int_0^t v_B(\Gamma'(s)+R)ds}\rho_0^B(\Gamma(0)+R,\Gamma'(0)+R)d\Gamma d\Gamma' dR)\rho_0^A(\gamma(0)+x,\gamma'(0)+y)d\gamma d\gamma' d\Gamma' d\Gamma' dR)$

By Fubini theorem (see theorem 2.2.3) and by the infinite dimensional oscillatory integral representation or the kernel of the density operator it is equal to $\int dR e^{-\epsilon R^2} \rho(t, x, y, R, R)$. By letting $\epsilon \to 0$ the conclusion follows.

Remark 2.3.2. It is typical of the difficulties in handling rigorously Feynman path integrals (as infinite dimensional oscillatory integrals) that the passages to the limit cause mathematical problems, because of the lack of the dominated convergence and limited availability of Fubinitype theorems. Our ϵ -cut-off trick was instrumental to perform such a type of computation.

2.4. Application to the Caldeira-Leggett model

Let us compute the influence functional $F(\gamma, \gamma', x, y)$ in the case:

$$v_B \equiv 0 , \ \rho_0^B(R,Q) \equiv \prod_{j=1}^N \rho_B^{(j)}(R_j,Q_j,0)$$

, where:

$$\rho_B^{(j)}(R_j, Q_j, 0) \equiv \sqrt{\frac{m\omega_j}{\pi\hbar\coth(\hbar\omega_j/2kT)}} e^{-\left(\frac{m\omega_j}{2\hbar\sinh(\hbar\omega_j/kT)}\left((R_j^2 + Q_j^2)\cosh\frac{\hbar\omega_j}{kT} - 2R_jQ_j\right)\right)}$$

 $\omega_j, j = 1 \dots n$ being the eigenvalues of the matrix Ω_B . By notation simplicity we put m = 1, the general case can be handled by replacing

$$\Omega_A, \Omega_B, C, v_A, v_B, \rho_0^A, \rho_0^B$$

by

$$\Omega_A', \Omega_B', C', v_A', v_B', \rho_{0,A}', \rho_{0,B}'$$

By inserting this into the general formula (2.55) the influence functional becomes:

$$F(\gamma,\gamma',x,y) = K(x,y,t)e^{-\frac{i}{2\hbar}\langle(\gamma-\gamma'),A(\gamma+\gamma')\rangle}e^{-\frac{i}{\hbar}\langle\gamma,CL^{N}(I_{N}-L_{B})^{-1}v_{C,x}\rangle} \times \\ \times e^{\frac{i}{\hbar}\langle\gamma',CL^{N}(I_{N}-L_{B})^{-1}v_{C,y}\rangle}e^{\frac{i}{2\hbar}C^{T}(x-y)\int_{0}^{t}\frac{\sin(\Omega_{B}t)\sin(\Omega_{B}(t-s))}{\Omega_{B}^{2}\cos(\Omega_{B}t)}C^{T}(\gamma(s)+\gamma'(s))ds} \times \\ \times \int_{\mathbb{R}^{N}}dh_{0}'\tilde{\rho}_{b}(h_{0}'-\frac{1}{2}a,h_{0}'+\frac{1}{2}a)e^{i(h_{0}-\frac{a}{2})\frac{1-\cos(\Omega_{B}t)}{\Omega_{B}^{2}\cos(\Omega_{B}t)}C^{T}x}e^{-i(h_{0}+\frac{a}{2})\frac{1-\cos(\Omega_{B}t)}{\Omega_{B}^{2}\cos(\Omega_{B}t)}C^{T}y} \times (2.59) \\ \times e^{i\hbar h_{0}'\frac{\sin\Omega_{B}t}{\Omega_{B}\cos\Omega_{B}t}a}e^{i\langle\gamma-\gamma',CL^{N}(I_{N}-L_{B})^{-1}h_{0}'G_{0}\rangle}$$

where

$$K(x,y,t) \equiv \pi^N 2^N e^{\frac{i}{2\hbar}C^T(x-y)\left(\frac{t}{\Omega_B^2} - \frac{\sin(\Omega_B t)}{\Omega_B^3}\right)C^T(x+y)}$$
(2.60)

and we have defined:

$$e^{-\frac{i}{2\hbar}\langle(\gamma-\gamma'),A(\gamma+\gamma')\rangle} \equiv e^{-\frac{i}{2\hbar}\langle C^{T}(\gamma-\gamma'),L^{N}(I_{N}-L_{B})^{-1}L^{N}C^{T}(\gamma+\gamma')\rangle} \times e^{+\frac{i}{2\hbar}\cos(\Omega_{B}t)\langle C^{T}(\gamma(s)-\gamma'(s)),(I_{N}-L_{B})^{-1}v\rangle\langle L^{N}(I_{N}-L_{B})^{-1}G_{0},C^{T}(\gamma(s)+\gamma'(s))\rangle} = (2.61)$$
$$= e^{\frac{i}{2\hbar}\int_{0}^{t}C^{T}(\gamma-\gamma')(s)\Omega^{-1}\int_{0}^{s}\sin(\Omega_{B}(s-r))C^{T}(\gamma+\gamma')(r)drds}$$

while a is set as follows:

$$a = -\cos(\Omega_B t) \frac{1}{\hbar} \int_0^t (I - L_B)^{-1} C^T(\gamma(s) - \gamma'(s)) ds) - \frac{1}{\hbar} (\Omega_B)^{-1} \sin(\Omega_B t) C^T(x - y))$$

By direct computation, we obtain:

$$F(\gamma,\gamma',x,y) = e^{\frac{i}{2\hbar}\int_0^t C^T(\gamma(s)+x-\gamma'(s)-y)\Omega_B^{-1}\int_0^s \sin(\Omega_B(s-r))C^T(\gamma(r)+x+\gamma'(r)+y)drds} \times e^{-\frac{1}{2\hbar}\int_0^t C^T(\gamma(s)+x-\gamma'(s)-y)\Omega_B^{-1}\coth(\frac{\hbar\Omega_B}{2kT})\int_0^s \cos(\Omega_B(s-r))C^T(\gamma(r)+x-\gamma'(r)-y)drds}$$
(2.62)

which yelds the result heuristically derived in [FV63].

Remark 2.4.1. (Kernel of the operator $I - L_A - A$) A vector $\gamma \in \mathcal{H}_t^d$ belongs to the kernel of the operator $I - L_A - A$, if it satisfies the following equation:

$$\gamma(s) + \int_{s}^{t} ds' \int_{0}^{s'} ds'' \int_{0}^{s''} C\Omega_{B}^{-1} \sin(\Omega_{B}(s''-r)) C^{T} \gamma(r) dr + - \int_{s}^{t} ds' \int_{0}^{s'} \Omega_{A}^{2} \gamma(s'') ds'' = 0 \qquad s \in [0,t]$$
(2.63)

with $\gamma(t) = 0$. Equation (2.63) is equivalent to:

$$\ddot{\gamma}(s) + \Omega_A^2 \gamma(s) - \int_0^s C \Omega_B^{-1} \sin(\Omega_B(s-r)) C^T \gamma(r) dr = 0$$
(2.64)

with the conditions: $\gamma(t) = 0, \dot{\gamma}(0) = 0.$

By differentiating equation (2.63), it is easy to see that its solution, if it exists, is a C^{∞} function and its odd derivatives, evaluated for s = 0, vanish, while the even derivatives satisfy the following relation

$$\gamma^{2(N+2)}(0) + \Omega_A^2 \gamma^{2(N+1)}(0) - \sum_{k=0}^N (-1)^k C \Omega_B^{2k} C^T \gamma^{2(N-k)}(0) = 0$$
(2.65)

By induction it is possible to prove that $\gamma^{2N}(0) = (-1)^N [\Omega^{2N}]_{d \times d} \gamma(0)$, where $[\Omega^{2N}]_{d \times d}$ denotes the $d \times d$ left upper block of the N-th power of the $n \times n$ matrix Ω^2 (where Ω^2 is given by equation (2.28)). One concludes that the solution of equation (2.63) is of the form $\gamma(s) = [\cos(\Omega s)]_{d \times d} \gamma(0)$.

By imposing the condition $\gamma(t) = 0$, one concludes that if $\det([\cos(\Omega s)]_{d \times d}) \neq 0$ then equation (2.63) cannot admit nontrivial solutions and the operator $I - L_A - A$ is invertible.

Remark 2.4.2. Using previous description of the Feynman-Vernon influence functional and results¹ stated in Ch.(7) Sec.(7.1.1) and Sec.(7.2), we can rigorously study the asymptotics for $\hbar \downarrow 0$ of the influence functional (2.6) in the rigorous path integral realization (2.49) given in Th.(2.3.4), i.e. its semiclassical limit, see [APM06b].

¹See also [AHK77, AB93].

CHAPTER 3

A Remark on the Semiclassical Limit for the Expectation of the Stochastic Schrödinger Equation

In this section we will use the semiclassical expansion developed in Ch.(7) in order to study the asymptotic behaviour of the solution to the stochastic Schrödinger equation associated to the Belavkin proposal, see [Bel89], in the framework given by the theory of infinite dimensional oscillating integrals as it is showed in Ch.(7).

Let us consider the Belavkin equation¹:

$$\begin{cases} d\psi = \frac{i}{\hbar} H \psi dt - \frac{\lambda |x|^2}{2} \psi dt + \sqrt{\lambda} x \psi dW(t) \\ \psi(0, x) = \psi_0(x) \qquad t \ge 0, x \in \mathbb{R}^d \end{cases}$$
(3.1)

which is a stochastic partial differential equation describing the behaviour of a non relativistic, quantum particle disturbed by a standard Brownian motion W, of intensity $\lambda > 0$ and where we have used the notation dW to indicate its Ito stochastic differential, see e.g. [oJ96, KS98].

Belavkin derives equation (3.1) by means of a one-dimensional bosonic field approach to the problem of modeling the measuring apparatus and by assuming a particular form for the interaction Hamiltonian between the field and the system on which the measurement is performed.

Using the Stratonovich theory of stochastic integration we can rewrite (3.1) as follows:

$$\begin{cases} d\psi = \frac{i}{\hbar} H\psi dt - \lambda \mid x \mid^2 \psi dt + \sqrt{\lambda} x \psi \circ dW(t) \\ \psi(0, x) = \psi_0(x) \qquad t \ge 0, x \in \mathbb{R}^d \end{cases}$$
(3.2)

In [AGM03] the study of (3.2) is given using the theory of infinite dimensional oscillatory

¹See [Bel89] and references therein.

integral² to rigorously realize the corrisponding Feynman path integral solution. In particular the following result holds³:

Theorem 3.0.1. Let V and ψ_0 be Fourier transforms of complex bounded variation measures on \mathbb{R}^d . Then there exists a strong solution of (3.2) given by:

$$\psi(t,x) = e^{-\frac{-i\Omega^2 |x|^2 t}{2\hbar} + \sqrt{\lambda}x \cdot \omega(t)} \int_{H} e^{\frac{i}{2\hbar} \langle l, (I+L)\gamma \rangle} e^{\langle \gamma, \gamma \rangle} e^{-i\int_{0}^{t} \Omega^2 x \cdot \gamma(s) ds} \times e^{-\frac{i}{\hbar} \int_{0}^{t} V(x+\gamma(s)) ds} \psi_0\left(\gamma(0)+x\right) d\gamma$$
(3.3)

where H is the Cameron-Martin space defined as the set of absolutely continuous paths γ : $[0,t] \mapsto \mathbb{R}^d$ which ends in 0, i.e. $\gamma(t) = 0$, and has finite kinetic energy, i.e. $\int_0^t |\gamma'(s)|^2 ds < \infty$, while the element $l \in H$ is defined by:

$$\langle l, \gamma \rangle \equiv \sqrt{\lambda} \int_{0}^{t} \omega(s) \cdot \gamma'(s) ds$$

The constant Ω is given by $\equiv \Omega^2 = -2i\lambda\hbar$ and L is the following operator defined on the complexification of the Cameron-Martin space H:

$$\langle \gamma_1, L\gamma_2 \rangle \equiv \Omega^2 \int_0^t \gamma_1(s) \cdot \gamma_2(s) ds \qquad \forall \gamma_1, \gamma_2 \in H$$

Above theorem can be extended to general initial vectors $\psi_0 \in L^2(\mathbb{R}^d)$ since the set $\mathcal{F}(\mathbb{R}^d)$ is a dense subset of $L^2(\mathbb{R}^d)$. Moreover formula (3.3) can be written as follows:

$$\psi(t,x) = \int e^{\frac{i}{2\hbar} \int_0^t |\dot{\gamma}(s)|^2 ds} e^{-\lambda \int_0^t |\gamma(s) - x|^2 ds} \times \\ \times e^{-\frac{i}{\hbar} \int_0^t V(\gamma(s) + x) ds} e^{\int_0^t \sqrt{\lambda} (\gamma(s) + x) \cdot dW(s)} \psi_0(\gamma(0) + x) d\gamma$$
(3.4)

which, according to the theory presented in [AHK77] see also Ch.(7), is the Feynman path integral solution of the problem (3.1), see [AGM03].

Proposition 3.0.1. Let us take a solutions ψ of (3.1) in the form (3.4) and $\mathbb{E}_W[\cdot]$ the expectation with respect to the standard Wiener measure W. Then the following holds:

$$\mathbb{E}_{W}\left[\psi(t,x)\right] = \widetilde{\int} e^{\frac{i}{2\hbar} \int_{0}^{t} |\dot{\gamma}(s)|^{2} ds} e^{-\lambda \int_{0}^{t} |\gamma(s)-x|^{2} ds} \times e^{-\frac{i}{\hbar} \int_{0}^{t} V(\gamma(s)+x) ds} \psi_{0}(\gamma(0)+x) \left(\mathbb{E}_{W}\left[e^{\int_{0}^{t} \sqrt{\lambda}(\gamma(s)+x) \cdot dW(s)}\right]\right) d\gamma$$
(3.5)

 $^2 \mathrm{See}\ \mathrm{Ch7}$ and references therein.

³See Th.3 of [AGM03].

Proof 3.0.1. This formula is first proven for the finite dimensional approximations of the oscillatory integral and the Wiener integral. We refer to [AHK76] for details.

Proposition 3.0.2. For any $\gamma \in \mathcal{H}$, $\lambda > 0$, $x \in \mathbb{R}^n$:

$$\mathbb{E}_{W}\left[e^{\int_{0}^{t}\sqrt{\lambda}(\gamma(s)+x)\cdot dW(s)}\right] = e^{\frac{\lambda}{2}\int_{0}^{t}(\gamma(s)+x)^{2}ds}$$
(3.6)

Proof 3.0.2. This is an easy consequence of $\eta(s) \equiv dW(s)$ being white noise, i.e. gaussian, mean zero and with covariance:

$$\mathbb{E}\left[\langle g_1, \eta \rangle \cdot \langle g_2, \eta \rangle\right] = \int_0^t g_1 \cdot g_2 ds$$

where $g_i \in L^2[0,t]$ for i = 1, 2. See e.g. [Kuo75].

Corollary 3.0.1. The expectation of the solution (3.4) of the Belavkin Stochastic Schrödinger equation is given by:

$$\mathbb{E}_{W}\left[\psi(t,x)\right] = e^{\frac{\lambda}{2}\int_{0}^{t}(\gamma(s)+x)^{2}ds} \times \\ \times \widetilde{\int} e^{\frac{i}{2\hbar}\int_{0}^{t}|\dot{\gamma}(s)|^{2}ds} e^{-\lambda\int_{0}^{t}|\gamma(s)-x|^{2}ds} e^{-\frac{i}{\hbar}\int_{0}^{t}V(\gamma(s)+x)ds} \psi_{0}(\gamma(0)+x)$$

Proof 3.0.3. This follows immediatly from Prop. (3.0.1), (3.0.2).

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Then we have obtained an expression which is of the form studied in Ch.7 Sec.7.2. Hence, assuming that the potential V and the initial condition $\psi(0, x) = \psi_0(x)$ chosen in (3.1) are such that we have only one non degenerate critical point for the corresponding phase (which can be shown to be the case for tg sufficiently small), we can perform the asymptotic expansion of the above infinite dimensional oscillating integral in the semiclassical limit $\hbar \to 0$ setting $\lambda \equiv \hbar^{-1}$ follows [AB93]. For details we refer to [APM06c].

CHAPTER 4

Laplace Method

4.1. One dimensional Laplace Method

As a first example of expansion methods to evaluate integrals which depend on *large positive parameters*, let us consider the following:

$$I(\lambda) \equiv \int_{a}^{b} g(x)e^{\lambda\phi(x)}dx , \qquad (4.1)$$

where the *amplitude* g(x) is a complex valued function, while the *phase*¹ $\phi(x)$ is a real valued one and we would like to study the asymptotics of (4.1) with respect to the limit $|\lambda| \to \infty, \lambda$ being a parameter. Is is assumed that $ge^{\lambda\phi}$ is Lebesgue integrable on the closed interval [a, b] of the real line. Let us start recalling the following fundamental lemma:

Lemma 4.1.1. (Watson Lemma) Set for $\epsilon > 0$:

$$S_{\epsilon} \equiv \left\{ \lambda \in \mathbb{C} : |\arg \lambda| \le \frac{\pi}{2} - \epsilon \right\}$$
(4.2)

Define for $0 < a < \infty$, $\alpha > 0, \beta > 0$ and $g \in C^{\infty}([0, a])$:

$$\tilde{I}(\lambda) \equiv \int_{0}^{a} g(x) x^{\beta - 1} e^{-\lambda x^{\alpha}} dx$$
(4.3)

The following asymptotic expansion of (4.3) for $\lambda \in S_{\epsilon}$, $|\lambda| \to \infty$ holds :

$$\tilde{I}(\lambda) = \frac{1}{\alpha} \sum_{k=0}^{\infty} \lambda^{-(\beta+k)/\alpha} \Gamma\left(\frac{\beta+k}{\alpha}\right) \frac{g^{(k)}(0)}{k!}$$

¹This terminology is strictly related to the subject of asymptotic expansions for one parameter-depending integral which naturally arise in several areas of mathematical physics. Traditionally the integrand term is viewed as a wave, so it is natural to name g and ϕ as we made.

$$\Gamma(z) = \int_{0}^{\infty} t^{z-1} e^{-t} dt$$

and then meromorphically continued to all $z \in \mathbb{C}$) and $g^{(k)}(0)$ denotes the k-th derivative of the function g evaluated at the point x = 0. The right hand side is understood in the sense of asymptotic series, i.e. :

$$\frac{1}{\alpha} \sum_{k=0}^{N} \lambda^{-(\beta+k)/\alpha} \Gamma\left(\frac{\beta+k}{\alpha}\right) \frac{g^{(k)}(0)}{k!} + \mathscr{R}_{N}(\lambda) ,$$

whit $|\mathscr{R}_N(\lambda)| \leq C_N \lambda^{N+1}$, as $\lambda \to +\infty$ for any N.

For a proof of Watson's lemma see e.g. Ch.4, Sec. 4.1 of [BH86].

Let ϕ be a sufficiently regular function, say $\phi \in C^{\infty}$ on the real positive axis, having a non degenerate maximum at an interior point $x_0 \in (a, b)$, i.e. $\phi'(x_0) = 0$ with $\phi''(x_0) \neq 0$ and $\phi''(x_0) < 0$. We can then perform the Taylor expansion of the function ϕ in a neighbourhood $U(x_0)$ of x_0 obtaining:

$$\phi(x) = \phi(x_0) + \phi''(x_0)\frac{(x-x_0)^2}{2} + o\left((x-x_0)^2\right)$$

It follows, see e.g. Ch.4 of [dB81] and [Foc54], that the main contribution to (4.1) comes from its evaluation $U(x_0)$, (due to its regularity, the function g(x) is almost constant near x_0 in such a way that we can replace it by its value at x_0). Extending the remaining integral to the whole real line and using the well known *Standard Gaussian Integral*, we obtain the main term of the asymptotics² for (4.1) when $\lambda \to +\infty$:

$$I(\lambda) \asymp \sqrt{\frac{2\pi}{-\lambda \phi''(x_0)}} g(x_0) e^{\lambda \phi(x_0)}$$
(4.4)

The idea on which the above is based goes back Laplace, namely if we have to evaluate an integral like $\int_a^b f(x,t)dx$ where the graph of f, considered as a function of x, has, somewhere in the interior of (a, b), a peak and that the contribution of some neighbourhood of the peak is almost equal to the whole integral when t is *large*, then we can try to approximate f by a suitable polynomial expression in that neighbourhood. Of course if we are able to perform better asymptotic expansions of the integrand, i.e. obtain more information from the asymptotic behaviour of ϕ for $x \to x_0$, then we could hope to recover more information about (4.1) when λ goes to infinity. To reach this goal let us consider the following general case:

$$I(\lambda) = \int_{-\infty}^{+\infty} g(x)e^{\lambda\phi(x)}dx$$
(4.5)

²In what follows we use the symbol \approx to relate two quantities that have the same limit.

with $ge^{\lambda\phi}$ Lebesgue integrable on the real line, $\lambda \in \mathbb{R}$, and let us assume, for semplicity, that $\phi(x)$ is the sum of a convergent power series:

$$\phi(x) = \sum_{n \ge 2} a_n x^n$$

in a neighbourhood of $x_0 = 0$, with $a_2 < 0$ and g is only an integrable function which is, as far as the interval $-\delta \leq x < \delta$ with $\delta > 0$ is concerned, is equal to the sum of the following convergent power series:

$$g(x) = \sum_{n \ge 0} b_n x^n \qquad b_n \in \mathbb{R}$$

We assume in addition that both power series are still absolutely convergent if $|x| = \delta$. In order to have negligible contributions from integrating over the intervals $(-\infty, -\delta), (\delta, +\infty)$ we assume³ that, for each positive integer M and for $\lambda \to +\infty$, we have:

$$\int_{-\infty}^{-\delta} g(x)e^{\lambda\phi(x)}dx = O(\lambda^{-M}), \quad \int_{\delta}^{+\infty} g(x)e^{\lambda\phi(x)}dx = O(\lambda^{-M})$$
(4.6)

Moreover we assume, without loss of generality, the existence of a positive number η such that⁴:

$$\phi(x) \le \eta x^2 \qquad (-\delta \le x \le \delta) \tag{4.7}$$

Considering $e^{\lambda a_2 x^2}$ as the main factor of (4.5) we have that the remainder:

$$S(\lambda x, x) \equiv g(x)e^{\lambda x^3(\sum_{i\geq 3}a_ix^{i-3})}$$
(4.8)

can be expanded in double power series in the two arguments λx^3 and x, which is convergent for $|x| \leq \delta$ and for all values of λx^3 . Thus:

$$S(\lambda x^3, x) = \sum_{m \ge 0} \sum_{n \ge 0} c_{mn} (\lambda x^3)^m x^n \quad ; \quad \mid x \mid \le \delta , \ \lambda \in \mathbb{R}$$

It is possible to uniformly approximate S by its partial sums restricting λx^3 to some bounded interval, e.g. we perform the power expansion if $|x| \leq T \equiv \lambda^{-\frac{1}{3}}$ and we may assume that $\lambda > \delta^{-3}$, whence $T \leq \delta$. It can be shown, see e.g. [dB81], that the contributions that come from integrating over $(-\delta, -T)$ and (T, δ) are negligible, moreover if $\eta > 0$ we have:

$$\int_{T}^{\infty} e^{-\eta\lambda x^{2}} dx = O\left(e^{-\eta\lambda^{\frac{1}{3}}}\right) , \qquad (4.9)$$

 $^{^{3}}$ We use this assumption for carrying on our calculations, without discussing when it can be implemented.

⁴This is not a restriction since the validity of this estimate can be proved on the basis that $\phi'(0) = 0$ using if necessary a smaller δ .

4.1 One dimensional Laplace Method

for some $\lambda > 0$.

The estimate (4.9) can be generalized in order to have, for $\lambda > 1$ and $N \ge 0$, that the following holds⁵:

$$\int_{T}^{\infty} e^{-\eta\lambda x^2} x^N dx = O\left(e^{-\frac{1}{2}\eta\lambda^{\frac{1}{3}}}\right)$$
(4.10)

Using (4.7), (4.10) and the fact that g is bounded in $-\delta \le x \le \delta$, it follows that for $\lambda > \delta^{-3}$:

$$\int_{T}^{\infty} g(x)e^{\lambda\phi(x)}dx + \int_{-\delta}^{-T} g(x)e^{\lambda\phi(x)}dx = O\left(e^{-\eta\lambda^{\frac{1}{3}}}\right)$$
(4.11)

Hence we are left with the contribution that comes from integrating over the interval (-T, T)where we will approximate S by its partial sums S_N . We choose a positive integer N and write:

$$S_N(\lambda x^3, x) = \sum_{\substack{m,n \ge 0 \\ m+n \le N}} c_{mn} (\lambda x^3)^m x^n$$
(4.12)

Then if $|x| < \delta$ we have, uniformly with respect to x and λ :

$$S - S_N = O((\lambda x^3)^{N+1}) + O(x^{N+1})$$
(4.13)

Equation (4.13) follows from the fact that if we have a double power series of the form:

$$\sum_{m,n\geq 0} c_{mn} z^m w^n \; ,$$

which converges for |z| < 2R and |w| < 2S, then the terms c_{mn} are bounded, i.e. :

$$c_{mn} = O\left(R^{-m}S^{-n}\right)$$

Therefore if $|z| < \frac{R}{3}$ and $|w| < \frac{S}{3}$, we have⁶:

$$\sum_{\substack{m,n \ge 0 \\ m+n > N}} c_{mn} z^m w^n = O\left(\sum \left|\frac{z}{R}\right|^m \left|\frac{w}{S}\right|^n\right) = O\left(\sum_{k=N+1}^{\infty} \left(\left|\frac{z}{R}\right| + \left|\frac{w}{S}\right|\right)^k\right) = O\left(\left(\left|\frac{z}{R}\right| + \left|\frac{w}{S}\right|\right)^{N+1}\right) = O\left(\left(|z| + |w|\right)^{N+1}\right) = O\left(\left(|z|^{N+1}\right) + O\left(|w|^{N+1}\right)$$

$$= O\left(\left(|z| + |w|\right)^{N+1}\right) = O\left(|z|^{N+1}\right) + O\left(|w|^{N+1}\right)$$

By (4.10), for fixed N and $\lambda \to +\infty$, we have:

$$\int_{-\infty}^{+\infty} S_N e^{\lambda a_2 x^2} dx - \int_{-T}^{+T} S_N e^{\lambda a_2 x^2} dx = O\left(\lambda^N e^{\frac{a}{2}a_2\lambda^{\frac{1}{3}}}\right) , \qquad (4.15)$$

 $^{^{5}}$ See Ch.4 Sec.4 of[dB81].

⁶The estimate is not uniform in N, for more details see Ch.4 Sec.4 [dB81].
a_2 being a negative constant⁷. Combining previous results we have that for all positive integers M the following estimate holds for $\lambda \to +\infty$:

$$\int_{-\infty}^{+\infty} g(x)e^{\lambda\phi(x)}dx - \int_{-\infty}^{+\infty} S_A e^{\lambda a_2 x^2} dx = O(\lambda^{-M}) + O(\int_{-\infty}^{+\infty} e^{\lambda a_2 x^2} (|\lambda x^3|^{N+1} + |x|^{N+1}) dx) ,$$

where the last O - term is $O(\lambda^{-\frac{1}{2}N-1})$, see Ch.4 Sec.1 of [dB81]. Hence, for $\lambda \to +\infty$ we have:

$$\int_{-\infty}^{\infty} g(x) e^{\lambda \phi(x)} dx = \sum_{\substack{m \ge 0, n \ge 0 \\ m+n \le N}} c_{mn} \epsilon_{mn} \lambda^{-\frac{1}{2}(m+n+1)} (-a_2)^{-\frac{1}{2}(3m+n+1)} \Gamma\left(\frac{1}{2}(3m+n+1)\right) + O(\lambda^{-\frac{1}{2}N-1}) + O(\lambda^{-M}) ,$$

where:

$$\epsilon_{mn} \equiv \begin{cases} 1 & \text{if } m+n \text{ is even} \\ 0 & \text{if } m+n \text{ is odd} \end{cases}$$

Since N, M are arbitrary we obtain the following asymptotic series for $\lambda \to +\infty$:

$$\int_{-\infty}^{+\infty} g(x)e^{\lambda\phi(x)}dx = \sum_{k\geq 0} \alpha_k \lambda^{-\frac{1}{2}-k}$$
(4.16)

where we have defined:

$$\alpha_k \equiv (-a_2)^{-k-\frac{1}{2}} \sum_{m=0}^{2k} c_{m,2k-m} (-a_2)^{-m} \Gamma\left(m+k+\frac{1}{2}\right)$$

It is easy to see that the main term, namely $\alpha_0 \lambda^{-\frac{1}{2}}$, equals $g(0)(-\frac{2\pi}{\lambda\phi''(0)})^{\frac{1}{2}}$. We can achieve the same result as before relaxing the assumption that the functions g, ϕ are analytic. Actually in order to have (4.16) it is sufficient that the following relations hold⁸:

$$g(x) \asymp \sum_{n \ge 0} b_n x^n \quad ; \quad \phi(x) \asymp \sum_{n \ge 2} a_n x^n \quad , \quad (x \to 0)$$

4.2. Multidimensional Laplace Method

What we have discussed in section (4.1) can be generalized to the multi-dimensional case in a rather direct manner. Let us start considering the following multiple integral:

$$I(\lambda) = \int_{J_1} \cdots \int_{J_n} e^{\lambda \phi(x_1, \dots, x_n)} dx_1 \cdots dx_n$$
(4.17)

 $^{^7 \}mathrm{See}$ Ch.4 Sec.1 of [dB81].

⁸See Ch.4 Sec.4 of [dB81].

where $\{J_i : i = 1, ..., n\}$ is a collection of bounded open intervals of \mathbb{R} and ϕ is a continuous function in the set $J \equiv J_1 \times J_2 \times \cdots \times J_n$. Without loss of generality we can assume that:

- (i) $J_i = (-1, 1)$ for each index i = 1, ..., n
- (ii) $\phi(0, \ldots, 0) = 0$
- (iii) $\phi(x_1,\ldots,x_n) < 0$ for all points in $J (0,\ldots,0)$
- (iv) all second order derivatives of ϕ exist and are continuous in a neighbourhood of the origin
- (v) the maximum of ϕ at the origin is of elliptic type

namely we can write:

$$\phi(x_1, \dots, x_n) = -\frac{1}{2} \sum_{i,j=1}^n a_{ij} x_i x_j + o\left(\sum_{i=1}^n x_i^2\right)$$

where the quadratic form defined by (a_{ij}) is strictly positive definite.

Remark 4.2.1. Assumption (i) can be obtained by scaling. Assumption (ii) is achieved shifting the critical point to the origin. Assumptions (iii) to (v) state that the origin is a local maximum for the function ϕ .

Under the above assumptions we can apply the same strategy as we have seen in the previous section in order to have:

$$I(\lambda) \asymp I\lambda^{-\frac{1}{2}n} \qquad (\lambda \to +\infty)$$

where:

$$I \equiv \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} e^{-\frac{1}{2}\sum_{i,j=1}^{n} a_{ij}x_ix_j} dx_1 \cdots dx_n$$
(4.18)

This is a standard type of non degenerate Gaussian integral and a well known calculation, see e.g. [Pra03], shows that:

$$I = \frac{(2\pi)^{\frac{n}{2}}}{\sqrt{\mid (a_{ij}) \mid}}$$

where $|(a_{ij})|$ is the determinant of the matrix (a_{ij}) (which is strictly positive by above assumption). Moreover if ϕ admits an expansion into powers of x_1, \ldots, x_n we have asymptotic results which correspond to those obtained in the 1-dimensional case, see Sec.(4.1) Eq.(4.16).

4.2.1. Detailed Multidimensional Laplace Method

We want to study the n – dimensional integral defined on a bounded simply connected subset $D \subset \mathbb{R}^n$:

$$I(\lambda) \equiv \int_{D} e^{\lambda \phi(x)} g_0(x) dx \tag{4.19}$$

when $\lambda \to +\infty$. We assume that the region *D* possesses a smooth boundary $\Gamma \equiv \partial D$, i.e. Γ is an (n-1) – dimensional hypersurface. We also assume that the amplitude function g_0 and the phase function ϕ are as smooth as we need below.

Let us define the Hessian matrix of ϕ by:

$$H = \left(\frac{\partial^2 \phi}{\partial x_i \partial x_j}\right)_{i,j} \qquad \text{where } i, j = 1, \dots, n$$

and assume that the quadratic form defined by H is negative definite in a neighbourhood of x_0 . Hence there exists an orthogonal matrix Q which diagonalizes H, i.e. such that:

$$Q^T H Q = (\lambda_1, \dots, \lambda_n) \cdot I_n$$

where $\lambda_1, \ldots, \lambda_n$ are the eigenvalues of H and I_n is the $n \times n$ unitary matrix. Let us define the following change of coordinates:

$$(x - x_0) \xrightarrow{\psi} \langle Q \cdot \left(\left(\sqrt{\alpha_1}, \dots, \sqrt{\alpha_n} \right) \cdot I_n \right)^t, z \rangle , \qquad (4.20)$$

where $\alpha_i \equiv |\lambda_i|^{-\frac{1}{2}}$ for $i = 1, \dots, n$, and:

$$\xi_i = h_i(z) \qquad \forall i \in \{1, \dots, n\}$$

$$(4.21)$$

where h_i are such that $h_i = z_i + o(|z|)$ for $z \to 0, i = 1, ..., n$ and:

$$\frac{1}{2}\sum_{i}h_i^2 = \phi(x_0) - \phi(x(z)) \equiv f$$

hence, near z = 0 we have that $f(z) \sim \frac{1}{2}z^2$. Since we have that x_0 is the only point in D such that $\nabla \phi$ vanishes, then

$$J(\xi) = \frac{\partial x}{\partial \xi} \qquad x = (x_1, \dots, x_n) \ \xi = (\xi_1, \dots, \xi_n)$$

is positive definite in all the image \hat{D} of the domain D under the action of the previous transformations ψ and h, moreover we have:

$$J(0) = \frac{1}{\sqrt{\| | H(x_0) | \|}}$$

where $\| \mid H(x_0) \mid \|$ is the absolute value of the determinant of the Hessian matrix H of ϕ , evaluated at $x = x_0$. The quantity in (4.19) can be rewritten as follows:

$$I(\lambda) = e^{\lambda \phi(x_0)} \int_{\hat{D}} G_0(\xi) e^{-\frac{\lambda}{2}\xi^2} d\xi$$
(4.22)

where $G_0(\xi) \equiv g_0(x(\xi))J(\xi)$ Let us define the following set of functions:

$$H_{1} \equiv \xi_{1}^{-1} \left(G_{0}(\xi_{1}, \dots, \xi_{n}) - G_{0}(0, \xi_{2}, \dots, \xi_{n}) \right)$$
$$H_{2} \equiv \xi_{1}^{-1} \left(G_{0}(0, \xi_{2}, \dots, \xi_{n}) - G_{0}(0, 0, \xi_{3}, \dots, \xi_{n}) \right)$$
$$\vdots$$
$$H_{n} \equiv \xi_{n}^{-1} \left(G_{0}(0, \dots, 0, \xi_{n}) - G_{0}(0, \dots, 0) \right)$$

and $H_0 \equiv (H_1, \ldots, H_n)$ in such a way that:

$$G_0(\xi) = G_0(0) + \xi \cdot H_0$$

Using the theorem of divergence up to M times and observing that the boundary terms, i.e. the ones which comes from integrating on $\partial \hat{D}$, are exponentially small in λ , we have:

$$I(\lambda) \asymp e^{\lambda \phi(x_0)} \left[\sum_{j=0}^{M-1} \frac{G_j(0)}{\lambda} \int_{\hat{D}} e^{-\frac{\lambda}{2}\xi^2} d\xi + \frac{1}{\lambda^M} \int_{\hat{D}} G_M(\xi) e^{-\frac{\lambda}{2}\xi^2} d\xi \right]$$

where we have recursively defined the functions:

$$G_j(\xi) \equiv G_j(0) + \xi \cdot H_j(\xi) \quad , \quad G_{j+1}(\xi) = \nabla H_j(\xi)$$

Hence we have an asymptotic expansion of $I(\lambda)$ in M terms when $\lambda \to +\infty$ with respect to the asymptotic sequence of contributions:

$$\left(\frac{1}{\lambda}\right)^{j} e^{\lambda\phi(x_{0})} \int_{\hat{D}} e^{-\frac{\lambda}{2}\xi^{2}} d\xi \qquad \forall j \in \mathbb{N}$$

$$(4.23)$$

Previous result is improved by the following proposition:

Proposition 4.2.1. Let $\xi = 0$ be an interior point of D, then, as $\lambda \to +\infty$:

$$\int_{D} e^{-\frac{\lambda}{2}\xi^{2}} d\xi = \left(\frac{2\pi}{\lambda}\right)^{\frac{n}{2}} + o\left(\left(\frac{1}{\lambda}\right)^{m}\right)$$

for any m.

Proof 4.2.1. Let r_1, r_2 be positive constants such that $B_{r_1}(0) \subset \hat{D} \subset B_{r_2}(0)$. Then for $\lambda > 0$:

$$\int_{B_{r_1}} e^{-\frac{\lambda}{2}\xi^2} d\xi \le \int_{\hat{D}} e^{-\frac{\lambda}{2}\xi^2} d\xi \le \int_{B_{r_2}} e^{-\frac{\lambda}{2}\xi^2} d\xi$$

$$(4.24)$$

Since:

$$\int_{B_{r_2}} e^{-\frac{\lambda}{2}\xi^2} d\xi = \left(\frac{2}{\lambda}\right)^{\frac{n}{2}} \left(\frac{2(\pi)^{\frac{n}{2}}}{\Gamma\left(\frac{n}{2}\right)}\right) \int_{0}^{r_2\sqrt{\frac{\lambda}{2}}} e^{-r^2} r^{n-1} dr$$
(4.25)

then we have the following upper bound:

$$\int_{B_{r_2}} e^{-\frac{\lambda}{2}\xi^2} d\xi \le \frac{2\left(\frac{2\pi}{\lambda}\right)^{\frac{n}{2}}}{\Gamma\left(\frac{n}{2}\right)} \int_0^\infty e^{-r^2} r^{n-1} dr = \left(\frac{2\pi}{\lambda}\right)^{\frac{n}{2}}$$
(4.26)

while:

$$\int_{B_{r_1}} e^{-\frac{\lambda}{2}\xi^2} d\xi = \left(\frac{2}{\lambda}\right)^{\frac{n}{2}} \frac{2}{\Gamma\left(\frac{n}{2}\right)} \left[\int_{0}^{\infty} e^{-r^2} r^{n-1} dr - \int_{r_1\sqrt{\frac{\lambda}{2}}}^{\infty} e^{-r^2} r^{n-1} dr\right]$$
(4.27)

Hence if $r_1\sqrt{\frac{\lambda}{2}} > 1$ and $n \ge 2$, we have:

$$\int_{B_{r_1}} e^{-\frac{\lambda}{2}\xi^2} d\xi \ge \left(\frac{2\pi}{\lambda}\right)^{\frac{n}{2}} \left[1 - \frac{e^{r_1^2 - \frac{\lambda}{2}}}{\Gamma\left(\frac{n}{2}\right)}\right]$$
(4.28)

Using equations (4.24), (4.26) and (4.28), we have, for λ sufficiently large, that:

$$\left(\frac{2\pi}{\lambda}\right)^{\frac{n}{2}} \left[1 - \frac{e^{r_1^2 - \frac{\lambda}{2}}}{\Gamma\left(\frac{n}{2}\right)}\right] \le \int_{\hat{D}} e^{-\frac{\lambda}{2}\xi^2} d\xi \le \left(\frac{2\pi}{\lambda}\right)^{\frac{n}{2}}$$
(4.29)

which concludes the proof of Prop. (4.2.1).

Prop. (4.2.1) implies that:

$$I(\lambda) \approx e^{\lambda \phi(x_0)} \sum_{j=0}^{M-1} (2\pi)^{\frac{n}{2}} \frac{G_j(0)}{\lambda^{\frac{n}{2}+j}}$$
(4.30)

In order to obtain an expression for (4.30) which can be as explicit as possible we observe that:

$$G_j(0) = \frac{1}{2^j} \Delta_{\xi}^j G_0 \mid_{\xi=0}$$
(4.31)

where we set $\Delta_{\xi} \equiv \sum_{i=1}^{n} \frac{\partial^2}{\partial \xi_i^2}$, in fact, recalling the definition of the functions $G_j(\xi)$ we have that:

$$\Delta_{\xi}^{j} G_{0} \mid_{\xi=0} = 2j \Delta_{\xi}^{j-1} G_{1} \mid_{\xi=0} = 2^{2} j(j-1) \Delta_{\xi}^{j-1} G_{2} \mid_{\xi=0} = \cdots = 2^{j} j! \Delta_{\xi}^{0} G_{j} \mid_{\xi=0} = 2^{j} j! G_{j} \mid_{\xi=0} (4.32)$$

Hence we can rewrite the expansion in (4.30) as follows:

$$I(\lambda) \approx e^{\lambda \phi(x_0)} \left(\frac{2\pi}{\lambda}\right)^{\frac{n}{2}} \sum_{j=0}^{M-1} \frac{\Delta_{\xi}^j G_0}{((j!)2\lambda)^j}$$
(4.33)

where:

$$\Delta_{\xi}^{0} G_{0} \mid_{\xi=0} = G_{0}(0) = \frac{g_{0}(x_{0})}{\sqrt{\parallel \mid H(x_{0}) \mid \parallel}}, \qquad (4.34)$$

From (4.33) and (4.34) we have that the leading term of our expansion reads:

$$I(\lambda) \approx \frac{e^{\lambda \phi(x_0)}}{\sqrt{\| | | H(x_0) | \|}} \left(\frac{2\pi}{\lambda}\right)^{\frac{n}{2}} g_0(x_0)$$

Remark 4.2.2. In Ch.(1) Sec.(1.2.1) the above described method for detailed expansions of Laplace type integrals is applied in order to study the Crystal problem.

Previous results are very useful not only for the study of systems of classical particles at low temperature, but also in many questions of probability theory such as, for example, when we have to deal with *large deviations*, see e.g. [Ell85, DS84]. In these cases more general assumptions are made but instead of asymptotic formulae like the one in (4.33) are one limit oneselve in controlling only the first terms of the expansions of interest.

In particular let us consider the following integral:

$$I(\lambda) \equiv \int_{D} g(x) e^{\lambda \phi(x)} dx$$

where g has compact support and ϕ is a continuous function, and define the domain:

$$\mathscr{D}_{c} \equiv \left\{ x \in \mathbb{R}^{n} : x \in supp (g), \phi(x) \ge \max_{x \in supp (g)} \{\phi(x) - c\} \right\} ,$$

where c is a positive constant. We have that:

$$\lim_{\lambda \to \infty} \frac{\ln I(\lambda)}{\lambda} = \max_{x \in supp (g)} \{\phi(x) - c\}$$

Moreover if the following condition holds, with $V(c) \equiv Vol(\mathscr{D}_c)$:

$$\lim_{c \to 0^+} \frac{\ln V(c)}{\ln c} = \alpha > 0$$

then:

$$\lim_{\lambda \to \infty} \ln I(\lambda) = \max_{x \in supp \ (g)} \{\phi(x) - c\}\lambda - \alpha \ln \lambda + o(\ln \lambda)$$
(4.35)

and the converse is also true provided V(0) = 0. Hence we have a rough, but simply, method to express the leading term for the asymptotics of the partition function of, let say, a classical system of n- particles interacting via a polynomial potential in a bounded box. In fact, see Ch.(1) Sec.(2) of [Fed89], if $\phi(x)$ is a polynomial then (4.35) holds.

4.3. Boundary Maximum Point

Let us return to discuss the asymptotics of the integral:

$$I(\lambda) = \int_{D} g(x)e^{\lambda\phi(x)}dx$$
(4.36)

for $\lambda \to +\infty$, where *D* is a bounded simply connected domain in \mathbb{R}^n such that $\Gamma \equiv \partial D$ is a (n-1)-dimensional hypersurface. Suppose that ϕ has a unique maximum point in $D \cup \Gamma$ and that this point belongs to Γ . In order to obtain the detailed asymptotics of (4.36) for $\lambda \to +\infty$ let us start with n = 2. In this case Γ is a smooth curve in \mathbb{R}^2 parametrized by:

$$(x_1(t), x_2(t))$$
 for $t \in [0, T]$ (4.37)

and we assume that, as t increases, Γ is run in the counterclock sense. Let us first suppose that $\nabla \phi \neq 0$ in $D \cup \Gamma$, and let $(x_1(0), x_2(0)) = x_0 \in \Gamma$ be the only maximum of ϕ in $D \cup \Gamma$. Then:

$$\nabla \phi \cdot \Gamma \mid_{t=0} = 0 \tag{4.38}$$

hence $\nabla \phi$ is normal to Γ at $x = x_0$. Taking $N(t) \equiv (\dot{x}_1(t), \dot{x}_2(t))$ we have⁹:

$$\nabla \phi(x_0) = | \nabla \phi(x_0) | N(0) \tag{4.39}$$

In the one dimensional case we have that if $\phi'(x) \neq 0 \quad \forall x \in D$ then the asymptotics is obtained integrating by parts, see e.g. Ch. 3 of [BH86]. A similar method can be used in the multidimensional scenario. Let us start with the 2 - dimensional case defining:

$$H_0 = g_0 \frac{\nabla \phi}{|\nabla \phi|^2} \tag{4.40}$$

with $g_0 \equiv g$. The divergence theorem gives:

$$I(\lambda) = \frac{1}{\lambda} \oint_{\Gamma} e^{\lambda \phi} H_0 \cdot N ds - \frac{1}{\lambda} \int_{D} e^{\lambda \phi} g_1 dx$$
(4.41)

⁹N(t) is the unit outward vector to Γ .

4.3 Boundary Maximum Point

where $g_1 \equiv \nabla \cdot H_0$. If we define:

$$J(\lambda) = \frac{1}{\lambda} \oint_{\Gamma} e^{\lambda \phi} H_0 \cdot N ds$$
(4.42)

then we define $\psi(t) \equiv \phi(x(t))$ and using Laplace's formula given in Eq. (5.2.1) of [BH86], with ϕ set equal to $-\psi$, we have¹⁰:

$$J(\lambda) \approx e^{\lambda \phi(x_0)} \sqrt{\frac{2\pi}{\lambda^3 \mid \phi''(0) \mid}} \left(H_0 \cdot N\right) \mid_{t=0}$$

$$(4.43)$$

Here we have assumed that t = 0 is a simple maximum point for ψ so that $\psi''(0) < 0$. By the divergence theorem we have:

$$I_1(\lambda) \equiv \frac{1}{\lambda} \int_D e^{\lambda\phi} g_1 dx = \frac{1}{\lambda^2} \oint_{\Gamma} e^{\lambda\phi} H_1 \cdot N ds - \frac{1}{\lambda^2} \int_D e^{\lambda\phi} g_2 dx$$
(4.44)

where we have defined:

$$H_1 \equiv g_1 \frac{\nabla \phi}{|\nabla \phi|^2} \quad \text{and} \quad g_2 \equiv \nabla \cdot H_1$$

$$(4.45)$$

Then, using Laplace's method, we can estimate the boundary integral in (4.44), hence:

$$\frac{1}{\lambda^2} \int_D e^{\lambda \phi} H_1 \cdot N ds = O\left(e^{\lambda \phi(x_0)} \lambda^{-2}\right)$$
(4.46)

which implies that $I_1 = O\left(e^{\lambda\phi(x_0)}\lambda^{-2}\right)$ and $I(\lambda) \simeq J(\lambda)$. Using (4.43) we have for the leading term:

$$I(\lambda) \simeq e^{\lambda \phi(x_0)} \sqrt{\frac{2\pi}{\lambda^3 \mid \phi''(0) \mid}} \left(H_0 \cdot N\right) \mid_{t=0}$$

$$(4.47)$$

Turning back to the original functions ϕ and g we have¹¹ for the leading term:

$$I(\lambda) \approx e^{\lambda\phi(x_0)}g(x_0)\sqrt{\frac{2\phi}{\lambda^3}} \left[\frac{\partial^2\phi}{\partial^2 x_1} \left(\frac{\partial\phi}{\partial x_2}\right)^2 - 2\frac{\partial^2\phi}{\partial x_1\partial x_2}\frac{\partial\phi}{\partial x_1}\frac{\partial\phi}{\partial x_2} + \frac{\partial^2\phi}{\partial^2 x_2} \left(\frac{\partial^2\phi}{\partial^2 x_1}\right)^2 \mp k(x_0) \mid \nabla\phi \mid^3\right]_{\substack{x=x_0\\(4.48)}}^{-\frac{1}{2}}$$

where $k(x_0)$ is the curvature of Γ at $x = x_0$. The sign taken in (4.48) for $k(x_0)$ is a minus (resp. a plus) if Γ is convex (resp. concave).

Remark 4.3.1. If the function g and ϕ belongs to $C^N(\mathbb{R}^n)$ it is possible to write an analogous of the formulae (4.30), (4.33) given in Sec.(4.2.1).

 $^{^{10}}$ See Ch.5 of [BH86].

¹¹See Sec.8.2 of [BH86].

4.3 Boundary Maximum Point

Let us consider the asymptotics of (4.36) where now $D \subsetneq \mathbb{R}^n$. We can repeat the steps done in the 2 – dimensional case. In particular the divergence theorem gives us:

$$I(\lambda) = \frac{1}{\lambda} \int_{\Gamma} (H_0 \cdot N) e^{\lambda \phi} d\Sigma - \frac{1}{\lambda} \int_{D} g_1 e^{\lambda \phi} dx \qquad (4.49)$$

where $g_0 \equiv g$, $H_0 \equiv g_0 \frac{\nabla \phi}{|\nabla \phi|^2}$, N is the unit outward normal vector to the hypersurface $\Gamma \equiv \partial D$, $d\Sigma$ is the differential of the volume function of Γ and $g_1 \equiv \nabla \cdot H_0$. If the functions g and ϕ are sufficiently differentiable then we have the following expansion¹²:

$$I(\lambda) = -\sum_{j=0}^{M-1} (-\lambda)^{-(j+1)} \int_{\Gamma} (H \cdot N) e^{\lambda \phi} d\Sigma + \frac{(-1)^M}{\lambda^M} \int_{D} g_M e^{\lambda \phi} dx$$
(4.50)

where for all j = 1, ..., M - 1 we have defined $H_j = g_j \frac{\nabla \phi}{|\nabla \phi|^2}$ and $g_{j+1} \equiv \nabla \cdot H_j$.

Suppose that $x = x_0$ is the only absolute maximum of ϕ and it belongs to Γ , then Γ can be parametrized by a smooth function $\sigma : \mathbb{R}^{n-1} \supseteq U \to \mathbb{R}^n$, with U open and 0 belongs to the interior of U, in such a way that: $\sigma(0) = x_0$ and we have:

$$\nabla \phi \cdot \frac{\partial x}{\partial \sigma_i} \mid_0 = 0 \quad \forall i = 1, \dots, n-1$$
(4.51)

Let us define the function $\psi(\sigma) \equiv \phi(x(\sigma))$ then by (4.51) we have:

$$\nabla \psi \mid_{\mathbf{0}} = 0 \tag{4.52}$$

where now the operator ∇ is defined with respect to the parametrization function σ , i.e. $\nabla = \nabla_{\sigma}$. The condition that 0 is a maximum point for ψ is given by assuming that its Hessian matrix is negative definite:

$$\langle (\sigma_1, \dots, \sigma_{n-1}), \mathscr{H} |_0 (\sigma_1, \dots, \sigma_{n-1}) \rangle < 0 \quad , \quad \forall (\sigma_1, \dots, \sigma_{n-1}) \in U$$

$$(4.53)$$

where:

$$\mathscr{H} \equiv \left(\frac{\partial^2 \psi}{\partial \sigma_i \partial \sigma_j}\right)_{i,j=1,\dots,n-1}$$

Then in terms of the previous parametrization each term $\int_{\Gamma} (H \cdot N) e^{\lambda \phi} d\Sigma$ in the sum appearing in the expansion (4.50) contains an integral of the type studied in Sec. (4.2.1). Then the desired asymptotics for (4.36) when $\lambda \to +\infty$ is obtained expanding those addends and proving that, compared to them, the term $\int_{D} g_M e^{\lambda \phi} dx$ is asymptotically small.

Remark 4.3.2. The case where the only absolute maximum point x_0 for the function ϕ is reached on Γ but with $\Delta \phi(x_0) = 0$ is complicated by the fact that now the boundary contributions are not asymptotically negligible. In particular we have:

¹²See Sec.8.3 of [BH86].

$$I(\lambda) \approx e^{\lambda \phi(x_0)} \left[\sum_{j=0}^{M-1} \left(\frac{G_j(0)}{\lambda^j} \int_D e^{-\frac{\lambda \xi^2}{2}} d\xi - \int_{\Gamma} \left(\frac{H_j \cdot N}{\lambda^{(j+1)}} \right) e^{-\frac{\lambda \xi^2}{2}} d\Sigma \right) + \frac{1}{\lambda^M} \int_D G_M(\xi) e^{-\frac{\lambda \xi^2}{2}} d\xi \right]$$
(4.54)

where the functions H_j and G_j are defined as in Sec. (4.2.1). The proof of (4.54) was given by Jones, see [Jon82, Jon97]. For the above discussion see also [Hsu48, Hsu51].

4.4. Morse Lemma and Laplace Method

In this section we would like to study the asymptotics¹³ of:

$$\int_{\Omega} g(x)e^{\lambda\phi(x)}dx \tag{4.55}$$

for $\lambda \to +\infty$, where Ω is a d - dimensional bounded and connected domain. Let us define $\forall 1 \leq i, j \leq n$:

$$\phi'(x) \equiv \nabla \phi(x) \quad and \quad \mathscr{H}(x) \equiv \left(\frac{\partial^2 \phi(x)}{\partial x_i \partial x_j}\right)$$

We call x_0 a non degenerate stationary point for the function ϕ iff $| \mathscr{H}(x_0) | \neq 0$. Let us suppose that the maximum of ϕ on the domain Ω is reached at only one point $x_0 \in \Omega$ such that x_0 is non degenerate, then it is possible to give an asymptotic expansion of (4.55) for $\lambda \to +\infty$ which is based on the following¹⁴ lemma:

Lemma 4.4.1. (Morse Lemma) Let x_0 be a non degenerate stationary point of ϕ . Then there exists a change of variables $x \to \xi(x), \xi \in C^{\infty}$, such that:

$$\xi(0) = x_0$$
 $det [\xi'(0)] = 1$

and the function ϕ reduces locally to the form:

$$\phi(x) = \phi(x_0) + \frac{1}{2} \sum_{j=1}^n \mu_j y_j^2$$

where μ_1, \ldots, μ_n are the eigenvalues of $\mathscr{H}(x_0)$.

The Inverse Function Theorem¹⁵ allows us to conclude that the inverse function $y = \psi(x)$ is of C^{∞} class, at least in a small neighbourhood of the point x_0 . Moreover if $\phi(x)$ is an

¹³Here we shall adopt a more geometric point of view compared with the one exploited in Sec. (4.2.1).

¹⁴See e.g. [Car76, Car92] for a detailed discussion about this geometrical result.

 $^{^{15}}$ See e.g. [Car92].

analytic function at x_0 , then also ξ and ψ are analytic functions at the point y = 0 and $x = x_0$, respectively.

As we have seen during Sec.(4.2) the asymptotics for $\lambda \to +\infty$ of (4.55) equals the sum of the contributions of the points x_1, \ldots, x_m at which ϕ reaches its maximum. In particular there exists a positive constant c such that the following holds:

$$I(\lambda) = \sum_{j=1}^{m} V_{x_j} + O\left(e^{\lambda(M-c)}\right)$$
(4.56)

where $M \equiv \max_{x \in \Omega} \phi(x)$, and for $j = 1, \dots, m$:

$$V_{x_j} \equiv \int_{U(x_j)} g(x) e^{\lambda \phi(x)} dx$$
(4.57)

is the contribution coming from integrating over a small neighbourhood $U(x_j)$ of x_j . Eq. (4.56) is the *Localization Principle*¹⁶ and can be viewed as an analogous of the *Residue Theorem*. Hence we can assume that the domain of integration Ω itself is a small neighbourhood of x_0 and by Morse lemma (4.4.1) we reduce (4.55) to the following form:

$$e^{-\lambda\phi(x_0)}I(\lambda) = \int_{V} \tilde{g}(y)e^{\frac{\lambda}{2}\sum_{j=1}^{n}\mu_j y_j^2} dy$$
(4.58)

where $\tilde{g}(0) = g(x_0)$. If we choose the original neighbourhood of x_0 so that V is a cube with $supp(\tilde{g}) \subset V$, then the integral in (4.58) can be treated applying the one-dimensional Laplace method sequentially with respect to the variables y_1, \ldots, y_n .

Proceeding as above we can prove the following¹⁷:

$$I(\lambda) = \left(\frac{2\pi}{\lambda}\right)^{\frac{n}{2}} (\| \| \mathscr{H}(x_0) \| \|)^{-\frac{1}{2}} \left[g(x_0) + O(\lambda^{-1})\right] e^{\lambda \phi(x_0)}$$
(4.59)

in the sector S_{ϵ} defined in (4.2), moreover the following expansion holds:

$$I(\lambda) = e^{\lambda \phi(x_0} \lambda^{-\frac{n}{2}} \sum_{k=0}^{\infty} C_k \lambda^{-k}$$

where the coefficients C_k are functions of the functions g and ϕ , assumed to be smooth, at the point $x = x_0$.

In the case where ϕ attains its maximum at a boundary point¹⁸, namely at a certain $x_0 \in \partial\Omega$, and with the same regularity assumptions on both g and ϕ we proceed as follows. From the smoothness of $\partial\Omega$ we can parametrize it at least in a neighbourhood U_{x_0} of the point

¹⁶See e.g.[Fed89] Sec.2.1.

 $^{^{17}}$ See e.g. Ch.1 of [Com82].

¹⁸In what follows we will assume that Ω has a sufficiently smooth boundary. For more detail see e.g. [LP79].

 x_0 by a smooth map $\xi : U_0 \subsetneq \mathbb{R}^{n-1} \to U_{x_0}$ which expresses the local coordinates of $U_{x_0} \cap \partial \Omega$ as functions of the (n-1)-dimensional parameters vector $\xi \equiv (\xi_1, \ldots, \xi_{n-1}) \in U_0$, namely $x_j = x_j(\xi) \quad \forall j = 1, \ldots, n$. Then, for each parameter ξ_j , the vector $v_j = (v_j^k) = \left(\frac{\partial x_j}{\partial \xi^k}\right)$, where $k = 1, \ldots n - 1$, is an element of the tangent space to $\partial \Omega$ at the point x_0 . Using again the smoothness of $\partial \Omega$ it is possible to define a *normal derivative* to $\partial \Omega$ at each of its points, hence the distance d = d(x) of a point x from $\partial \Omega$ is well defined and by the latter $\partial \Omega$ is characterized to be the *locus* of the point x with $d(x) = 0 = d(x(\xi))$ for all $\xi \in U_0$, while for any other point $y \in \Omega - \partial \Omega$ we have d(y) > 0. As a consequence we obtain that the vector field:

$$n \equiv \frac{\left(\frac{\partial d}{\partial x_i}\right)}{\mid \left(\frac{\partial d}{\partial x_i}\right) \mid}$$

is orthonormal¹⁹ to each element of the tangent bundle of $\partial\Omega$. Given a certain point $x \in \partial\Omega$ we choose n(x) as the inward, normalized, normal vector with respect to the tangent space $T_x\partial\Omega$. By Taylor's theorem ϕ can be expanded as follows in a neighbourhood of a non degenerate boundary maximum point:

$$\phi(x) = \phi(x_0) + (\partial_n \phi(x_0)) n + \frac{1}{2} (\partial_n^2 \phi(x_0)) n^2 + (\partial_n \partial_\xi \phi(x_0)) \cdot (\xi - \xi_0) n + \frac{1}{2} (\xi - \xi_0) \cdot (\partial_\xi^2 \phi(x_0)) (\xi - \xi_0) + o(|\xi - \xi_0|^3)$$

where x_0 is such that $x(\xi_0) = x_0$. Using this expansion for ϕ we replace the integral $I(\lambda)$ by a corresponding one performed on a smaller neigbourhood of x_0 . Then we use as integration variables the set of couples $\{(\xi_k, n) : k = 1, ..., n - 1\}$ instead of the x_i 's and neglet the third order terms in the latter Taylor series. As before we also replace g by $g_0 \equiv g(x_0)$ and extend the integration to the whole $\mathbb{R}^+ \times \mathbb{R}^{n-1}$ obtaining a multidimensional, standard *Gaussian* integral. Taking $\lambda \to +\infty$, we have that:

$$I(\lambda) \approx -\lambda^{-(n+1)/2} (2\pi)^{(n-1)/2} e^{\lambda \phi(x_0)} \frac{(-\mid \partial_{\xi}^2 \phi(x_0) \mid)^{-1/2}}{(\partial_n \phi(x_0))^{-1}} J(x_0) g_0$$
(4.60)

where $J(x_0)$ is the change of variables Jacobian evaluated in x_0 . Hence we have:

Theorem 4.4.1. Let $g, \phi \in C^{\infty}(\Omega)$ and let $x_0 \in \partial\Omega$ be a nondegenerate maximum boundary point for ϕ , then, as $\lambda \to +\infty$, with $\lambda \in S_{\epsilon} \equiv \{\lambda \in \mathbb{C} : | \arg \lambda | \leq \frac{\pi}{2} - \epsilon\}$, the following asymptotic expansion holds:

$$I(\lambda) = \lambda^{-(n+1)/2} (2\pi)^{(n-1)/2} e^{\lambda \phi(x_0)} \sum_{k \ge 0} a_k \lambda^{-k}$$

with coefficients a_k which depend on the derivatives of the functions g, ϕ at $x = x_0$.

See e.g. Sec. (2.3) of [Fed77], Sec.2 of Ch.IX in [Won89] or [Jon82] for a proof of (4.60) and Th. (4.4.1).

¹⁹It easy to see that n is always a non-zero vector field in the sense that it produces non-zero orthonormal vector n(x) to each tangent vector of $w(x) \in T_x \partial \Omega$, for all $x \in \partial \Omega$.

CHAPTER 5

Stationary Phase and Saddle Point Method

5.1. Oscillatory Integrals

5.1.1. A first glance

In this section we shall consider integrals similar to those involved in the Laplace method analysis but with an oscillating term containing the phase. In particular we would like to evaluate the *accurate* asymptotics for quantities of the following type:

$$I(\lambda) \equiv \int_{J} g(x)e^{i\lambda\phi(x)}dx$$
(5.1)

when the parameter λ goes to infinity along the real line and where $J \subset \mathbb{R}$ is a connected interval of the real line. We will refer to the functions g and ϕ as amplitude and phase respectively as we made for the integrals of the type in eq.(4.1). It is straightforward to note that the growth of λ determines the fast varying of the term $e^{i\lambda\phi}$ in such a way that the contributions to (5.1) oscillate more and more, hence we expect that the greater contribution comes from neighbourhoods of the points in which ϕ has vanishing derivative. Let us recall the following

Lemma 5.1.1. (*Riemann-Lebesgue*) if $g \in L_1((a, b))$, then¹:

$$\int\limits_{a}^{b}g(x)e^{i\lambda x}dx \xrightarrow{\lambda \to \infty} 0$$

In order to obtain the asymptotics of (5.1) for $\lambda \to \infty$, let us state²:

¹See e.g. [Fed89, Sir71].

²See e.g. [Erd56, LP79, tS73].

Lemma 5.1.2. (Erdélyi Lemma) Let $\alpha \ge 1$ and $\beta > 0$. Let $g \in C^{\infty}([0, a])$ such that $g^{(n)}(a) = 0$ for all $n \in \mathbb{N}$. Then the following asymptotic expansions for $\lambda \to \infty$ holds:

$$\int_{0}^{a} x^{\beta-1} g(x) e^{i\lambda x^{\alpha}} dx = \sum_{n=0}^{\infty} C_n \lambda^{-\frac{(n+\beta)}{\alpha}}$$
(5.2)

where the coefficients C_n are given by:

$$C_n \equiv \frac{g^{(n)}(0)}{n!} \Gamma\left(\frac{n+\beta}{\alpha}\right) e^{\frac{i\pi(n+\beta)}{2\alpha}}$$

Remark 5.1.1. Previous Lemma is obtained by integrating by parts and it is still valid as $|\lambda| \rightarrow \infty$ if $arg(\lambda) \in [0, \pi]$, uniformly with respect to $arg(\lambda)$. Watson's Lemma (4.1.1), considered in Ch.(4) Sec.(4.1), can also be derived from Lemma (5.1.2).

Suppose now that $g, \phi \in C^{\infty}(J)$, where J is the interval of integration in (5.1), and let $x_0 \in (a, b) \subset J$ the unique stationary point of order n of ϕ , i.e.

$$\phi'(x_0) = \phi^{(2)}(x_0) = \dots = \phi^{(n-1)}(x_0) = 0, \qquad \phi^{(n)}(x_0) \neq 0 \quad \text{for} \quad n \ge 2$$

Then:

$$I(\lambda) = I_a(\lambda) + I_b(\lambda) + I_{x_0}(\lambda) + O\left(\lambda^{-\infty}\right)$$

where $I_a(\lambda)$ and $I_b(\lambda)$ are the boundary contributions to the asymptotics of (5.1) and can be evaluated integrating by parts, see e.g. Ch.3 of [BH86]or Sec.(1) of [Fed89]. By a suitable change of variables $x \to t$ in a neighbourhood of x_0 contained in (a, b), we reduce ϕ to the form $\phi(x_0) \pm t^n$. Then it is possible to apply Lemma (5.1.2). In particular if x_0 is a nondegenerate stationary point for ϕ , i.e. $\phi''(x_0) \neq 0$ the leading term in the asymptotics of (5.1) for $\lambda \to \infty$ is given by³:

$$I_{x_0}(\lambda) = \sqrt{\frac{2\pi}{\lambda \mid \phi''(x_0) \mid}} e^{i\lambda\phi(x_0) + \frac{i\pi}{4}\delta(x_0)} \left[g(x_0) + O\left(\lambda^{-1}\right)\right]$$
(5.3)

where $\delta(x_0) \equiv sgn(\phi''(x_0))$. Let now define the coefficients:

$$C_n \equiv e^{\frac{i\pi n}{2}\delta(x_0)} \frac{\Gamma\left(n+\frac{1}{2}\right)}{(2n)!} \left[\left(\sqrt{2\frac{(\phi(x)-\phi(x_0))\delta(x_0)}{\phi'(x)}} \right)^{-1} \frac{d}{dx} \right]^{2n} \left[\sqrt{2\frac{(\phi(x)-\phi(x_0))\delta(x_0)}{\phi'(x)}} \right]_{x=x_0}$$

then:

$$I_{x_0}(\lambda) = \frac{1}{\sqrt{\lambda}} e^{i\lambda\phi(x_0) + \frac{i\pi}{4}\delta(x_0)} \sum_{n=0}^{\infty} C_n \lambda^{-n}$$
(5.4)

³See e.g. Ch.6 Sec.(1) of [BH86] or Sec.(3.2) of [Fed89].

5.1.2. Boundary Points

A simpler case to deal with is the one in which the set of critical values for (5.1) is empty, in fact is sufficient, up to natural smoothness conditions of g and ϕ which may be refined if the integration interval is infinite, to integrate by parts to get⁴:

Theorem 5.1.1. Let $\phi'(x) \neq 0$ for all points $x \in J$, then in the sens of asymptotic series as $\lambda \to +\infty$:

$$I(\lambda) = \sum_{k \ge 0} (i\lambda)^{-(k+1)} \left(-\frac{1}{\phi'(x)} \right)^k \left(\frac{\partial}{\partial x} \right)^k \left(\frac{g(x)}{\phi'(x)} \right) e^{i\phi(x)} |_J$$

where $|_J$ indicates that we have to evaluate latter quantities with respect to the initial and final points of the interval J if it is bounded or we have to take a limit, when J is not bounded.

5.1.3. Multidimensional Case

We would like to extend previous, unidimensional, result obtained for integrals of type (5.1) to the case where J is replaced by a domain $\Omega \subset \mathbb{R}^d$, i.e. for the asymptotics of:

$$I(\lambda) = \int_{\Omega} g(x)e^{i\lambda\phi(x)}dx$$
(5.5)

Let us start recalling the following Lemma⁵:

Lemma 5.1.3. Let Ω be a connected domain in \mathbb{R}^d , $g \in C_0^{\infty}(\Omega)$ and $\phi \in C^{\infty}(\Omega)$ such that $\forall x \in supp(g)$ it holds $\nabla(\phi)(x) \neq 0$, then as $\lambda \to +\infty$:

$$I(\lambda) = O\left(\frac{1}{\lambda^{\infty}}\right)$$

Lemma (5.1.3) implies that if $g, \phi \in C^{\infty}(D \cup \partial D)$ then the main contributions to the asymptotics of (5.5) come integrating on the neighbourhoods which contain the stationary points of ϕ and on the boundary $\Gamma \equiv \partial D$. Other contributions appear if $g^{(n)}$ or $\phi^{(n)}$ have discontinuities for some $n \in \mathbb{N}$. The whole set of above mentioned points form the set of *critical points* for (5.5). Let us suppose that there exists only a finite set (x_1, \ldots, x_k) of such critical points. Then we can construct a C^{∞} partition of unity with k + 2 functions $\eta_j, j = 1, \ldots, k$ and $\eta_{\Gamma}, \tilde{\eta}$ such that, for all $j = 1, \ldots, k, x \in D \cup \Gamma$, the following conditions are satisfied:

- η_j has compact support $D_j \equiv supp(\eta_j)$
- · each critical point x_i belongs to exactly one D_i

⁴See see e.g. Ch.3 of [BH86] or Sec.(1) of [Fed89].

⁵Its proof is done by integration by parts, see e.g. Sec.(3) of [Fed89].

- $\cdot D_j \cap \Gamma = \emptyset$
- · $\eta_j \equiv 1$ at least in a neighbourhood of x_j contained in D_j

$$\cdot \sum_{j=1}^{k} \eta_j(x) + \eta_{\Gamma}(x) + \tilde{\eta}(x) = 1$$

The function η_{Γ} is identically zero in some strip close to the boundary Γ and it is equal to 1 in a smaller strip containing Γ . The function $\tilde{\eta}$ has compact support on which $\nabla \phi \neq 0^6$ Let us define the following integrals:

$$I_{x_j}(\lambda) \equiv \int_D g(x)\eta_j(x)e^{i\lambda\phi(x)}dx \quad \text{and} \quad I_{\Gamma}(\lambda) \equiv \int_D g(x)\eta_{\Gamma}(x)e^{i\lambda\phi(x)}dx \tag{5.6}$$

where, for j = 1, ..., k, $I_{x_j}(\lambda)$ expresses the contribution to (5.5) coming from the critical points x_j , while $I_{\Gamma}(\lambda)$ gives the contribution from the boundary Γ .

Applying Lemma (5.1.3) we have that⁷:

$$I(\lambda) = \sum_{j=1}^{k} I_{x_j}(\lambda) + I_{\Gamma}(\lambda) + O\left(\lambda^{-\infty}\right)$$
(5.7)

Let us consider one, say x_0 , of the stationary points $x_j, j = 1, ..., k$ and assume that x_0 is a nondegenerate critical point for ϕ . Then, for $\lambda \to \infty$, the following asymptotic expansion holds:

$$I_{x_0} = e^{i\phi(x_0)} \sqrt{\frac{1}{\lambda^n}} \sum_{m=0}^{\infty} \frac{C_m}{\lambda^m}$$
(5.8)

and the leading term is given by:

$$I_{x_0} = e^{i\phi(x_0)} \left(\frac{2\pi}{\lambda}\right)^{\frac{n}{2}} \left|\phi''(x_0)\right|^{-\frac{1}{2}} \cdot e^{\frac{i\pi}{4} sgn[\phi''(x_0)]} \left[g(x_0) + O\left(\lambda^{-1}\right)\right]$$
(5.9)

where $sgn[\phi''(x_0)]$ represents the difference between the number of positive and negative eigenvalues of the $n \times n$ square matrix $\phi''(x_0)^8$. Let us now treat the asymptotic behaviour in λ as $\lambda \to \infty$ of the quantity $I_{\Gamma}(\lambda)$. If Γ contains a nondegenerate critical point of ϕ then the result (5.9) has to be multiplied by a $\frac{1}{2}$ factor, see e.g. Sec.(3.3) of [Fed89]. If Γ does not contain stationary points of ϕ then the following result holds⁹:

$$I_{\Gamma}(\lambda) = \sum_{m=1}^{M} \int_{\Gamma} e^{i\lambda\phi(x)}\omega_m + O\left(\lambda^{-(M+1)}\right)$$
(5.10)

⁶For the general construction of a partition of unity see e.g. [BM97]. For our purpose is not essential to give explicitly such functions η 's.

⁷This is the analogous of the principle of localization stated by Eq. (4.56) in Sec. (4.4) of Ch.(4).

⁸For a proof of the results stated by (5.8) and (5.9) see e.g. Sec.(3.3) of [Fed89].

 $^{{}^{9}}See Sec.(3.3) of [Fed89].$

where $M \geq 1$ is an integer and ω_j are differential forms given, for all $j = 1, \ldots, M$, by

$$\omega_j(x) = |\nabla\phi(x)|^{-2} \sum_{m=1}^n \frac{\partial\phi}{\partial x_m} \left((L^*)^{m-1} g \right) dx_1 \wedge \dots \wedge \widehat{dx_m} \wedge \dots \wedge dx_n$$

and L^* is the transpose of the operator L defined by:

$$L\left(e^{i\lambda\phi}\right) = i\lambda e^{i\lambda\phi}$$

We would like to underline the major difference between the asymptotic analysis of integrals of the *complex oscillatory type* and of the *Laplace* type defined by eq.(4.1) or their multidimensional generalizations, relies in the fact that in the oscillatory case we have to take into account all their *critical points*, whereas in the *Laplace* case only the absolute maxima.

In fact if we consider the following:

$$I(\lambda) \equiv \int_{\mathscr{D}} g(x) e^{i\lambda\phi(x)} dx \tag{5.11}$$

where \mathscr{D} is a bounded connected domain in \mathbb{R}^n then, in order to study the behaviour of 5.11, we have to take care of:

- $\cdot \{x \in \mathscr{D} : \nabla \phi(x) = 0\}$
- · all $x \in \Gamma \equiv \partial \mathscr{D}$
- · all $x \in \mathscr{D}$ where ϕ and/or g are not smooth

Remark 5.1.2. The determination of the critical points for the phase ϕ , i.e $\nabla \phi(x) = 0$ involves, in general, solving a trascendental equation. In order to have explicit expansions often parametric methods are used, see Sec. (8.5) of [BH86].

5.1.4. Degenerate Stationary Point

In the case where the Hessian matrix of the function ϕ evaluated at the critical point x_0 is singular, i.e. it has zero eigenvalues, we cannot use the Morse lemma. As a replacement we can apply¹⁰ the following:

Lemma 5.1.4. (Splitting Lemma) Let $\phi : \mathbb{R}^n \to \mathbb{R}^n$ be a C^{∞} function and let x_0 a stationary point of ϕ such that $Rank(\mathscr{H}(x_0)) = r$ for some $r \in \mathbb{N}$, then there exists neighbourhoods U, Vof the points u = 0 and $x = x_0$ and a diffeomorphism $h : U \to V$ such that:

$$\phi(h(u)) = \sum_{i=1}^{r} \pm u_i^2 + p(u_{r+1}, \dots, u_n)$$
(5.12)

where $p: \mathbb{R}^{n-r} \to \mathbb{R}$ is a C^{∞} function.

¹⁰See [PS78] and [Dui74, Arn91].

5.1 Oscillatory Integrals

Lemma (5.1.4) splits the problem of finding the asymptotic behaviour of (5.5) in two part. The first can be treated geometrically as we made in Sec. (4.4), i.e. we use the principle of localization and the Morse lemma on a set of r variables. The second one requires a different approach. Let us consider the case in which $Rank(\mathscr{H}(x_0)) = n - 1$ and assume $\Omega = \mathbb{R}^n$ (so there are no boundary points to investigate). Let x_0 be the only critic point. Without loss of generality we can also assume that g has compact support in a neighbourhood of x_0 . Using (5.12) in (5.5) we have:

$$I(\lambda) = \int_{\Omega} \tilde{g}(u) e^{i\lambda \sum_{i=1}^{n-1} \pm u_i^2 + i\lambda p(u_n)} du$$

where \tilde{g} is the product of g and the Jacobian of the change of variables in lemma (5.1.4). The asymptotic expansion of $I(\lambda)$ in the first n-1 variables follows the way shown above using theory developed during Sec.(5.1.3) and we are left we the study of the asymptotics, for $\lambda \to +\infty$, of:

$$\int\limits_{\mathbb{R}} \bar{g}(u) e^{i\lambda p(u)} du$$

where \bar{g} is a C^{∞} function having compact support in a neighbourhood¹¹ of u = 0 and $\bar{g}'(0) = \bar{g}''(0) = 0$ and we can apply the discussion made in Sec.(4.1).

Remark 5.1.3. In [Won89], Ch.IX, Sec.4, one can find examples where the previous procedure cannot be applied, namely:

$$\phi(x_1, x_2) = x_1 x_2^2$$
 and $\phi(x_1, x_2, x_3) = \prod_{i=1}^3 x_i$

In these cases we have namely $Rank(\mathscr{H}) = 0$.

Let us consider the case in which the phase function has the following form:

$$\phi(x) = \left(\prod_{i=1}^{n} x_i^{\alpha_i}\right) \psi(x) \tag{5.13}$$

where ψ is an invertible real analytic function. By the theorem of Hironaka on the resolution of singularities, see e.g. [Ati70], every function real analytic ϕ which is not indentically zero can be represented in the form (5.13).

Without loss of generality one can assume that $\psi(x) \equiv 1$ and $supp(g) \in [-1,1]^n$. For $0 < c < \frac{1}{2}$, we have:

$$\frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \mu^{-z} \Gamma(z) e^{i\pi \frac{z}{2}} dz = e^{i\mu}$$
(5.14)

¹¹We suppose that the critic point is in 0 for the variable u.

whether μ is positive or negative. In fact since the Mellin transform of $e^{ix} = \Gamma(z)e^{\frac{iz}{2}}$, for $0 < \Re(z) < 1$ then Eq.(5.14) can be obtained using the fact that the Mellin transform of the functions:

$$Si(x) = \frac{\pi}{2} - \int_{x}^{\infty} \frac{\sin t}{t} dt$$
 and $Ci(x) = -\int_{x}^{\infty} \frac{\cos t}{t} dt$

are given by:

$$-\sin\left(\frac{2\pi}{2}\right)\frac{\Gamma(z)}{z}$$
 for $-1 < \Re(z) < 0$

and

$$-\cos\left(\frac{z\pi}{2}\right)\frac{\Gamma(z)}{z}$$
 for $0 < \mathscr{R}(z) < 1$

resepctively.

If μ is negative the principal value of μ^{-z} must be taken in (5.14). Let us define $Q_1 = [0, 1]^n$, $m \equiv \min\{\frac{1}{2}, \frac{1}{\alpha_1}, \ldots, \frac{1}{\alpha_n}\}$ and:

$$I_1(\lambda) = \int_{Q_1} g(x)e^{i\lambda x^{\alpha}} , \qquad (5.15)$$

where $\alpha = (\alpha_1, \ldots, \alpha_n)$ and $x^{\alpha} \equiv \prod_{i=1}^n x_i^{\alpha_i}$. Then, using (5.14) with $0 < c_0 < m$, we have:

$$I_1(\lambda) = \int_{Q_1} g(x) \frac{1}{2\pi i} \left(\int_{c_0 - i\infty}^{c_0 + i\infty} (\lambda x^{\alpha})^{-z} \Gamma(z) e^{i\frac{\pi}{2}} dz \right) dx$$
(5.16)

We note that the function:

$$\int_{Q_1} (x^{\alpha})^{-z} g(x) dx$$

is analytic and bounded in $\Re(z) < \delta < m$ and since $g((1, \ldots, 1)) = 0$ by partial, repeated integration, we obtain, for any multi-index $k = (k_1, \ldots, k_n)$, the following equation:

$$\int_{Q_1} (x^{\alpha})^{-z} g(x) dx = \prod_{j=1}^n \left(\prod_{i=1}^{k_j} \frac{1}{\alpha_j z - i} \right) \int_{Q_1} x^{-\alpha z + k} \mathcal{D}^k g(x) dx$$

where we have indicated by D^k the k-th derivative operator and used the fact that the poles of $\int_{Q_1} (x^{\alpha})^{-z} g(x) dx$ are at the points $\frac{i}{\alpha_j}$. The asymptotics of $I_1(\lambda)$ can be then obtained traslating the contour of integration to the right as shown in Ch.III Sec.7 of [Won89].

Suppose that $\frac{1}{\alpha_1} < \frac{1}{\alpha_j}$ for j > 1, then α_1^{-1} is a simple pole and we obtain, after calculating the corresponding residue and applying Fubini theorem to (5.16), the following equality:

$$I_{1}(\lambda) = -\lambda^{\alpha_{1}^{-1}} \Gamma\left(\alpha_{1}^{-1}\right) e^{i\frac{\pi}{2\alpha_{1}}} r(\alpha_{1}^{-1}) + \frac{1}{2\pi i} \int_{c_{1}-i\infty}^{c_{1}+i\infty} \lambda^{-z} \Gamma(z) e^{i\pi\frac{z}{2}} \int_{Q_{1}} (x^{\alpha})^{-z} g(x) dx dz$$
(5.17)

where:

$$r(\alpha_1^{-1}) = -\frac{1}{\alpha_1} \int_0^1 \cdots \int_0^1 x_2^{-\frac{\alpha_2}{\alpha_1}} x_n^{-\frac{\alpha_n}{\alpha_1}} g(0, x_2, \dots, x_n) dx_2 \cdots dx_n$$

is the residue of $\int_{Q_1} (x^{\alpha})^{-z} g(x) dx$ at the pole $z = \alpha_1^{-1}$. Since the last integral in (5.17) is $o(\lambda^{\alpha_1^{-1}})$, we have found the leading term in the asymptotic expansion of $I_1(\lambda)$ for $\lambda \to +\infty$. Such calculations can be generalized in order to have higher order terms, moreover it applies not only to the unit cube Q_1 , but also to any similar cube $\times_{i=1}^n I_i$, where each interval I_i can be equal to [0, 1] or [-1, 0]. The final asymptotics is obtained summing over all such cubes, see e.g. [Won89] Ch. IX, Sec.4.

See also e.g. [Arn91, AGZV88] for a theory of asymptotics for phase functions which are degenerate.

5.1.5. The Saddle Point Method

The Saddle Point Method is also known under other names. Some authors, depending on their scientific education, prefer to call it Method of steepest descent, some other use the term Stationary Phase Method also for this case, here after we will follow the terminology used in $[dB81]^{12}$.

Our aim is to evaluate the asymptotics of integrals of the following type:

$$I(\lambda) = \int_{\gamma} g(z) e^{\lambda \phi(z)} dz$$
(5.18)

as λ goes to infinity and where $\gamma \subset \mathbb{C}$ is a contour in a neighbourhood of which both functions g and ϕ are holomorphic. A priori we assume that γ, g, ϕ all depend on the parameter $\lambda \in \mathbb{R}$. As we will see later on problems of the type (5.18) have less direct solutions than their *real* homologous. In particular a topological discussion of the situation has to be done before any explicit calculations. Namely it will be necessary to perform an accurate discussion of the *chosen path* to evaluate (5.18) which is the flywheel to a second stage composed of more or less standard calculations that rely on the *Laplace Method*.

At very rough first level we may think of the Saddle Point Method as a way to deform the integration contour γ in such a way that the main contribution to the asymptotics of (5.18) comes from neighbourhoods of a finite number of points. In order to perform mathematically this type of argument one has to request that both functions g and ϕ are holomorphic. Once the just described operation has been done, then we are in a situation very similar to the one described in Ch.(4) Sec.(4.1).

 $^{^{12}}$ As in the case of [Din73], this is a standard reference to the asymptotic expansions subject and several parts of these two books has been extensively used writing this section.

5.1 Oscillatory Integrals

But why deforming ? Let us define:

$$f(z) \equiv g(z)e^{i\phi(z)} \tag{5.19}$$

then the answer is given by *Cauchy's Theorem* together with the following estimate which holds if the length $|\gamma|$ of the path γ is finite, and g, ϕ satisfy the regularity conditions stated before:

$$|I(\lambda)| \leq \int_{\gamma} |f(z)| |dz| \leq |\gamma| \max_{\gamma} |f(z)|$$
(5.20)

Could we get better estimates changing the path of integration ? In fact (5.20) is actually not very accurate and it is quiet natural to use the *Cauchy Theorem* in order to find a more suitable route for our integration trip. Deformed paths must have the same endpoints of the original one. Besides, the *continuous deformation process* has to be done in such a way that the subsequent paths lie, at each step, in the analyticity domain of f. Hence the challenge consist in finding a new path γ' such that ¹³ the following quantity is minimized:

$$\mid \gamma' \mid \max_{\gamma'} \mid f(z) \mid$$

It should be noticed that since the length of both γ and its deformations γ' are finite, our attention as to (5.20) has to be concentrated to the, possibly, wild variations of f with respect to even small modifications of the integration path. Therefore our strategy will be focused in discovering those paths γ' which minimize $\max_{\gamma'} | f(z) |$. Since the solution to the previous step may be not unique, we have to choose the one to which *Laplace Method* better applies. The method to complete this final step is known as *Method of Steepest Descent*.

5.1.6. Analytic Part I

In order to really develop the mathematical details of previous discussion let us recall that:

- (1) The quantities involved in (5.18) are all λ -dependent
- (2) The deformation of the path γ must be done according to the analyticity domain of the functions of interest, namely g and ϕ
- (3) The contour length $|\gamma|$ is not the important part
- (4) Since the variations of the function ϕ dramatically depend on λ and ϕ controls the behaviour of the exponential term, then we expect that ϕ dominates g

¹³We have to keep in mind that all the quantities involved in the evaluation of the asymptotics of (5.18) depend on the parameter λ , hence γ as well as γ' should be read as $\gamma(\lambda)$, $\gamma'(\lambda)$ respectively.

Finally it is realistic to work towards the achievement of an estimate of the following type:

$$|I(\lambda)| \le c(\gamma, g) \inf_{\gamma' \text{ allowable}} \left\{ \max_{z \in \gamma} e^{\lambda \mathscr{R}\phi(z)} \right\}$$
(5.21)

where γ' is an *allowable* deformation of the original integration path γ according to the discussion done in (5.1.5), while $c(\gamma, g)$ is a constant which depends only on the original contour γ and the function g. The procedure behind estimate (5.21) relies on the existence of a so called *minimax contour*, i.e. a path γ' which passes through a point z_0 in which $\Re \phi$ attains its maximum and such that this maximum be the lowest one among the maxima. If such a contour actually exists then we have:

$$|I(\lambda)| \le c(\gamma, g) e^{\lambda \mathscr{R}\phi(z_0)}$$
(5.22)

and Cauchy's theorem guarantes us that:

$$I(\lambda) = \int\limits_{\gamma'} g(z) e^{\lambda \phi(z)} dz$$

The asymptotics of this integrals for large λ can be evaluated by *Laplace Method* as discussed in Ch.(4).

Definition 5.1.1. A point $z_0 \in \mathbb{C}$ is a saddle point of $\phi : \mathbb{C} \to \mathbb{C}$ iff $\phi'(z_0) = 0$, moreover it is called simple iff $\phi''(z_0) \neq 0$.

If z_0 is an *interior* saddle point then the asymptotics of (5.18) can be evaluated¹⁴ simply by replacing the *minimax contour* γ' with a smaller arc $\gamma'' \subset \gamma'$ which still contains z_0 , then we use the analyticity of ϕ in order to perform its *Taylor expansion* in a neighbourhood $U_{z_0} \supseteq \gamma''$ and by *Laplace Method* we get:

$$I(\lambda) = \sqrt{-\frac{2\pi}{\lambda\phi''(z_0)}} e^{\lambda\phi(z_0)} \left(g(z_0) + O\left(\frac{1}{\lambda}\right)\right)$$

If z_0 is the initial point of the contour γ and $\max_{z \in \gamma} \mathscr{R}(\phi(z)) = \mathscr{R}(\phi(z_0))$ and $\phi'(z_0) \neq 0$, then, as $\lambda \to \infty$, we have ¹⁵:

$$I(\lambda) = -\frac{1}{\lambda \phi'(z_0)} e^{\lambda \phi(z_0)} \left(g(z_0) + O\left(\frac{1}{\lambda}\right) \right)$$
(5.23)

For the contribution given by Eq.(5.23) the following expansion holds:

$$I(\lambda) = e^{\lambda \phi(z_0)} \sum_{k=0}^{\infty} \frac{(-1)^k}{\lambda^{k+1}} \left(\frac{1}{\phi'(z)} \frac{d}{dx} \right)^k \frac{g(z)}{\phi'(z)} |_{z=z_0}$$
(5.24)

¹⁴The main idea is clear: one would like to translate in the complex domain notions which are developed in the real case where the Laplace Method has been established.

 $^{^{15}}$ See e.g. Sec.(4.3) of [Fed89], Sec.(5.5) of [dB81].

5.1.7. Topological Part

As we have seen in (5.1.6) the concrete evaluation of the asymptotics for (5.18) depends on finding the *minimax contour*. The latter could not exist at all so that we are forced to find a *minimax* solution for the extended problem:

$$\min_{\gamma' \text{ allowable } x \in \gamma'} \max_{x \in \gamma'} g(z) e^{\mathscr{R}\phi(z)}$$

which actually becomes a topological challenge. 16 .

Lemma 5.1.5. ¹⁷ Let $\phi : \mathbb{C} \to \mathbb{C}$ be a holomorphic function in a neighbourhood U_{z_0} of a point z_0 in which $\phi'(z_0) \neq 0$, then there exists a neighbourhood $V_{z_0} \subseteq U_{z_0}$ such that the level curves:

$$\mathscr{R}\phi(z)\mid_{V_{z_0}}=\mathscr{R}\phi(z_0)\quad;\quad\mathscr{I}\phi(z)\mid_{V_{z_0}}=\mathscr{I}\phi(z_0)$$

are analytic and orthogonal to each other at z_0 .

Lemma 5.1.6. Let z_0 be a such that $\phi^{(i)}(z_0) = 0$, $\forall i = 1, ..., n$ and $\phi^{n+1}(z_0) \neq 0$, then there exists a neibourhood U_{z_0} of z_0 in which the level curve $\Re\phi(z) = \Re\phi(z_0)$ consists of n + 1 analytic curves that intersect at z_0 dividing U_{z_0} in 2(n + 1) sectors of angular amplitude equal to $\pi(n + 1)$ in which the sign of $\Re\phi(z) = \Re\phi(z_0)$ alternates.

In order to better understand the previous lemma we turn back to (5.1.5). If we are in the simple point case ¹⁸ we know that it is possible to apply the Inverse Function Theorem in order to find a function which express the local coordinates z. In other words there exists ψ which is smooth in a neighbourhodd of 0 such that $z = \psi(w)$, $\psi(0) = z_0$, $\psi'(0) \neq 0$ and $\phi(\psi(w)) = \psi(z_0) + w^2$. Hence the curve $\Re \phi(z) = \Re \phi(z_0)$ is described by $\Re w^2 = 0$ which identifies the locus of complex points composed by two mutually orthogonal paths at z_0 , e.g. $\gamma_{\pm} \equiv (1 \pm it)$ where t run in a time interval whose length is determined by the Implicit Function Theorem. The general statement follows as shown in Sec.(4.5) of [Fed89]. See also Ch.7 of [BH86], Sec.(2.6) of [Sir71] and [dW51] where the saddle point method is treated by different techniques.

¹⁶In order to have a naive description of the following described idea, namely the *Steepest Descent Method*, a fruitful reading can be found in Ch.5 of [dB81].

¹⁷From the hypotheses it follows that $r(z) \equiv \phi(z) - \phi(z_0)$ is holomorphic in a neighbourhood of z_0 , then the *Inverse Function Theorem* applies and $\psi \equiv u + iv = r^{-1}$ is holomorphic in a neighbourhood of the origin. Therefore the arc of the level curve $\Re \phi(z) = \Re \phi(z_0)$ is defined by $\psi(0, v)$ and is analytic. Analogously for $\mathscr{I}\phi$ with respect to $\psi(u, 0)$. Orthogonality of the two level curves follows since these two curves are actually conformal maps.

¹⁸Namely $\phi'(z_0) = 0$ and $\phi''(z_0) \neq 0$.

5.2. Steepest Descent Method

Using previous definitions and lemmas let us go deeper in the concrete topological part of the Saddle Point $Method^{19}$.

Definition 5.2.1. Let ϕ be a complex valued function. A curve $\gamma : [0,T] \to \mathbb{C}$ in \mathbb{C} such that $\gamma(0) = z_0 \in \mathbb{C}$, is called curve of steepest descent of the function $\mathscr{R}\phi$ iff for all points $z \neq z_0$ in γ one has:

- (i) $\mathscr{I}\phi(z)$ is constant
- (ii) $\mathscr{R}\phi(z) < \mathscr{R}\phi(z_0)$

Proposition 5.2.1. Let $z_0 \in \mathbb{C}$, ϕ be analytic in a neighbourhood U_{z_0} such that

$$\phi^{(i)}(z_0) = 0$$
, $\forall i = 1, \dots n$ and $\phi^{(n+1)}(z_0) \neq 0$

Then there exist exactly n + 1 curves of steepest descent each of which relies in one and only one of the sectors determined by $\Re \phi(z) < \Re \phi(z_0)$

Lemma 5.2.1. Let ϕ be a holomorphic function on a finite contour γ such that the points which realize: $\max_{z \in \gamma} \mathscr{R}\phi(z)$ are neither saddle points nor endpoints of the path γ . Then there exists γ' such that:

$$\int_{\gamma} g(z) e^{\lambda \phi(z)} dz = \int_{\gamma'} g(z) e^{\lambda \phi(z)} dz$$

and

$$\max_{z \in \gamma'} \mathscr{R}\phi(z) < \max_{z \in \gamma} \mathscr{R}\phi(z)$$

5.2.1. Analytic Part II

Lemma 5.2.2. Let ϕ be an holomorphic function on γ such that $\max_{z \in \gamma} \mathscr{R}\phi(z) \geq C$, then for $\lambda \geq 1$ one has:

$$I(\lambda) = O(\lambda e^C)$$

Let us divide the considerations in two different situations, namely where we have to deal with a boundary saddle point or with an interior one:

 $^{^{19}}$ The basic idea of the steepest descent method can be found in [Rie53], see also [Deb09] for first further developments and [Olv70], where very interesting numerical estimates are obtained.

Theorem 5.2.1. (Boundary Saddle Point) Let $\gamma : [0,T] \to \mathbb{C}$ be a smooth path such that $\gamma(0) = z_0 \in \mathbb{C}$ and let g, ϕ be analytic at z_0 , with $\mathscr{R}\phi(z_0) > \mathscr{R}\phi(z)$ and $\phi'(z_0) \neq 0$, then as $\lambda \to +\infty$:

$$I(\lambda) = e^{\lambda \phi(z_0)} \sum_{k \ge 0} a_k \lambda^{-(k+1)}$$

where the coefficients a_k are defined as follows:

$$a_k \equiv -\left(-\frac{1}{\phi'(z_0)}\frac{\partial}{\partial z}\right)^k \frac{g(z)}{\phi'(z)} \mid_{z=z_0}$$

Theorem 5.2.2. (Interior Saddle Point) Let γ be a smooth curve in \mathbb{C} , $z_0 \in \gamma$, g, ϕ analytic at z_0 with $\mathscr{R}\phi(z_0) > \mathscr{R}\phi(z)$ for all $z \in \gamma$. Let $\phi'(z_0) = 0 \neq \phi''(z_0)$ and γ goes trough two different sectors in a neighbourhood of z_0 where $\mathscr{R}\phi(z) < \mathscr{R}\phi(z_0)$, then it follows, as $\lambda \to +\infty$:

$$I(\lambda) = e^{\lambda \phi(z_0)} \sum_{k \ge 0} a_k \lambda^{-(k+\frac{1}{2})}$$

In order to evaluate the coefficients a_k we use the results discussed in sections (5.1.6) and (5.1.7), in particular we know the existence of a smooth coordinates change: $z = \psi(w)$ such that $\phi(\psi(w)) = \psi(z_0) - \frac{w^2}{2}$ holds at least in a sufficiently small neighbourhood of the point z_0 . Changing integration variable in (5.18) and using the *Cauchy Theorem* in order to allowably deforming the path integration γ until the steepest descent contour has been reached, we get as $\lambda \to +\infty$:

$$I(\lambda) = e^{\lambda \phi(z_0)} \int_{I} e^{-\lambda w^2} g(\psi(w)) \psi'(w) dw + O\left(\frac{1}{\lambda}\right)$$

The analyticity of both g and ϕ allows us to write down the following Taylor expansion in terms of ψ :

$$g(\psi(w))\psi'(w) = \sum_{k\geq 0} c_k w^k$$

so that the coefficients a_k remain determined as:

$$a_k \equiv 2^{k+\frac{1}{2}} \Gamma\left(k+\frac{1}{2}\right) c_{2k}$$

One can easily merge results contained in asymptotics (5.2.1) and (5.2.2) in order to state the following *generalization* to the case of multiple *critical points*:

Theorem 5.2.3. Let $\gamma : [0,T] \to \mathbb{C}$ be a smooth contour and g, ϕ be analytic functions in a open set containing γ . Let $\max_{z \in \gamma} \mathscr{R}\phi(z)$ be attained at $\{z_j\}$ which are either $\gamma(0), \gamma(T)$ or saddle points each of which possess a contour where $\mathscr{R}\phi(z) < \mathscr{R}\phi(z_j)$, then as $\lambda \to +\infty$:

$$I(\lambda) = \sum_{z_j} I(\lambda, z_j)$$

where the single asymptotic contribution due to the point z_j is called $I(\lambda, z_j)$ and is evaluated as stated in asymptotics (5.2.1) and (5.2.2).

5.2.2. Constant Altitude Paths

What happens when the *minimax contour* contains a path of constant $\Re \phi$ -altitude ? Namely consider the following integral:

$$\int_{a}^{b} e^{\phi(z)} dz \tag{5.25}$$

where $a, b \in \mathbb{C}$ are connected by a smooth curve $\gamma : [0, T] \to \mathbb{C}$ such that $\gamma(0) = a$, $\gamma(T) = b$ and $\forall t \in [0, T]$, $\mathscr{R}\phi(\gamma t) = const$, then γ is the minimax solution. It is possible then to show that γ can be deformed so as to give a path with only a finite number of highest point, so that we have are back ²⁰ into the scenario discussed in Th.(5.2.3).

Remark 5.2.1. If we have to calculate the asymptotics of (5.1) in the case of a closed path we clearly have no contributions coming from endpoints. If the integrand function is analytic all over the path of integration, then (5.1) is obviously zero. Otherwise we proceed as follows:

If there exists a smooth transformation $\gamma \xrightarrow{\Phi} \gamma'$ of the integration path γ in a new path γ' such that γ' crosses just one saddle point which is higher than the other points of γ' and we can apply the results obtained in Sec.(5.2.1), since we have no contribution from the ending point.

If we have a closed path of the type in Sec. (5.25) we do not solve the minimum problem as it can be shown by considering e.g. ²¹ the phase function $\phi(z) \equiv z^{-2}$. In this case any circle centered in z = 0 is a curve of constant altitude which does not solve the minimum problem.

5.2.3. Precision in determing Saddle Points

If the exact determination of the saddle point of a certain phase function ϕ involved in (5.1) is not possible and/or we can be satisfied by some type of approximation²² we can perform an approximated saddle point technique. Let us start defining the range of a saddle point. If ξ is a saddle point of the function ϕ then we define the δ – range of ξ as follows:

$$\mathbf{R}_{\delta}(\xi) \equiv \left\{ z \in \mathbb{C} : \mid \phi^{(2)}(\xi) \cdot (z - \xi)^2 \mid < \delta \right\}$$

where $\delta > 0$ and $\phi^{(2)}$ indicates the second derivative of the function ϕ . If we consider the expansion:

$$\phi(z) = \phi(\xi) + \frac{1}{2}\phi^{(2)}(\xi) \cdot (z-\xi)^2 + \frac{1}{6}\phi^{(3)}(\xi) \cdot (z-\xi)^3 + o\left(|z-\xi|^3\right)$$

²¹See [dB81] Sec.(5.9).

 $^{^{20}}$ See Sec.(5.1) of [dB81] for an explicit example of this technique.

 $^{^{22}}$ See e.g. [dB81] Sec.(5.10)

and the sum $\sum_{n=3}^{\infty} \frac{1}{n!} \phi^{(n)}(\xi) \cdot (z-\xi)^n$ is small, with respect to asymptotic parameter λ , compared with the one of the second order, at least in a sufficiently small δ – range of ξ , then we can apply methods seen in Sec.(5.1.5) and the integral can be successfully compared to²³:

$$\int_{\gamma_{\xi}} e^{\phi(\xi) + \frac{\phi''(\xi)}{2}} (z - \xi)^2 dz = \sqrt{2\pi} \alpha \mid \phi''(\xi) \mid e^{\phi(\xi)}$$
(5.26)

where γ_{ξ} is defined as the axis of the saddle point and the integration is made running through γ_{ξ} in accordance with the direction in which γ crosses the saddle point.

The parameter α , which indicates the direction of γ_{ξ} is such that $|\alpha| = 1$. For the special case in which $\phi(z) = th(z)$ with h independent of the real parameter t, $h'(\xi) = 0$ and $h''(\xi) \neq 0$ see Sec.(5.7) of [dB81].

In the other case, i.e. when $\sum_{n=3}^{\infty} \frac{1}{n!} \phi^{(n)}(\xi) \cdot (z-\xi)^n$ is not small compared to the term $\frac{1}{2}\phi''(\xi) (z-\xi)^2$, it is difficult to obtain approximated asymptotics following previous procedure. This general difficulty could be caused by the presence of other saddle points in some small δ – range of ξ or by singularities of the function ϕ near ξ . An example of such a situation is discussed in Sec.(5.12) of [dB81].

5.2.4. A case in point

Let $\Omega \subset \mathbb{C}$ be simply connected, g, ϕ holomorphic in Ω and consider the following integral:

$$I(\lambda) = \int_{a}^{b} g(z)e^{\lambda\phi(z)}dz$$
(5.27)

for which we would like to find the asymptotic behaviour for large λ . Suppose that z_0 is a simple point for ϕ , then we can determine, according to the theory discussed in the previous sections, two sectors:

$$S_{\pm} \equiv 0 < |z - z_0| < \rho, \ |\arg(z - z_0) \pm \frac{\pi}{2} + \frac{1}{2} \arg \phi''(z_0)| < \frac{\pi}{2} - \delta$$

where δ is independent of λ and such that $0 < \delta < \frac{\pi}{4}$ and $\rho = \rho(\delta) > 0$ such that there are two *opposite* sectors in $B_{\rho}(z_0)$ of amplitude equal to $\frac{\pi}{2} - 2\delta$, both symmetric with respect to the axis of z_0 . In these sectors $|e^{\lambda\phi}| < |e^{\lambda\phi(z_0)}|$, i.e. $\Re\phi(z) < \Re(z_0)$. For both S_+ and S_- we have:

$$| arg(-(z-z_0)^2 \phi''(z_0)) | < \frac{\pi}{2} - 2\delta$$

hence:

$$\mathscr{R}(-(z-z_0)^2 \phi''(z_0)) > |z-z_0|^2 \cdot |\phi''(z_0)\sin(2\delta)$$

 $^{^{23}}$ See e.g. Sec.(5.10) of [dB81].

and we get:

$$\mathscr{R}\phi(z) - \mathscr{R}\phi(z_0) < -\frac{1}{2} |z - z_0|^2 \cdot \phi''(z_0)\sin(2\delta) + O(|z - z_0|^3)$$

which is negative as soon as ρ is sufficiently small. Now let $a_1 \in S_+$ and $b_1 \in S_-$ such that the path $\gamma_{a_1 \to b_1}$ joining these two points is still in Ω . Then we can replace $\gamma_{a_1 \to b_1}$ by a new path which is composed by the following three parts:

- $(\gamma_1) \ a_1 \to a_2$ such that the final point a_2 belongs to the axis inside S_+
- $(\gamma_2) \ a_2 \to b_2$ crossing the saddle point along the axis until we reach $b_2 \in S_-$
- (γ_3) $b_2 \rightarrow b_1$ by a curve inside S_-

Along γ_1 and γ_2 we have that $\mathscr{R}[\phi(z) - \phi(z_0] < -c$, hence as $\lambda \to +\infty$:

$$\int_{\gamma_1 \cup \gamma_2} g(z) e^{\lambda \phi(z)} dz = O\left(e^{\lambda(\mathscr{R}\phi(z_0) - c)}\right)$$

while the contribution due to integrating along γ_3 can be evaluated by Laplace Method. In fact γ_3 can be reparametrized by:

$$z = z_0 + \alpha x, \bar{a} \le x \le \bar{b} \quad \left(-\rho < \bar{a} < 0 < \bar{b} < \rho, \ \alpha = e^{\frac{i}{2} \left[\pi - arg(\phi''(z_0)) \right]} \right)$$

getting:

$$\int_{\gamma_3} g(z) e^{\lambda \phi(z)} dz = \alpha \int_{\bar{a}}^{\bar{b}} g(z_0 + \alpha x) e^{\lambda \phi(z_0 + \alpha x)} dx \stackrel{\lambda \to \infty}{\asymp} \frac{e^{\lambda \phi(z_0)}}{\sqrt{\lambda}} \sum_{k \ge 0} \frac{c_k}{\lambda^k}$$

where we used the Taylor expansion of ϕ around z_0 :

$$\phi(z_0 + \alpha x) = \phi(z_0) + \frac{1}{2}\phi''(z_0)\alpha^2 x^2 + O\left(|x|^3\right)$$

and the coefficients c_k are determined as in Sec.(4.4) of [dB81]. If $g(z_0) \neq 0$ then the leading asymptotics as $\lambda \to +\infty$ is:

$$\int_{\gamma_3} g(z) e^{\lambda \phi(z)} dz = \alpha \sqrt{\frac{2\pi}{\lambda \mid \phi''(z_0) \mid}} g(z_0) e^{\lambda \phi(z_0)} \left(1 + O\left(\frac{1}{\lambda}\right)\right)$$
(5.28)

where α is a complex number of unit modulus and its argument indicates the direction on the axis from S_+ to S_- .

Remark 5.2.2.

- $\frac{e^{\lambda\phi(z_0)}}{\sqrt{\lambda}}\sum_{k\geq 0}\frac{c_k}{\lambda^k}$ is the saddle point contribution [with respect to (5.27)]. It depends on the direction chosen to cross z_0 by our integration path: reversing the direction causes a 1 factor in front.
- The question whether the asymptotics of (5.18) can be represented by saddle point contributions cannot be answered by studying small neighbourhoods of their associated critical points. Nevertheless it is affermative in all those cases in which we can link a to a_1 and b to b_1 in such a a way that along these paths the condition $\max_{z \in \gamma} \mathscr{R}\phi(z) < \max_{z \in \gamma} \mathscr{R}\phi(z_0)$ is fulfilled since , in this case, their contributions can be neglected.

In the case of a boundary point our discussion is simplified. In particular if:

$$g(a) \neq 0$$
 and $\phi'(a) \neq 0$

and the path which starts from a in a direction in which $\Re \phi$ decreases, then the leading asymptotics, due to the contribution of a neighbourhood of a, can be evaluated using Laplace Method and it equals:

$$g(a)e^{\lambda\phi(a)}\left(-\lambda\phi('(a)\right)^{-1}$$

as shown in Ch.(4), see also Sec.(4.3) of [dB81].

5.2.5. Airy Functions

As a classical application of the *steepest descent* method let us introduce the study of the *Airy* $function^{24}$:

$$\mathscr{A}(x) \equiv \frac{1}{\pi} \int_{0}^{+\infty} \cos\left(\frac{z^3}{3} + zx\right) dz \tag{5.29}$$

for which we would like to find the asymptotics as $x \to +\infty$. With a suitable change of variable (5.29) can be written as:

$$\mathscr{A}(x) = \frac{\sqrt{x}}{2\pi} \int_{-\infty}^{+\infty} e^{i\left(\frac{z^3}{3} + zx\right)} dz$$

which allows us to consider an integral of the form (5.18), where $\phi(z) = i\left(\frac{z^3}{3} + z\right)$, $\lambda \equiv x^{\frac{3}{2}}$ and the path γ is replaced by the real axis. We note that the function ϕ has exactly two saddle points, namely $z_{+,-} \equiv \pm i$ where it attains, respectively, the values $\phi(z_{+,-}) = \pm \frac{2}{3}$.

²⁴For a deeper introduction to this class of *special functions* see e.g. [Leb72], Ch.5, Sec.(17)., [SV98] or [Fri54].

5.2 Steepest Descent Method

We note that $\Re \phi(z_{-}) > 0 = \max_{z \in \gamma} \Re \phi(z)$ which implies that the z_{-} contribution to the asymptotics of (5.29) can be neglected. Since we have to integrate over an infinite contour it is necessary to study the behaviour of $\Re \phi(z)$ at infinity dividing the complex plane in the following three sectors:

$$S_1 \equiv \{z \in \mathbb{C} : \arg(z) \in (o, \frac{\pi}{3})\}$$
$$S_2 \equiv \{z \in \mathbb{C} : \arg(z) \in (\frac{2\pi}{3}, \pi)\}$$
$$S_3 \equiv \{z \in \mathbb{C} : \arg(z) \in (-\frac{4\pi}{3}, -\frac{2\pi}{3})\}$$

where, along any ray which lies in D_1, D_2 or D_3 and such that its origin is in z = 0, it has to hold $\mathscr{R}\phi(z) \to -\infty$ as $|z| \to \infty$. Vice versa, in the remaining sectors, we have $\mathscr{R}\phi(z) \to +\infty$ along any ray. Coming back to the previous discussion, see (5.1.7), we can deform γ to any line of the type $\mathscr{I}(z) = c > 0^{25}$, e.g. to a path $\tilde{\gamma}$ such that $\mathscr{I}z = 1$ which passes through the saddle point z_+ . Since $\tilde{\gamma}$ is only a translation of the real axis we can parametrize it in a linear way, i.e. $\forall z \in \tilde{\gamma}$ we have $z = i + t, t \in \mathbb{R}$, moreover:

$$\forall z \in \tilde{\gamma} \Rightarrow \mathscr{R}\phi(z) = -\frac{2}{3} - t^2$$

which implies not only that $\max_{z \in \tilde{\gamma}} \mathscr{R}\phi(z)$ is attained solely at the saddle point $z_+ = i$, but also that the asymptotics of (5.29) is given by the z_+ contribution. Using (5.28) ²⁶ we find as $x \to \infty$:

$$\mathscr{A}(x) = \frac{1}{2x^{\frac{1}{4}}\sqrt{\pi}} e^{-\frac{2}{3} \cdot x^{\frac{3}{2}}} \left(1 + O(x^{-\frac{3}{2}})\right)$$
(5.30)

In fact in a sufficiently small neighbourhood U_+ of z_+ we have $\phi(z) - \phi(z_+) \sim -(z-i)^2$ and in U_+ the line of steepest descent $\bar{\gamma}$ has the form $\mathscr{I}(z-i) \simeq 0$ which implies that both $\tilde{\gamma}$ and $\bar{\gamma}$ have the same tangent at the point z_+ where $\arg \sqrt{-\phi''(z_+)} = 0$. According to the expansion given in Th.(5.2.2) we have:

$$\mathscr{A}(x) = \frac{1}{2\pi x^{\frac{1}{4}}} e^{-\frac{2}{3} \cdot x^{\frac{3}{2}}} \sum_{k \ge 0} (-1)^k \frac{\Gamma\left(\frac{3k+1}{2}\right)}{3^{3k}(2k)!} x^{-\frac{3k}{2}}$$
(5.31)

Let us turn back to the analysis of the phase function $\phi(z) = i\left(\frac{z^3}{3} + z\right)$ for which we have found the *critical points* $z_{\pm} = \pm i$. Writing our local coordinates $z = \xi + i\eta$ we have that:

$$\mathscr{I}\phi(z) = \frac{\xi^3}{3} - \xi\eta^2 + \xi \,, \,\, \mathscr{I}\phi(\pm i) = 0$$

so that the steepest paths are given as the closed set in the Zariski topology²⁷ associated to the equation: $\xi(\xi^2 - 3\eta^2 + 3) = 0$ which represents a degenerate cubic formed by the imaginary axis

 $^{^{25}\}mathrm{Clearly}$ this kind of paths are parallel to the real axis.

²⁶Where $\lambda = x^{\frac{2}{3}}, g \equiv 1, \phi(z) = i\left(\frac{z^3}{3} + z\right).$

 $^{^{27}}$ See e.g. [Zar44].

and the two branches of an hyperbola. Following the directions along which $\Re \phi(z)$ decreases we note that the global landscape can be divided into two antisymmetric parts with respect to the real axis. The hyperbola's asymptotes are given by $\xi = \mp \sqrt{3}\eta$ and the original integration path can be modified in the branch of the hyperbola which lies in the upper half of the complex plane and running from $\infty \cdot e^{\frac{5i\pi}{6}}$ to $\infty \cdot e^{\frac{i\pi}{6}}$. Along the latter *route* we can easily see that (5.29) converges whenever $\Re x > 0$ and we can write:

$$\frac{2\pi\mathscr{A}\left(x^{\frac{2}{3}}\right)}{x^{\frac{1}{3}}} = \int_{i}^{\infty \cdot e^{\frac{i\pi}{6}}} e^{x\phi(z)}dz - \int_{i}^{e^{\frac{5i\pi}{6}}} e^{x\phi(z)}dz = I(x)_{1} - I(x)_{2}$$
(5.32)

which can be evealuated by Laplace method, see e.g. Ch.(4). Since both in $I(x)_1$ and in $I(x)_2$ we have that $\tilde{\phi} \equiv \phi(z) - \phi(z_+)$ is real, attains its maximum at $z = z_+$ and $\frac{d}{dz} [\phi(z) - \phi(z_+)] < 0$, then:

$$\tilde{\phi}(z) = -\frac{2}{3} - i\left(\frac{z^3}{3} + z\right) = (z-i)^2 - \frac{1}{3}i(z-i)^3$$

and we can define:

$$\pm \tilde{\phi}^{\frac{1}{2}} = (z-i) \left[1 - \frac{1}{3}i \left(z - i \right) \right]^{\frac{1}{2}}$$

where:

- · $\tilde{\phi}^{\frac{1}{2}}$ is the positive square root
- $\left[1 \frac{1}{3}i(z-i)\right]^{\frac{1}{2}}$ is the value which reduces to a at $z_{+} = i$
- the positive specification for $\tilde{\phi}^{\frac{1}{2}}$ holds for $I(x)_1$ while the negative one holds for $I(x)_2$.

By a standard Taylor expansion we have that, at least in a sufficiently small neighbourood of z_+ , $z - i = \sum_{k\geq 0} b_k \left(\pm \tilde{\phi}^{\frac{1}{2}}\right)^k$ where kb_k is the coefficient of $(z-i)^{k^{-1}}$ in the expansion of $\left[1 - \frac{i(z-i)}{3}\right]^{-\frac{k}{2}}$ in powers of z - i, so that:

$$z - i = \sum_{k \ge 1} \frac{i^{k^{-1}} \Gamma\left(\frac{3k-2}{2}\right)}{3^{k^{-1}} k! \Gamma\left(\frac{k}{2}\right)} \left(\pm \tilde{\phi}^{\frac{1}{2}}\right)^k$$
(5.33)

are the expansions with respect to $I(x)_1$, for the + sign, and for $I(x)_2$, for the - sign. By the results stated in Ch.(4), the fact that $e^{-x\phi(z_+)}I(x)_{1,2} = \int_0^\infty e^{-x\tilde{\phi}}\frac{dz}{d\tilde{\phi}}d\tilde{\phi}$ and using (5.33) it is possible to write down the asymptotics expansions of $I(x)_{1,2}$, namely the following holds:

$$e^{\frac{2}{3}x}I(x)_{1,2} = \int_{0}^{+\infty} e^{-x\tilde{\phi}} \sum_{k\geq 1} \frac{(\pm 1)i^{n-1}\Gamma\left(\frac{3k-2}{2}\right)}{3^{k-1}2(k-1)!\Gamma\left(\frac{k}{2}\right)} \tilde{\phi}^{\frac{k}{2}-1} d\tilde{\phi} \sim \sum_{k\geq 0} \frac{(\pm 1)i^{n-1}\Gamma\left(\frac{3k-2}{2}\right)}{3^{k-1}2(k-1)!x^{\frac{k}{2}}}$$

where we have integrated term-by-term. Since $\mathscr{A}\left(x^{\frac{2}{3}}\right) = 2\pi x^{\frac{1}{3}}\left(I(x)_{1} - I(x)_{2}\right)$ then we have:

$$\mathscr{A}(z) \sim \frac{1}{2\pi z^{\frac{1}{4}}} e^{-\frac{2}{3}z^{\frac{3}{2}}} \sum_{k \ge 0} \frac{\Gamma\left(3k + \frac{1}{2}\right)}{(2k)!} \left(-9z^{\frac{3}{2}}\right)^{-k}$$

which holds uniformly in $\arg z$ as $z \to \infty$ and $|\arg z| \le \frac{\pi}{3} - \delta$ for all positive δ .

What happens to $\mathscr{A}(x)$ when $x \to -\infty$? it is possible to work as in the latter situation, $x \to +\infty$ with the only difference that, now, we have to deal with an infinite path of integration γ where $|e^{\lambda\phi(z)}| \equiv 1$, hence the integral is only conditionally convergent.

More interesting is the *full-complex* asymptotic case, i.e. the scenario in which we want to take care of the asymptotics of $\mathscr{A}(z)$ when $z \in \mathbb{C}$ and $|z| \to +\infty$. Let us define:

$$\bar{\mathbb{C}} \equiv \mathbb{C} - \{ z \in \mathbb{C} : \mathscr{I}z = 0, \mathscr{R}z \in (-\infty, 0] \}$$

In order to make a useful change of variable consider the complex function \sqrt{z} for which we choose a positive, real, definition in $\overline{\mathbb{C}}$, i.e. $\mathscr{R}[\sqrt{z}|_{z\in\overline{\mathbb{C}}}] > 0$.

The saddle points of the new phase function $\phi(t, z) \equiv it\left(\frac{t^2+3z}{3}\right)$ are equal to $t_{\pm} \equiv \pm i\sqrt{z}$.

Since we choose the branch of \sqrt{z} in such a way that it is positive for any, positive, real argument, then t_{\pm} belong, respectively, to the upper and lower half-space. Let us deform our integration contour according to what we have done for (5.29) in the case of $x \in \mathbb{R}, x \to +\infty$, namely we consider the contour $\tilde{\gamma}$ which is a line parallel to the *original* one and passes through $t_{\pm}(z)$. Over $\tilde{\gamma}$ we have:

$$t = i\sqrt{z} + \tau \quad -\infty < \tau < +\infty \quad \phi(t,z) = -\frac{2}{3}z^{\frac{3}{2}} + i\frac{\tau^3}{3} - \tau^2\sqrt{z}$$

hence:

$$\mathscr{A}(z) = \frac{1}{2\pi} e^{-\frac{2}{3}z^{\frac{3}{2}}} \int_{-\infty}^{+\infty} e^{i\frac{t^{3}}{3} - t^{2}\sqrt{z}} dt = \frac{1}{\pi} e^{-\frac{2}{3}z^{\frac{3}{2}}} \int_{0}^{+\infty} e^{-t^{2}\sqrt{z}} \cos\frac{t^{3}}{3} dt$$

To the latter integral we can apply Lemma (4.1.1) in order to obtain the asymptotics (5.31) for $|z| \rightarrow +\infty$ where $|\arg z| \leq \pi - \epsilon < \pi$, uniformly in $\arg z$.

What happens in $\mathbb{\tilde{C}}_{\epsilon} \equiv |\arg(-z)| \leq \epsilon$? By the discussion done for the real case when we took the limit $x \to -\infty$ for $\mathscr{A}(x)$, we have that the desired asymptotics is due to the sum of the contributions of both saddle points $t_{\pm} = 1, 2$, the same is also valid in the present case where we replace x by z. Let us define $\alpha = \arg(-z)$, hence, in the part of the complex plane in which we are working, we have $|\alpha| \leq \epsilon$. As seen before, choose a branch of \sqrt{z} so that $\sqrt{z} = |\sqrt{z}| ie^{i\frac{\alpha}{2}}$. Take $\alpha \geq 0$ and change the integration contour into:

$$\tilde{\gamma} \equiv [i\sqrt{z}, i\sqrt{z} + \infty) \cup (-i\sqrt{z}(-\infty), -i\sqrt{z}] \cup [-i\sqrt{z}, i\sqrt{z}]$$

on the first two components of $\tilde{\gamma}$ we have:

$$\mathscr{R}t = i\sqrt{z} + \tau \quad 0 \le \tau < \infty \quad \mathscr{R}\phi(t,z) = -\frac{1}{2}\mathscr{R}z^{\frac{3}{2}} - \tau^2 \mathscr{R}\sqrt{z}$$

hence $\Re \phi(t, z)$ attains its maximum at $\tau = 0$. Vice versa over the segment $[-i\sqrt{z}, i\sqrt{z}]$ we have:

$$t = i\sqrt{z}\rho \quad -1 \le \rho \le 1 \quad \phi(t,z) = \left(\frac{\rho^3}{3} - \rho\right)z^{\frac{3}{2}}$$

Since $\Re z^{\frac{3}{2}} = |z|^{\frac{3}{2}} \cos\left(\frac{3\alpha}{2}\right) > 0$ and $\frac{\rho^3 - 3\rho}{3}$ is monotonically decreasing with a maximum in $\rho = -1$, then $\phi(t, z)$ takes its maximum value at the saddle point $t_{-}(z)$.

Analogously if $\alpha \leq 0$ then $\Re \phi(t, z)$ attains its maximum at $t_+(z)$, hence $\forall z \in \overline{\mathbb{C}}$ we have that $\tilde{\gamma}$ is a *saddle contour*, and the asymptotic of the Airy functions is given as the sum of the contributions of these points.

It follows that $\mathscr{A}(z)$ has different asymptotic forms in different sectors of the complex plane, i.e. our function reveals the so called *Stokes phenomenon*, see next section and Ch.(6) Sec.(6.2.4).

Moreover something else can happen when we have the freedom of choice among several path of integration. One situation is very delicate and it is related to the case where a line of steepest descent which comes from a saddle point passes through another saddle point, then both contributions compete for the asymptotics. This is the case for $\mathscr{A}(z)$ when we take, in $\phi(t, z) = it \frac{t^2+3z}{3}$, $\arg t = \frac{2\pi}{3}$ so that our integration contour goes through the saddle point located in the lower half-space, i.e. z_- . In this situation, contrary to what happens if $\arg t = \frac{\pi}{3}$ when the path passes only through one saddle point namely z_+ , we have to take into account a second contribution. The addendum due to z_- does not affect the whole asymptotics which actually remains the same, but the Borel²⁸ summability is lost. Finally when we increase the angle and t reaches π , both z_+ and z_- takes place in the asymptotics. The theory developed to take care of the loss of Borel summability in asymptotic expansions of integrals is the so called *Resurgence Theory*, see e.g. [É81, CNP93] and references therein.

5.2.6. Stokes Phenomenon

Let us return on the concept of *Stokes Phenomenon* already seen in the study of asymptotics of the Airy's functions (5.29). If we consider the following differential equation of Airy:

$$\frac{d^2y}{dz^2} = zy(z) \tag{5.34}$$

its solution is approximated, for large |z| by a linear combination of

$$u_{\pm} = z^{-\frac{1}{4}} e^{\pm x} \tag{5.35}$$

²⁸See the original work of Borel [Bor28], and Hardy [Har49]. See also [SW94] for an extensive review on the subject.

for $x = 2\frac{z^2}{3}$, see [Olv74]. The functions u_{\pm} are multivalued with a branchpoint at z = 0, nevertheless the solutions y(z) of (5.34) are entire. Therefore if a specific solution y(z) is approximated at $\bar{z} \neq 0$ by $c_1u_+ + c_2u_-$ we cannot use the same approximation at $z = \bar{z}e^{2\pi}$. The latter is the basic Stokes Phenomenon.

The solutions of (5.34) arise as Fourier components, actually, except when x is purely imaginary, the functions:

$$U_{+} = e^{-i\omega t} = z^{-\frac{1}{4}} \quad \text{and} \quad u_{-}e^{-i\omega t} = z^{-\frac{1}{4}}e^{-x-i\omega t}$$
(5.36)

represent waves, of frequency ω with approximate wavelength $3\frac{pi}{z^{\frac{1}{2}}}$ which varies with spatial position with a corrispondent variation of the approximate amplitudes $c_1 z^{-\frac{1}{4}}$ and $c_2 z^{-\frac{1}{4}}$. If x is purely imaginary, the functions defined in (5.36) represent purely progressive waves. The wave character of the solutions of (5.34) is their most important property and is the fundamental reason why we take multivalued approximation for an entire function.

Analogous considerations hold²⁹ for the general linear differential equation of the second order:

$$\lambda^2 \frac{d^2 w}{dz^2} - p(z)w(z) = 0$$
(5.37)

with analytic coefficient p(z) and parameter λ . The corresponding³⁰ wave approximations³¹ are:

$$v_{\pm} = p^{-\frac{1}{4}} e^{\pm x}$$
 and $x = \frac{1}{\lambda} \int \sqrt{p(s)} ds$ (5.38)

If p(z) has a root z_0 and is analytic at this point then w(z) is also analytic at the same point. Nevertheless the functions v_{\pm} have branchpoints at $z = z_0$, they approximate the solutions of (5.37) only for $z \neq z_0$ and sufficiently large $|x - x(z_0)|$. Moreover they approximate locally single-valued solutions by locally multivalued functions which turn to be domain-dependent approximations, i.e. the Stokes phenomenon arises again.

Another examples of the Stokes phenomenon happens in the canonical representation of the Hamiltonian oscillators in terms of action angle, see [Gol50]. Let us rewrite (5.37) in the following *standard* form:

$$\frac{d^2W}{dx^2} - (1+\lambda^2\phi)W = 0 \quad \text{and} \quad \phi(x) = -p^{-\frac{3}{4}}\frac{d^2\left(p^{-\frac{1}{4}}\right)}{dz^2}$$
(5.39)

where $W(x) \equiv p(z)^{\frac{1}{4}}w(z)$ with $x \equiv \frac{1}{\lambda} \int \sqrt{p(s)} ds$. Let us assume that we have to deal with only one singular point, in the above sense, at x = 0. Let $r(\lambda x)$ denote a definite branch, in the complex x - plane cut from 0 to ∞ , of the fourth root of the coefficient function p(z). Moreover

 $^{^{29}}$ See [Mey89].

³⁰See [Olv74] for rigorous derivation of the result.

³¹This is the WKB method, see e.g. Ch.2 of [Fed89].

let $\psi(x)$ in (5.39) be understood as the corresponding branch. Then the wave approximations to v_{\pm} in (5.38) are:

$$V_{+}(x) = e^{x}$$
 and $V_{-}(x) = e^{-x}$

By the WKB theorem³², the following:

$$W_{\pm} \equiv a_{\pm}(x;\lambda)e^{\pm x}$$

is a fundamental system of solutions of (5.39) with the property that $|a_{\pm}|$ are bounded for large |x|. Hence we have that the approximating functions V_{\pm} are entire, while ψ has a branchpoint at x = 0 and the same happens for W. It follows that the coefficients in the approximation $c_1V_+ + c_2V_-$ to W must jump across the cut, this is called³³ Stokes curve or Stokes line.

The study of Stokes phenomena naturally arise in the analysis of the classical functions of mathematical physics which possess concrete integral representations. Since their asymptotics is studied by the application of the steepest descent method, as we seen in the case of the Airy functions in Subsec. (5.2.5), one has to deal with asymptotic approximations of wave character which exhibit Stokes behaviour. In the case of more than one singular point we have to perform a more complicated description of the Stokes phenomenon, see e.g. [Olv78], which is even more difficult when the integrals of interest depend on some extra parameters. Actually, in the latter case, it could be possible that different singular points coalesce according to the variation of the parameters which trigger the asymptotics of our integrals, see e.g. [BH93, QW00] and references therein for a detailed study of the subject.

5.2.7. Steepest Descent Method in Multidimensional Scenario

In this section we would like to carry on the methods of Sections from (5.2.1) to (5.2.6) towards, hallowing problems on multi dimensional complex domains. We shall discuss some problems of the steepest descent method for the case of oscillating integrals see [AHK77, AB93]. We will see that new topological problems arise in the sense of the multidimensional steepest descent method.

Let us consider the following integral in many dimensions:

$$I(\lambda) \equiv \int_{\gamma^n} g(z) e^{\lambda \phi(z)} dz$$
(5.40)

where $z \in \mathbb{C}^n$ and γ^n is a n-dimensional complex, smooth and compact manifold. We will assume that both g and the phase ϕ are *sufficiently* smooth at least in some domain D which contains the integration manifold γ^n .

 $^{^{32}}$ See [Olv74] for details.

³³For a detailed discussion on how choose these cuts of the complex plane, see e.g. [Sto50, Olv74, MP83, Mey89, Mey92].

5.2 Steepest Descent Method

Of course, viewed as a real manifold, γ^n doubled its dimension so it is quiet difficult to try a graphical sketch of the present scenario even if $z = (z_1, z_2) \in \mathbb{C}^2$, nevertheless the main idea of the saddle point method can be applied, namely the searching of a saddle minimax contour. Let us assume that both g and ϕ are polynomial function and that $\partial \gamma^n$ is connected. Applying Poincaré's theorem we know that the value of (5.40) does not change if we replace γ^n with a new manifold $\tilde{\gamma}^n$ provided the latter has the same boundary $\partial \gamma^n$. Let us suppose that, among all the possible deformations of γ^n , we can pick up $\tilde{\gamma}^n$ with the minimax property, i.e. the value:

$$\min_{\tilde{\gamma}^n} \max_{z \in \tilde{\gamma}^n} \mathscr{R}\phi(z) = M_{\tilde{\gamma}^n}$$

is attained on $\tilde{\gamma}^n$. Hence if:

$$\tilde{\gamma}_M^n \equiv \{ z \in \tilde{\gamma}^n : \mathscr{R}\phi(z) = M_{\tilde{\gamma}^n} \}$$

then $\tilde{\gamma}_M^n$ must contain either a saddle point or a boundary point of the integration manifold. If $z_0 \in \tilde{\gamma}^n$ is a simple saddle point one can use the Morse's lemma, see Ch.(4) Sec.(4.4), in order to have³⁴:

$$\phi(z) = \sum_{i=1}^{n} z_i^2 \Rightarrow \mathscr{R}\phi(z) = \sum_{i=1}^{n} x_i^2 - y_i^2 \qquad \mathscr{I}\phi(z) = 2\sum_{i=1}^{n} x_i y_i$$

at least in a neighbourhood U_{z_0} of z_0 . It follows that, if the dimension n is greater than one, the steepest descent paths are replaced by planes Π characterized by having $x_i = 0$ for all i = 1, ..., n.

To give a glance of the situation let us suppose that $z_0 = 0$ lies in γ^n and it is the only point at which $\Re \phi(z)$ attains its maximum. Then we can deform γ^n in order to make it coincide with ϕ in a sufficiently small neighbourhood of z_0 and (5.40) takes the form, as $\lambda \to +\infty$:

$$\int_{|y| \le \delta} g(y) e^{-\lambda \sum_{j=1}^n y_j^2} dy + O\left(e^{-\lambda c}\right)$$

for some constant c > 0. The final asymptotic can be developed using the Laplace method.

Suppose that $\max_{z \in \gamma^n} \mathscr{R}\phi(z)$ is attained only at the point z_0 which is both an interior and a simple saddle point for γ^n . then the asymptotic expansion for (5.40) is (see [Fed77]):

$$I(\lambda) = \frac{1}{\sqrt{|\phi''(z_0)|}} \left(\frac{2\pi}{\lambda}\right)^{\frac{n}{2}} e^{\lambda\phi(z_0)} \left[g(z_0) + \sum_{k\geq 1} c_k \lambda^{-k}\right]$$

where the choice of the branch for the root depends on the orientation of the contour.

In [Fed77] some theorems for choosing saddle points are developed, but a set of general rules is still missing, one which can help us in solving the problem of the existence of a *necessary* saddle point as we have done in the unidimensional complex case.

 $^{^{34}}$ See Sec.(4.5) of [Fed89].
For the multidimensional investigation of a certain class of integrals see [Fed89], Sec.(4.5)., where there is also an interesting example which emphasizes the differences between the one dimensional and the multidimensional case, see [Fed89], Sec 4.5.

CHAPTER 6

Uniform Asymptotic Expansions

6.1. Introduction

Let us consider the Hankel functions of type j = 1, 2, argument kr and order ka:

$$H_k a^{(j)}(kr) \equiv \frac{1}{\pi} \int_{\gamma_j} e^{ik\left[r\cos z + a\left(z - \frac{\pi}{2}\right)\right]} dz$$
(6.1)

where the path of integration γ_1 , seen as a function from $(\frac{\pi}{2}, \frac{3}{2}\pi)$ to the real axis, is such that $\lim_{t\to\frac{\pi}{2}^+}\gamma_1(t) = -\infty$, there exists a point $t_0 \in (\pi, \frac{3\pi}{2})$ such that $\lim_{t\to t_0^-}\gamma_1(t) = +\infty$ and a point $\overline{t} \in (\frac{\pi}{2}, \pi)$ in which γ_1 equals 0, i.e. the path γ_1 intersects the real axis. The path γ_2 is symmetric to γ_1 with respect to the axis $t = \frac{\pi}{2}$. We are interested in the limit behaviour for $k \to \infty$, i.e. the high frequency limit behaviour. It is appropriate to take the order and the argument parameter as a function of ka and kr respectively. If we make the following substitutions:

$$\lambda = kr \quad \text{and} \quad \beta = \frac{a}{r}$$

and define:

$$w(z,\beta) \equiv i \left[\cos z + \beta \left(z - \frac{\pi}{2} \right) \right]$$

for j = 1, 2, we have:

$$H_{ka}^{(j)}(kr) = I_j(\lambda,\beta) = \frac{1}{\pi} \int_{\gamma_j} e^{\lambda w(z,\beta)} dz$$
(6.2)

We shall consider the case in which $\lambda \in \mathbb{R}$, $\lambda \to \infty$ and $0 < \beta < 1$. By the definition of the paths of integration we have that the only critical points are saddle points of w, and since:

$$w'(z) = i \left[-\sin z + \beta\right]$$
 and $w''(z) = -i \cos z$

we have that in the strip $-\frac{\pi}{2} < \mathscr{R}(z) < \frac{3\pi}{3}$, what two simple points z_{\pm} such that¹:

$$\sin z_{\pm} = \beta$$
 and $0 < z_{+} < \frac{\pi}{2}$ and $\frac{\pi}{2} < z_{-} = \pi - z_{+} < \pi$

We then have:

$$w(z_{\pm}) = \pm i \left[\sqrt{1 - \beta^2} + \beta \left(\sin^{-1} \beta - \frac{\pi}{2} \right) \right]$$

where $\sin^{-} 1$ is the $\sin - inverse$ function. Since $w''(z) = \pm i\sqrt{1-\beta^2}$ it follows that the steepest descent direction at the two saddle points are:

$$\theta(z_+) = -\frac{\pi}{4}, \frac{3\pi}{4} \text{ and } \theta(z_-) = \frac{\pi}{4}, -\frac{3\pi}{4}$$

Along the corresponding paths of steepest descent u(x, y) + iv(x, y) we have:

$$u(x,y) = \mathscr{R}(w) = \sin x \sinh y - \beta y$$

$$v(x,y) = \mathscr{I}(w) = \cos x \cosh y + \beta \left(x - \frac{\pi}{2}\right)$$
(6.3)

Analyzing equations (6.3) we find qualitative informations about the way of deforming the original paths of integration $\gamma - 1$, γ_2 in order to apply the method of steepest descent which allows to state the following asymptotics :

$$H_{ka}^{(j)}(kr) \asymp \sqrt{\frac{2}{\pi\lambda}} \frac{e^{(-1)^{j+1}i\left[k\sqrt{r^2 - a^2} - ka\cos^{-1}\left(\frac{a}{r}\right) - \frac{\pi}{4}\right]}}{(r^2 - a^2)^{\frac{1}{4}}} \tag{6.4}$$

where $\frac{a}{r} < 1$ and for j = 1, 2. This result is no longer valid if $\frac{a}{r} = 1$, i.e. when the order and the argument of th *Hankel* functions coincide. In particular in this case $z_{-} = z_{+}$ and instead of having two different saddle points of order one, we have only one saddle point of higher order. Nevertheless we can treat this case by deforming the original paths of integration in a different manner with respect to what we have done above. Finally, for j = 1, 2, we find:

$$H_{ka}^{(j)}(ka) \approx -\frac{\Gamma\left(\frac{1}{3}\right)}{\pi(ka)^{\frac{1}{3}}} \left(\frac{4}{3}\right)^{\frac{1}{6}} e^{(-1)^{j+1}\frac{2\pi i}{3}}$$
(6.5)

Hence the corrisponding expression $I_j(\lambda,\beta)$ for the Hankel functions are of the order $O(\lambda^{-\frac{1}{2}})$ if $0 < \beta < 1$ and of order $O(\lambda^{-\frac{1}{3}})$ if $\beta > 1$. Latter transition in the determination of the asymptotics for the Hankel functions with respect to the variation of the parameter $\beta = \frac{a}{r}$, suggests to develop a more sofisticated method of investigation. Actually we would like to have an asymptotic expansion which remains valid even if the parameter triggering our integrals crosses some critical values. In the case of the Hankel function the problem arises because of the coaelescence of the saddle points z_{\pm} when the parameter β approaches 1. Nevertheless the latter is not the only situation in which anomalies in the asymptotics of the integrals of interest arise. Different problems can be caused by the coaelescence of saddle points to a boundary point of the path of integration, or to some singularity points of the integrand functions.

¹For the analysis of the other saddle points, which give negligible contributions to the required asymptotics, see Ch.7 of [BH86].

6.2. Two Nearby Saddle Points

We would like to consider the following integral 2 :

$$I_{\mathscr{C}}(\lambda,\alpha) \equiv \int_{\mathscr{C}} g(z) e^{\lambda \phi(z,\alpha)} dz$$
(6.6)

where $\lambda \in \mathbb{R}^+$, g(z) and $\phi(z, \alpha)$ are analytic functions of z in some simply connected complex domain containing the integration path \mathscr{C} and the points $z = \alpha_+$, $z = \alpha_-$, which are non degenerate sadde points of the phase function $\phi(z, \alpha)$.

We shall try to find an asymptotic expansion for (6.6) in the large values of the asymptotic parameter λ which are uniform in the complex parameter α . In particular the saddle points α_{\pm} are free to move in a simply connected domain D_1 in which we allow them to *coalesce* in order to form a degenerate saddle point of order two. Moreover we suppose that, for each choice of $\alpha_{\pm} \in D_1$ there exists a domain $D_2 \supset D_1$, outside of which all other saddle points of the phase function ϕ lie and that their contribution to the asymptotic expansion of (6.6) can be neglected in comparison to that of $z = \alpha_{\pm}$.

Of course the major problem in reaching our purpose is to find an asymptotic expansion which remains valid even if $\alpha_{+} = \alpha_{-}$, i.e. even if the parameter $d \equiv |\alpha_{+} - \alpha_{-}| = 0 = d_{c}$, i.e. dtakes the *the critical value* 0.

6.2.1. First Underlying Principle

It is possible to state some general principles which can help us to solve the asymptotic expansion problem for integrals of the type (6.6). The first ingredient consists in finding a suitable, sufficiently smooth, change of variable, e.g. z = z(t), which allows us to change the phase function $\phi(z, \alpha)$ with a new one that could be *simpler*. For example if we have *n* saddle points for the function ϕ , each of which is counted with its algebraic multiplicity, in many cases it is possible to substitute ϕ with a polynomial function $\overline{\phi}$ of degree equal to n+1. This *new phase*, according to [BH86], will be called *canonical exponent* since a whole class of problems could be reduced to consider a particular $\overline{\phi}$. We shall see that in the case of two nearby saddle points the *canonical exponent* will be a polynomial of degree three.

In order to find the appropriate *canonical exponent* we have to ask for a change of variable z = z(t) which possesses the following properties:

(i) z = z(t) should yield a conformal map of some disc $D_{\alpha} \subset D_2$, containing $z = \alpha_{\pm}$, onto a domain \overline{D}_{α} in the *new* complex t plane.

²What follows is essentially based on [CFF57], Ch.9 of[BH86], [Urs70], [Urs65] and [Olv54]. Moreover a good introduction to the subject can be found in Ch.4 of [Jon97] in the framework of *non-standard analysis*.

(ii) The new phase function $\bar{\phi}(t, \alpha) = \phi(z(t), \alpha)$ should have in \bar{D}_{α} two simple saddle points for $\alpha_+ \neq \alpha_-$ which, eventually, can coalesce to a single saddle point, of higher order, for $d = d_c = 0$.

One hopes to find a *convenient* change of variable, i.e. one which gives a simpler phase function $\bar{\phi}$ compared with the original one ϕ . Following this idea let us consider the following cubic transformation defined in implicit form:

$$\phi(z,\alpha) = -\left(\frac{t^3}{3} - (\gamma(\alpha))^2 t\right) + \rho(\alpha) = \bar{\phi}(t,\alpha)$$
(6.7)

where the coefficients γ , ρ have to be determined according to the values of α . From (6.7), differentiating with respect to t, we have:

$$\frac{dz}{dt} = \frac{\gamma^2 - t^2}{\frac{d}{dz}\phi(z,\alpha)} \tag{6.8}$$

If property (i) has to be satisfied then the derivative in (6.8) must be finite and nonzero $\forall (t, z) \in \overline{D}_{\alpha} \times D_{\alpha}$. We can encounter problems in the following two cases: first if $z = \alpha_{\pm}$, when the above ratio explodes, second if $t = \pm \gamma$. In order to avoid this situation we request that:

$$t = \pm \gamma \leftrightarrow z = \alpha_{\pm}$$

Putting the latter condition in our cubic transformation we can make explicit γ and ρ , namely:

$$\gamma = \frac{3}{4}\sqrt[3]{\phi(\alpha_+, \alpha) - \phi(\alpha_-, \alpha)} \quad ; \quad \rho = \frac{1}{2}\left(\phi(\alpha_+, \alpha) + \phi(\alpha_-, \alpha)\right) \tag{6.9}$$

The result in (6.9) might look unsatisfactory due to the fact that the parameter γ is not uniquely determined, since $\alpha_+ \neq \alpha_-$. Different choices for γ lead us to pick up different branches in (6.7), fortunately, however, the following result holds³:

Theorem 6.2.1. For each α_{\pm} in D_1 the transformation:

$$\phi(z,\alpha) = -\left(\frac{t^3}{3} - (\gamma(\alpha))^2 t\right) + \rho(\alpha) = \bar{\phi}(t,\alpha)$$

has just one branch which defines a conformal map of some disc D_{α} containing α_{\pm} . On this branch the points $z = \alpha_{+}$ and $z = \alpha_{-}$ correspond to $t = +\gamma$ and $t = -\gamma$ respectively.

Once we have chosen the *right* value for γ we can take into account the behaviour of z = z(t) at the saddle points $t = \pm \gamma$.

If $\alpha_+ \neq \alpha_-$ then $\gamma \neq 0$ and we have:

$$0 \neq \frac{d^2 z}{dt^2} \mid_{t=\pm\gamma, z=\alpha_{\pm}} = \frac{\mp 2\gamma}{\frac{d^2}{dz^2}\phi(\alpha_{\pm}, \alpha)} < \infty$$

³See [CFF57] Th.1 for a proof.

(while, if $\alpha_+ = \alpha_-$ we have: $0 \neq \frac{d^3 z}{dt^3} |_{t=0,z=\alpha_+} = \frac{-2}{\frac{d^3}{dz^3}\phi(\alpha_+,\alpha)} < \infty$). Applying (6.7) to (6.6) we obtain:

$$I_{\mathscr{C}}(\lambda,\alpha) = \int_{\mathscr{\overline{C}}} g(z(t)) \left(\frac{\gamma^2 - t^2}{\frac{d}{dz}\phi(z,\alpha)}\right) e^{\lambda\bar{\phi}(t,\gamma)} dt + \mathscr{R}$$
(6.10)

where $\bar{\mathscr{C}} \equiv \mathscr{C} \cap \bar{D}_{\alpha}$ and \mathscr{R} is asymptotically negligible being by assumption exponentially smaller than $I(\lambda, \alpha)$ itself. Let us define the following function:

$$g_0(t,\alpha) \equiv g(z(t)) \left(\frac{\gamma^2 - t^2}{\frac{d}{dz}\phi(z,\alpha)}\right) = g(z(t))\frac{dz}{dt} = a_0 + a_1t + h_0(t,\alpha)(t^2 - \gamma^2)$$
(6.11)

The coefficients a_0, a_1 and the function h_0 will be determined in the next section.

6.2.2. Second Underlying Principle

The change of variable z = z(t) brings on a new function, namely g_0 defined by (6.11), which will plays the role of a new *amplitude function*. The next step in our analysis consists in finding a finite expansion in power of α , of this function fulfilling the following requests:

- (1) The remainder should vanish at all the critical points which are involved in the uniform expansion of (6.6) with respect to the parameter α .
- (2) The smoothness of the remainder must be the same as the one of the transformed amplitude.

If (1),(2) are satisfied then the integral involving the remainder can be uniformly integrated by parts producing a *new remainder integral* which has the same form as (6.6) and is multiplied by the inverse power of the large parameter λ . Since the boundary terms are either zero or asymptotically small compared with $I(\lambda, \alpha)$, it follows that the leading term of the uniform expansion involves a finite sum of *canonical integrals*. Namely each of the latter integrals is asymptotically equivalent to a well studied special function. Moreover if we work with sufficiently smooth functions, i.e. the original phase $\phi(z, \alpha)$ and amplitude g(z), we can repeat the process applying it to the remainder integral obtained at the previous step in order to find an infinite expansion.

Turning back to (6.11) let us suppose that the function h_0 is a regular function in D_{α} , then we have:

$$\lim_{t \to \pm \gamma} h_0(t, \alpha)(t^2 - \gamma^2) = 0$$

Setting $t = \pm \gamma$ we then obtain:

$$a_{0} = \frac{g_{0}(\gamma, \alpha) + g_{0}(-\gamma, \alpha)}{2} \quad ; \quad a_{1} = \frac{g_{0}(\gamma, \alpha) - g_{0}(-\gamma, \alpha)}{2\gamma} \tag{6.12}$$

Since g_0 is smooth we have:

$$\lim_{\gamma \to 0} a_0 = g_0(0, \alpha) \quad ; \quad \lim_{\gamma \to 0} a_1 = \frac{d}{dt} g_0(0, \alpha) \tag{6.13}$$

hence we can determine h_0 :

$$h_0 = \frac{g_0(t,\alpha) - a_0 - a_1 t}{t^2 - \gamma^2}$$

which is regular in \bar{D}_{α} with a removable singularity at $t = \pm \gamma$ as one can see by:

$$\lim_{t \to \pm \gamma} h_0(t, \alpha) = \pm \frac{\frac{d}{dt}g_0(\pm \gamma, \alpha) - a_1}{2\gamma}$$

Using (6.11) in (6.10) where $\bar{\phi} = -\left(\frac{t^3}{3} - \gamma^2 t\right) + \rho$ as defined in (6.7), we have:

$$I(\lambda,\alpha) = e^{\lambda\rho} \int_{\widehat{\mathscr{C}}} (a_0 + a_1 t) e^{-\lambda \left(\frac{t^3}{3} - \gamma^2 t\right)} dt + \mathscr{R}_0(\lambda,\alpha)$$
(6.14)

where the remainder \mathscr{R}_0 is equal to:

$$\mathscr{R}_0(\lambda,\alpha) = e^{\lambda\rho} \int_{\bar{\mathscr{C}}\cap\bar{D}_\alpha} (t^2 - \gamma^2) h_0(t,\alpha) e^{-\lambda \left(\frac{t^3}{3} - \gamma^2 t\right)} dt$$

The integral in (6.14) is over the whole path $\hat{\mathscr{C}}$ since the difference with its restriction to the set $\hat{\mathscr{C}} \cap \bar{D}_{\alpha}$ equals an asymptotically small error. There remains to be evaluated an integral which can be expressed in terms of the Airy function⁴ \mathscr{A} and its derivative:

$$I(\lambda,\alpha) \approx 2\pi i e^{\lambda\rho} \left[\frac{a_0}{\sqrt[3]{\lambda}} \mathscr{A}(\sqrt[3]{\lambda^2}\gamma^2) + \frac{a_1}{\sqrt[3]{\lambda^2}} \mathscr{A}'(\sqrt[3]{\lambda^2}\gamma^2) \right] + \frac{e^{\lambda\rho}}{\lambda} I_1(\lambda,\alpha)$$
(6.15)

where:

$$I_1(\lambda,\alpha) \equiv \int_{\vec{\mathscr{C}} \cap \bar{D}_{\alpha}} \left(\frac{d}{dt} h_0(t,\alpha) \right) e^{-\lambda \left(\frac{\gamma^3}{3} - \gamma^2 t\right)} dt$$
(6.16)

In fact, in (6.14), the remainder \mathscr{R}_0 can be evaluated integrating by parts and the asymptotically negligible contributions from boundary terms can be discarded.

Setting $g_1(t,\alpha) \equiv \frac{d}{dt}h_0(t,\alpha)$ we see that $I_1(t,\alpha)$ is of the form (6.10) multiplied by the λ^{-1} factor. Hence it is natural to establish an iterated set of steps, to expand I_1 in the way already described for I, in order to obtain a third integral $I_3(t,\alpha)$ again of the form (6.10) but multiplied by a λ^{-2} factor and so on. Following this scheme we obtain the following asymptotic expansion for $I_{\mathscr{C}}(\lambda,\alpha)$:

$$I_{\mathscr{C}}(\lambda,\alpha) = 2\pi i e^{\lambda\rho} \left[\frac{\mathscr{A}(\sqrt[3]{\lambda^2}\gamma^2)}{\sqrt[3]{\lambda}} \sum_{n=0}^{N} \frac{a_{2n}}{\lambda^n} + \frac{\mathscr{A}'(\sqrt[3]{\lambda^2}\gamma^2)}{\sqrt[3]{\lambda^2}} \sum_{n=0}^{N} \frac{a_{2n+1}}{\lambda^n} \right] + \mathscr{R}_N(\lambda,\alpha)$$
(6.17)

⁴See Ch.(5) Sec.(5.2.5).

where

$$\mathscr{R}_N \equiv \lambda^{-(N+1)} e^{\lambda \rho} \int_{\bar{\mathscr{C}} \cap \bar{D}_{\alpha}} g_{n+1}(t,\alpha) e^{-\lambda \left(\frac{t^3}{3} - \gamma^2 t\right)} dt$$

The coefficients $a_j, j \in \mathbb{N}$, are given recursively by:

$$a_{2n} \equiv \frac{g_n(+\gamma,\alpha) + g_n(-\gamma,\alpha)}{2} \quad ; \quad a_{2n+1} \equiv \frac{g_n(+\gamma,\alpha) - g_n(-\gamma,\alpha)}{2\gamma}$$

and

$$g_n(t,\alpha) \equiv a_{2n} + a_{2n+1}t + (t^2 - \gamma^2)h_n(t,\alpha) \quad ; \quad g_{n+1} \equiv \frac{d}{dt}h_n(t,\alpha)$$

The following theorem⁵ states that (6.17) is uniformly valid for $d = |\alpha_{+} - \alpha_{-}| \rightarrow 0$:

Theorem 6.2.2. The previous recursive system yields an asymptotic expansion of $I(\lambda, \alpha)$, as $\lambda \to \infty$, with respect to the asymptotic sequence:

$$\left\{\phi_n(\lambda,\alpha) = e^{\Re\mathfrak{e}(\lambda\rho)} \left[\lambda^{-n-\frac{1}{3}} \mid \mathscr{A}(\sqrt[3]{\lambda^2}\gamma^2) \mid +\lambda^{-n-\frac{2}{3}} \mid \mathscr{A}'(\sqrt[3]{\lambda^2}\gamma^2) \mid \right]\right\}_{n \in \mathbb{N}}$$

Moreover, this expansion is uniformly valid for small $d = |\alpha_+ - \alpha_-|$.

6.2.3. Last Underlying Principle

The transformation (6.7) modifies the phase function $\phi(z, \alpha)$ in a polynomial of degree n + 1and leaves us the task of determining n + 2 constants. If our change of variable is such that the n saddle points of ϕ are mapped into n saddle points of $\overline{\phi}$, then there remains a free constant which can be chosen in order to obtain the possible *simplest integral*. Namely, in our abstract example we choose a polynomial of degree 3 for which the coefficient of t^2 is set to zero, this choice leads us to work with a *canonical integral* of the form (6.10) expressed via the Airy function and its derivative.

6.2.4. Stokes Phenomenon, again !

We have seen that in order to develop the asymptotic expansion for large values of the parameter λ of (6.6) we first start with the application of the standard method of *steepest descent*, nevertheless, since our phase function ϕ depends on a *second parameter* α we have that, varying α , it is possible for the two saddle points $z_{\pm} =$ to coalesce, say $z_{\pm} = 0$ for $\alpha = 0$.

It follows that the expansions of our integral, for a sufficiently large value of $\lambda > \lambda_0(\alpha)$, give rise to expansions involving exponential functions. But since the index $N_0(\alpha)$ goes to infinity when α approaches 0, then we have obtained a non-uniform expansion. Moreover if $\alpha = 0$ we have a different asymptotic expansion, see e.g. [Wat41] Sec. 8.21.

⁵See [CFF57] §5, [BH86] Th. 9.2.2 and [Olv54].

The study of this *breakdown*, in a domain of the complex plane which contains $\alpha = 0$, is the key point of our previous discussion and results as those shown in (6.17) expressed in terms of Airy function \mathscr{A} . But what type of Airy function we have to chose? The answer is not unique, since it depends on the contour of integration and slightly different solutions had been obtained by different authors. Anyway, compared to previous approaches like the ones of [Nic10], [Wat41] or [Olv54], in [CFF57] one can find a consistent improvement due to the fact that, instead of having an expansion in a region which shrinks to $\alpha = 0$ when $\lambda \to \infty$, the latter authors obtain an expansion which is uniform in a ball $B_{R_{\alpha}}(0)$ independently of λ .

Nevertheless this improvement cannot save us from the *Stokes Phenomenon*. As we have seen in Sec. (5.29) the Airy integral:

$$\int_{-\infty e^{-\frac{1}{3}\pi i}}^{\infty e^{+\frac{1}{3}\pi i}} e^{\lambda\left(\frac{1}{3}z^3 - \alpha z\right)} dz \tag{6.18}$$

possesses an asymptotic expansion which seems to be discontinuous, see the remarks at the end of this section, since its form changes in different sectors of the plane, i.e. for different values of the parameter α that determines the behaviour of the two saddle points $z_{\pm}(\alpha) = \pm \sqrt{\alpha}$. In particular the contribution due to z_{\pm} becomes relevant when $\arg(\alpha)$ increases through $\frac{2}{3}\pi$ and there is an apparent discontinuity, which constitutes namely the *Stokes phenomenon*.

Anyway this is only an apparent problem. Indeed the contribution from z_+ , for:

$$\frac{2}{3}\pi < \arg(\alpha) < \pi - \epsilon,$$

is exponentially large, compared to the one of z_- . Along $\arg(\alpha) = \pi$ the two contributions are comparable. When $\arg(\alpha)$ increases to $\frac{4}{3}\pi$ the contribution from z_- becomes dominant. When $\arg(\alpha) = \frac{4}{3}\pi$ the path of steepest descent thorugh z_- passes from z_+ , i.e. we have a new *Stokes phenomenon*. No *Stokes phenomenon* occurs when the path of (6.18) goes from $\infty e^{-\frac{1}{3}\pi i}$ to $\infty e^{+\frac{1}{3}\pi i}$. Of course one could have another *Stokes phenomenon* for different limits of integration in (6.18). Since the previous considerations depend on the values taken by $\arg(\alpha)$, one has that the whole complex plane in general and the domain D_{α} in particular, are divided into three different regions by the *Stokes lines*: $\arg(\alpha) \in \{0, \frac{2}{3}\pi, \frac{4}{3}\pi\}$. The same happens for integrals of the general form (6.6). To fix ideas suppose that the integral over \mathscr{C} equals the one from $\infty(-\frac{1}{3}\pi)$ to $\infty(\frac{1}{3}\pi)$, then \mathscr{C} can be deformed into an equivalent set of steepest descent paths which pass only through one of the saddle points z_{\pm} or through both of them provided α is restricted to lie in D_{α} as mentioned before. With the same reasoning done for (6.18) we can see that D_{α} is divided into three different regions by the following three *Stokes lines*: $\arg(\sqrt{\gamma}) \in \{0, \frac{2}{3}\pi, \frac{4}{3}\pi\}$.

Remark 6.2.1. A different proof of the analyticity of the change of variables z = z(t) introduced by (6.7) is stated in [Urs70]. In [Fri59] it is possible to find an extensive treatment of the material above and in [BH86] (Example 9.2.1) an application to the Hankel functions case is given.

An improvement of the result given in [CFF57] is done in [Urs65] where the validity of the used Airy function expansion is extended to a larger region which may be unbounded according to the regularity of the involved phase and amplitude functions.

It is interesting to note that in several papers dealing with the Stokes phenomenon the change in the asymptotic expansions of the integral under investigation is often interpreted as discontinuos. Actually this is not the case as it is shown in [Ber88, Ber89, McL92], see also Sec.11 and 12 of [Boy99] and references therein. In the latter a clear explanation of the Stokes phenomenon using the Airy functions is given together with an extensive list of references on the Stokes phenomenon subject with links to the new developments in the Resurgence theory, see e.g. [CNP93, É81, Vor93], and Hyperasymptotics, see e.g. [BH91, Boy90, Daa98].

CHAPTER 7

Infinite Dimensional Integrals

7.1. Introduction

In this chapter we recall some basic notions about the rigourous derivation of the Feynman path integrals as the infinite dimensional analogue of the usual finite dimensional oscillating integrals in \mathbb{R}^n :

$$\int_{\mathbb{R}^n} e^{i\frac{\Phi(x)}{\hbar}} f(x) dx,$$
(7.1)

where $\Phi : \mathbb{R}^n \to \mathbb{R}$, $f : \mathbb{R}^n \to \mathbb{C}$ and $\hbar > 0$ is a parameter. Since a complete treatment of the Feynman path integrals subject is out of the purposes of this work, we refer the reader to [AHK76] and references therein, for a detailed description of the topic.

The integral (7.1) is strongly related to those discussed in Ch.5 and its study, originated in optics, is a classical topic which ranges from mathematical physics to functional analysis. We can define (7.1) also in the case in which f is not absolutely integrable as follows ¹:

Definition 7.1.1. The oscillatory integral of a Borel function $f : \mathbb{R}^n \to \mathbb{C}$ with respect to a phase function $\Phi : \mathbb{R}^n \to \mathbb{R}$ is defined if and only if for each test function $\phi \in \mathcal{S}(\mathbb{R}^n)$ such that $\phi(0) = 1$ the integral

$$I_{\epsilon}(f,\phi) \equiv \int_{\mathbb{R}^n} e^{i\frac{\Phi(x)}{\hbar}} f(x)\phi(\epsilon x)dx$$
(7.2)

exists for all $\epsilon > 0$ and the limit $\lim_{\epsilon \to 0} I_{\epsilon}(f, \phi)$ exists and is independent of ϕ . In this case the limit is called the oscillatory integral of f with respect to Φ and denoted by

$$\int_{\mathbb{R}^n}^{\circ} e^{i \frac{\Phi(x)}{\hbar}} f(x) dx \equiv I(f, \Phi)$$

¹See [Hör71] and references therein.

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In the case where $\Phi(x) = |x^2|$ one calls: $(2\pi i\hbar)^{-\frac{n}{2}}I(f,\Phi)$ Fresnel (or normalized oscillatory), integral of f. One also uses the notation:

$$(2\pi i\hbar)^{-\frac{n}{2}} I(f,\Phi) = \int_{\mathbb{R}^n}^{\infty} e^{\frac{i}{2\hbar}|x|^2} f(x) dx$$

The symbol ~ reminds us to the presence of the normalizing factor $(2\pi i\hbar)^{n/2}$. Let us introduce the following class of functions:

Definition 7.1.2. A Borel measurable function $f : \mathcal{H} \to \mathbb{C}$ is called \mathcal{F}^{\hbar} integrable if for each sequence $\{P_n\}_{n\in\mathbb{N}}$ of projectors onto n-dimensional subspaces of \mathcal{H} , such that $P_n \leq P_{n+1}$ and $P_n \to I$ strongly as $n \to \infty$ (I being the identity operator in \mathcal{H}), the finite dimensional approximations of the oscillatory integral of f

$$\mathcal{F}_{P_n}^{\hbar}(f) = \int_{P_n\mathcal{H}}^{\circ} e^{\frac{i}{2\hbar}|P_nx|^2} f(P_nx) d(P_nx) \Big(\int_{P_n\mathcal{H}}^{\circ} e^{\frac{i}{2\hbar}|P_nx|^2} d(P_nx)\Big)^{-1},$$

are well defined in the sense of the previous definition and the limit $\lim_{n\to\infty} \mathcal{F}_{P_n}^{\hbar}(f)$ exists and is independent on the sequence $\{P_n\}$.

In this case the limit is called the infinite dimensional oscillatory integral of f and is denoted by

$$\mathcal{F}^{\hbar}(f) = \int_{\mathcal{H}}^{\circ} e^{\frac{i}{2\hbar}|x|^2} f(x) dx$$

Even though a complete description of the class of all \mathcal{F}^{\hbar} integrable functions is still missing (even in finite dimension), it is possible to show that this class includes $\mathcal{F}(\mathcal{H})$, the class of Fresnel integrable functions defined in Ch.(2), Sec. (2.2). In particular the following theorem, see [AHK76], holds:

Theorem 7.1.1. Let $L : \mathcal{H} \to \mathcal{H}$ be a self-adjoint trace class operator such that (I - L) is invertible (I being the identity operator in \mathcal{H}). Let us assume that $f \in \mathcal{F}(\mathcal{H})$. Then the function $g : \mathcal{H} \to \mathbb{C}$ given by

$$g(x) = e^{-\frac{i}{2\hbar}(x,Lx)} f(x), \qquad x \in \mathcal{H}$$

is \mathcal{F}^{\hbar} integrable and the corresponding infinite dimensional oscillatory integral $\mathcal{F}^{\hbar}(g)$ is given by the following Cameron-Martin-Parseval type formula:

$$\int_{\mathcal{H}}^{\infty} e^{\frac{i}{2\hbar}(x,(I-L)x)} f(x) dx = (\det(I-L))^{-1/2} \int_{\mathcal{H}} e^{-\frac{i\hbar}{2}(x,(I-L)^{-1}x)} d\mu_f(x)$$
(7.3)

where $\det(I - L) = |\det(I - L)| e^{-\pi i \operatorname{Ind}(I - L)}$ is the Fredholm determinant of the operator (I - L), $|\det(I - L)|$ its absolute value and $\operatorname{Ind}((I - L))$ is the number of negative eigenvalues of the operator (I - L), counted with their multiplicity.

Moreover, see [AHK76], it is also possible to define the normalized infinite dimensional oscillatory integral with respect to an invertible operator B on \mathcal{H} as follows:

Definition 7.1.3. A Borel function $f : \mathcal{H} \to \mathbb{C}$ is called \mathcal{F}_B^{\hbar} integrable if and only for each sequence $\{P_n\}_{n\in\mathbb{N}}$ of projectors onto n-dimensional subspaces of \mathcal{H} , such that $P_n \leq P_{n+1}$ and $P_n \to I$ strongly as $n \to \infty$ (I being the identity operator in \mathcal{H}) the finite dimensional approximations

$$\int_{P_n\mathcal{H}}^{\circ} e^{\frac{i}{2\hbar}(P_n x, BP_n x)} f(P_n x) d(P_n x),$$

are well defined and the limit

$$\lim_{n \to \infty} (\det P_n B P_n)^{\frac{1}{2}} \int_{P_n \mathcal{H}}^{\circ} e^{\frac{i}{2\hbar}(P_n x, B P_n x)} f(P_n x) d(P_n x)$$
(7.4)

exists and is independent on the sequence $\{P_n\}$. In this case the limit is called the normalized oscillatory integral of f with respect to B and is denoted by:

$$\int_{\mathcal{H}}^{B} e^{\frac{i}{2\hbar}(x,Bx)} f(x) dx$$

Moreover if $f \in \mathcal{F}(\mathcal{H})$ then $f \in \mathcal{F}_B^{\hbar}$ and we have the following analogous of formula (7.3):

Theorem 7.1.2. Let us assume that $f \in \mathcal{F}(\mathcal{H})$. Then f is \mathcal{F}_B^{\hbar} integrable and the corresponding normalized oscillatory integral is given by the following Cameron-Martin-Parseval type formula:

$$\int_{\mathcal{H}}^{B} e^{\frac{i}{2\hbar}(x,Bx)} f(x) dx = \int_{\mathcal{H}} e^{-\frac{i\hbar}{2}(x,B^{-1}x)} d\mu_f(x)$$
(7.5)

Remark 7.1.1. Theorem (7.1.2) shows that definitions (7.1.2) and (7.1.3) are not equivalent. Indeed theorem (7.1.2) makes sense even if the operator $L \equiv I - B$ is not trace class (in which case the Fredholm determinant det(I - B) cannot be defined).

In fact it is possible to introduce different normalization constants in the finite dimensional approximations and the properties of the corresponding infinite dimensional oscillatory integrals are related to the trace properties of the operator associated to the quadratic part of the phase function [AB95]. For example let us consider, for all integer $p \ge 2$, the class of bounded linear operators in \mathcal{H} such that:

$$||L||_p = \left(Tr(L^*L)^{\frac{p}{2}}\right)^{\frac{1}{p}} < \infty$$

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For such an operator we define:

$$\det_{(p)}(I+L) = \det\left((I+L)\exp\left[\sum_{j=1}^{p-1}\frac{(-1)^j}{j}L^j\right]\right)$$

and the following normalized quadratic form on \mathcal{H} :

$$N_p(L)(x) = (x, Lx) - i\hbar Tr \sum_{j=1}^{p-1} \frac{L^j}{j}, \qquad x \in \mathcal{H}$$

$$(7.6)$$

then the following definition is well posed, see [AHK76]:

Definition 7.1.4. Let $p \in \mathbb{N}$, $p \geq 2$, L a bounded linear operator in \mathcal{H} , $f : \mathcal{H} \to \mathbb{C}$ a Borel measurable function. The class p normalized oscillatory integral of the function f with respect to the operator L is well defined if for each sequence $\{P_n\}_{n\in\mathbb{N}}$ of projectors onto n-dimensional subspaces of \mathcal{H} , such that $P_n \leq P_{n+1}$ and $P_n \to I$ strongly as $n \to \infty$ (I being the identity operator in \mathcal{H}) the finite dimensional approximations

$$\int_{P_n\mathcal{H}}^{\circ} e^{\frac{i}{2\hbar}|x|^2} e^{-\frac{i}{2\hbar}N_p(P_nLP_n)(P_nx)} f(P_nx) d(P_nx),$$
(7.7)

are well defined and the limit

$$\lim_{n \to \infty} \int_{P_n \mathcal{H}}^{\circ} e^{\frac{i}{2\hbar}|x|^2} e^{-\frac{i}{2\hbar}N_p(P_n L P_n)(P_n x)} f(P_n x) d(P_n x)$$
(7.8)

exists and is independent of the sequence $\{P_n\}$. In this case the limit is denoted by

$$\mathcal{I}_{p,L}(f) = \int_{\mathcal{H}}^{\widetilde{p}} e^{\frac{i}{2\hbar}|x|^2} e^{-\frac{i}{2\hbar}(x,Lx)} f(x) dx.$$

and it remains defined the class of p – normalized oscillatory integrals.

Previous results and definitions can be used in order to prove that, under suitable assumptions on the initial datum ϕ , the solution of the Schrödinger equation for an anharmonic oscillator potential:

$$\begin{cases} i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\Delta\psi + (\frac{1}{2}xA^2x + V(x))\psi\\ \psi(0,x) = \phi(x) \end{cases}$$
(7.9)

which $A^2 \geq 0$ and $V \in \mathscr{F}(\mathbb{R}^n)$, can be represented by a well defined infinite dimensional oscillatory integral on the Hilbert space $(\mathcal{H}_t, (,))$ of real continuous functions $\gamma(\tau)$ from [0, t]to \mathbb{R}^d such that $\frac{d\gamma}{d\tau} \in L_2([0, t]; \mathbb{R}^d)$ and $\gamma(t) = 0$ with inner product

$$(\gamma_1, \gamma_2) = \int_0^t \frac{d\gamma_1}{d\tau} \cdot \frac{d\gamma_2}{d\tau} d\tau$$

Let us define the following operator L on \mathcal{H}_t :

$$(\gamma, L\gamma) \equiv \int_{0}^{t} \gamma(\tau) A^{2} \gamma(\tau) d\tau,$$

and the function $v: \mathcal{H}_t \to \mathbb{C}$

$$v(\gamma) \equiv \int_{0}^{t} V(\gamma(\tau) + x) d\tau + 2xA^{2} \int_{0}^{t} \gamma(\tau) d\tau, \qquad \gamma \in \mathcal{H}_{t}, x \in \mathbb{R}^{d}$$

The following theorem holds 2 :

Theorem 7.1.3. Let $\phi \in \mathcal{F}(\mathbb{R}^d) \cap L^2(\mathbb{R}^d)$ and let $V \in \mathcal{F}(\mathbb{R}^d)$. Then the function $f_x : \mathcal{H}_t \to \mathbb{C}$, $x \in \mathbb{R}^d$, given by

$$f_x(\gamma) = e^{-\frac{i}{\hbar}v(\gamma)}\phi(\gamma(0) + x)$$

is the Fourier transform of a complex bounded variation measure μ_{f_x} on \mathcal{H}_t and the infinite dimensional Fresnel integral of the function $g_x(\gamma) = e^{-\frac{i}{2\hbar}(\gamma,L\gamma)}f_x(\gamma)$

$$\int_{\mathcal{H}_t}^{\infty} e^{\frac{i}{2\hbar}(\gamma,(I-L)\gamma)} e^{-\frac{i}{\hbar}v(\gamma)} \phi(\gamma(0)+x) d\gamma.$$

is well defined, in the sense of (7.1.2), and is equal to

$$\det(I-L)^{-1/2} \int_{\mathcal{H}_t} e^{-\frac{i\hbar}{2}(\gamma,(I-L)^{-1}\gamma)} d\mu_{f_x}(\gamma).$$

Moreover it is a representation of the solution of equation (7.9) evaluated at $x \in \mathbb{R}^d$ at time t.

We would like to point out that definition (7.1.2) is more general than definition (7.1.3) given in Ch.2. In [AM04b, AM05a] a further extension is given which provides a direct rigorous Feynman path integral definition for the solution of the Schrödinger equation for an anharmonic oscillator potential $V(x) = \frac{1}{2}xA^2x + \lambda x^4$, $\lambda > 0^{-3}$.

²See [AHK76, ET84].

³See [AHK76], Sec.10.2 for a detailed description of the subject of Fresnel integrals and applications.

7.1.1. Semiclassical Expansion

The theory of infinite-dimensional oscillatory integrals allows the rigorous generalization of the Stationary Phase Method to the infinite dimensional scenario, see [AHK77, AB93]. This means, in particular, that one can study the asymptotic semiclassical expansion of the solution⁴ of the Schrödinger equation in the limit $\hbar \rightarrow 0$.

In [AHK77] the authors consider Fresnel integrals of the form

$$I(\hbar) = \int_{\mathcal{H}} e^{\frac{i}{2\hbar}|x|^2} e^{-\frac{i}{\hbar}V(x)} g(x) dx, \qquad (7.10)$$

where \mathcal{H} is a real separable Hilbert space and V and g are in $\mathcal{F}(\mathcal{H})$, and prove, under additional regularity assumptions on V, g, that if the phase function $\frac{1}{2}|x|^2 - V(x)$ has only non degenerate critical points, then $I(\hbar)$ is a C^{∞} function of \hbar and its asymptotic expansion at $\hbar = 0$ depends only on the derivatives of V and g at these critical points. In particular the following holds⁵:

Theorem 7.1.4. Let \mathcal{H} be a real separable Hilbert space, and V and g in $\mathcal{F}(\mathcal{H})$, i.e. there are bounded complex measures on \mathcal{H} such that

$$V(x) = \int_{\mathcal{H}} e^{ix\alpha} d\mu(\alpha) \qquad g(x) = \int_{\mathcal{H}} e^{ix\alpha} d\nu(\alpha)$$

Let us assume V and g C^{∞} , i.e. all moments of μ and ν exist, and that $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$, where dim $\mathcal{H}_2 < \infty$, and if $d\mu(\beta, \gamma), d\nu(\beta, \gamma)$ are the measures on $\mathcal{H}_1 \times \mathcal{H}_2$ given by μ and ν . Then there is a λ such that $\|\mu\| < \lambda^2$ and

$$\int\limits_{\mathcal{H}} e^{\sqrt{2}\lambda|\beta|} d|\mu|(\beta,\gamma) < \infty, \qquad \int\limits_{\mathcal{H}} e^{\sqrt{2}\lambda|\beta|} \ d|\nu|(\beta,\gamma) < \infty.$$

Then if the equation dV(x) = x has only a finite number of solutions x_1, \ldots, x_n on the support of the function g, such that none of the operators $I - d^2V(x_i)$, $i = 1, \ldots, n$, has zero as an eigenvalue, then the function

$$I(\hbar) = \widetilde{\int}_{\mathcal{H}} e^{\frac{i}{2\hbar}|x|^2} e^{-\frac{i}{\hbar}V(x)}g(x)dx$$

is of the following form

$$I(\hbar) = \sum_{k=1}^{n} e^{\frac{i}{2\hbar}|x_k|^2 - V(x_k)} I_k^*(\hbar)$$

⁵See [AHK77].

⁴For a detailed description of the subject see, eg. [AHK77, AB93, ABHK82, AdMBB82] and references therein.

where $I_k^*(\hbar) \ k = 1, \dots, n$ are C^{∞} functions of \hbar such that

$$I_k^*(0) = e^{\frac{i\pi}{2}n_k} |\det(I - d^2 V(x_k))|^{-\frac{1}{2}} g(x_k)$$

where n_k is the number of negative eigenvalues of the operator $d^2V(x_k)$ which are larger than 1.

Moreover if V(x) is gentle, that is there exists a constant $\overline{\lambda} > 0$ with

$$\|\mu\| < \bar{\lambda}^2 \qquad and \qquad \int_{\mathcal{H}} e^{\sqrt{2}\bar{\lambda}|\alpha|} d|\mu|(\alpha) < \infty, \tag{7.11}$$

then the solutions of equation dV(x) = x have no limit points.

In [AHK77] Th.7.1.4 is applied to the study of the asymptotic behavior of the solution of the Schrödinger equation (7.9), by using the Feynman path integral representation. In particular the following theorem is proved:

Theorem 7.1.5. Consider the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\Delta\psi + V(x)\psi$$

where the potential V is the Fourier transform of some complex measure ν such that

$$V(x) = \int\limits_{\mathbb{R}^d} e^{ix\beta} d\nu(\beta)$$

with

$$\int_{\mathbb{R}^d} e^{|\beta|\epsilon} d|\nu|(\beta) < \infty$$

for some $\epsilon > 0$. Let the initial condition be

$$\psi(y,0) = e^{\frac{i}{\hbar}f(y)}\chi(y)$$

with $\chi \in C_0^{\infty}(\mathbb{R}^d)$ and $f \in C^{\infty}(\mathbb{R}^d)$ and such that the Lagrange manifold $L_f \equiv (y, -\nabla f)$ intersects transversally the subset Λ_V of the phase space made of all points (y, p), such that pis the momentum at y of a classical particle that starts at time zero from x, moves under the action of V and ends at y at time t.

Then $\psi(t, x)$, given by the Feynman path integral

$$\widetilde{\int}_{\gamma(t)=x} e^{\frac{i}{2\hbar} \int_0^t \dot{\gamma}(\tau)^2 d\tau} e^{-\frac{i}{\hbar} \int_0^t V(\gamma(\tau)) d\tau} \psi(\gamma(0), 0) d\gamma = \widetilde{\int}_{\gamma(t)=x} e^{\frac{i}{\hbar} S(\gamma)} \psi(\gamma(0), 0) d\gamma,$$

(which can be made precise as Fresnel integral as in Th.(7.1.3), with L = 0, see Ch.10 of [AHK76]). has an asymptotic expansion in powers of \hbar , whose leading term is the sum of the values of the function

$$\left|\det\left(\left(\frac{\partial\bar{\gamma}_{k}^{(j)}}{\partial y_{l}^{(j)}}(y^{(j)},t)\right)\right)\right|^{-1/2}\left(e^{-\frac{i}{2}\pi m^{(j)}}e^{-\frac{i}{\hbar}S}e^{-\frac{i}{\hbar}f}\chi\right)(\bar{\gamma}^{(j)})$$

taken at the points $y^{(j)}$ such that a classical particle starting at $y^{(j)}$ at time zero with momentum $\nabla f(y^{(j)})$ is in x at time t. $S(\bar{\gamma}^{(j)})$ is the classical action along this classical path $\bar{\gamma}^{(j)}$ and $m^{(j)}(\bar{\gamma}^{(j)})$ is the Maslov index of the path $\bar{\gamma}^{(j)}$, i.e. $m^{(j)}$ is the number of zeros of $\det\left(\left(\frac{\partial \bar{\gamma}_k^{(j)}}{\partial y_i^{(j)}}(y^{(j)},\tau)\right)\right)$ as τ varies on the interval (0,t).

If some critical point of the phase function is degenerate, the study of the asymptotic behavior of the integral $I(\hbar)$ in (7.10) becomes more complicated. Fo example in [AB93] the study of the degeneracy is reduced on a finite dimensional subspace of the Hilbert space \mathcal{H} , then the same tecniques of Ch.5 Sec.5.1.5 are applied.

The authors of [AB93] assume that $\frac{1}{2}(x, Bx) - V(x)$ has the point $x_c = 0$ as the unique, degenerate, stationary point and under suitable assumptions on B and V that the set:

$$Z \equiv \operatorname{Ker}(B - d^2V)(0) \neq \{0\}$$

is finite dimensional. By taking the subspace $Y \equiv B(Z^{\perp})$ and applying the Fubini theorem one has

$$I(\hbar) = \int_{\mathcal{H}}^{\circ} e^{\frac{i}{2\hbar}(x,Bx)} e^{-\frac{i}{\hbar}V(x)} g(x) dx =$$
$$= C_B \int_{Z}^{\circ} e^{\frac{i}{2\hbar}(z,B_2z)} \int_{Y}^{\circ} e^{\frac{i}{2\hbar}(y,B_1y)} e^{-\frac{i}{\hbar}V(y+z)} dy dz, \quad (7.12)$$

where B_1 and B_2 are defined by

$$B_1 y = (\pi_Y \circ B)(y), \qquad y \in Y,$$
$$B_2 z = (\pi_Z \circ B)(z), \qquad z \in Z,$$

and $C_B = (\det B)^{-1/2} (\det B_1)^{1/2} (\det B_2)^{1/2}$. By assuming that $V, g \in \mathcal{F}(\mathcal{H}), V = \hat{\mu}$ and $g = \hat{\nu}$, and under some growth conditions on μ and ν , one has that the phase function

$$y \mapsto \frac{1}{2}(y, B_1 y) - V(y+z)$$

of the oscillatory integral $J(z,\hbar) = \widetilde{\int_Y^{\circ}} e^{\frac{i}{2\hbar}(y,B_1y)} e^{-\frac{i}{\hbar}V(y+z)} dy$ has only one nondegenerate stationary point $a(z) \in Y$. By applying then the theory developed for the nondegenerate case one has

$$J(z,\hbar) = e^{\frac{i}{2\hbar}(a(z),B_1a(z))}e^{-\frac{i}{\hbar}V(a(z)+z)}J^*(z,\hbar),$$

$$J^*(z,0) = \left[\det\left(B_1 - \frac{\partial^2 V}{\partial^2 y}(a(z)+z)\right)\right]^{-1/2}g(a(z)+z).$$

As $I(\hbar) = \widetilde{\int_Z^{\circ}} e^{\phi(z)} J^*(z,\hbar) dz$, where $\phi(z) = \frac{i}{2\hbar} (z, B_2 z) + \frac{i}{2\hbar} (a(z), B_1 a(z)) - \frac{i}{\hbar} V(a(z) + z)$, the main ingredient for the asymptotic behavior of $I(\hbar)$ comes from $J^*(z,0)$.

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The phase function ϕ has z = 0 as a unique degenerate critical point and one can use the finite dimensional theory in order to investigate the higher derivatives of ϕ at 0. For example if $\dim(Z) = 1$ and $\frac{\partial^3 V}{\partial^3 z}(0) \neq 0$ then

$$I(\hbar) \sim C\hbar^{-1/6}, \quad \text{as} \quad \hbar \to 0.$$

More generally it is possible to handle other cases, taking into account the classification of different types of degeneracies, see, e.g. [AB93]).

In [ABHK82, AdMBB82] the Feynman path integral representation $I(t, \hbar)$ for the trace of the Schrödinger group $\mathrm{T}re^{-\frac{i}{\hbar}Ht}$ and the corrisponding asymptotics as $\hbar \to 0$ is studied. In particular in [AdMBB82] the oscillatory integral

$$I(t,\hbar) = \int_{\mathcal{H}_{p,t}}^{\widetilde{o}} e^{\frac{i}{\hbar}\Phi(\gamma)} d\gamma,$$

is considered, where $\mathcal{H}_{p,t}$ is the Hilbert space of periodic functions $\gamma \in H^1(0,t;\mathbb{R}^d)$ such that $\gamma(0) = \gamma(t)$, with norm $|\gamma|^2 = \int_0^t \dot{\gamma}(\tau)^2 d\tau + \int_0^t \gamma(\tau)^2 d\tau$, and $\Phi(\gamma) = \frac{1}{2} \int_0^t \dot{\gamma}(\tau)^2 d\tau - \int_0^t V_1(\gamma(\tau)) d\tau$, $V_1(x) = \frac{1}{2} x \Omega^2 x + V_0(x)$ being the classical potential. If $V_1 : \mathbb{R}^d \to \mathbb{R}$ is of class C^2 , then one proves that the functional Φ is of class C^2 and a path $\gamma \in \mathcal{H}_{p,t}$ is a stationary point for Φ if and only if γ is a solution of the Newton equation

$$\ddot{\gamma}(\tau) + V_1'(\gamma(\tau)) = 0 \tag{7.13}$$

satisfying the periodic conditions

$$\gamma(0) = \gamma(t), \qquad \dot{\gamma}(0) = \dot{\gamma}(t). \tag{7.14}$$

 V_1 is also assumed to satisfy the following conditions:

- 1. V_1 has a finite number critical points c_1, \ldots, c_s , and each of them is non-degenerate, i.e. det $V_1''(c_j) \neq 0$;
- 2. t > 0 is such that the function γ_{c_j} , given by $\gamma_{c_j}(\tau) = c_j, \tau \in [0, t]$, is a non-degenerate stationary point for Φ ;
- 3. any non-constant t-periodic solution γ of (7.13) and (7.14) is a non-degenerate periodic solution, i.e. $\dim \operatorname{Ker}(\Phi''(\gamma)) = 1$, see [Eke90].

Under additional assumptions, the authors prove that the set M of stationary points of the phase function Φ is a disjoint union of the following form:

$$M = \{x_{c_1}, \dots, x_{c_s}\} \cup \bigcup_{k=1}^r M_k,$$

where x_{c_i} , $i = 1, \ldots s$, are nondegenerate and M_k are manifolds (diffeomorphic to S^1) of degenerate stationary points, on which the phase function is constant. Under some regularity on V they also prove that, as $\hbar \to 0$

$$I(t,\hbar) = \sum_{j=1}^{s} e^{\frac{i}{\hbar}tV_{1}(c_{j})}I_{j}^{*}(\hbar) + (2\pi i\hbar)^{-1/2} \left[e^{\frac{i}{\hbar}\Phi(b_{k})} |M_{k}I_{k}^{**}(\hbar) + O(\hbar) \right]$$

where c_j are the points in condition 1, $b_k \in M_k$ are all noncongruent *t*-periodic solutions of (7.13) and (7.14) as in condition 3, $|M_k|$ is the Riemannian volume of M_k , I_j^* and I_k^{**} are C^{∞} functions of $\hbar \in \mathbb{R}$ such that, in particular,

$$I_j^*(0) = \left(\det\left[2\left[\cos\left(t\sqrt{V''(c_j)}\right) - 1\right]\right]\right)^{-1/2},$$
$$I_k^{**}(0) = \left(\frac{d}{d\epsilon}\det(R_{\epsilon}^k(t) - I)|_{\epsilon=1}\right)^{-1/2},$$

where $R^k_{\epsilon}(t)$ denotes the fundamental solution of

$$\begin{cases} \ddot{x}(\tau) = -\epsilon V''(b_k(\tau))x(\tau), & \tau > 0, \\ x(0) = x_0, & \dot{x}(0) = y_0 \end{cases}$$

written as a first order system of 2d equations for real valued functions.

Remark 7.1.2. The problem of corresponding asymptotic expansions in powers of \hbar for the case of the Schrödinger equation with a quartic potential requires a different treatement. For the corresponding finite dimensional approximation a detailed presentation, including Borel summability, is given in [AM05b]. The case of the Schrödinger equation itself is discussed in [APM06a].

7.2. Further Infinite Dimensional Asymptotics

In this section we will consider the semiclassical limit of a particular class of infinite dimensional oscillating integrals. Our study is based on the following work [AHK76, AHK77, AB93].

Let us start recalling the definition of the following spaces of symmetric linear continuous operator from \mathcal{H} into itself:

$$L^{+}(\mathcal{H}) \equiv \{T : \mathcal{H} \to \mathcal{H}s.t.\langle Tx, x \rangle \ge 0, \ T^{*} = T\}$$

$$(7.15)$$

$$L_1^+(\mathcal{H}) \equiv \left\{ T \in L^+(\mathcal{H}) : Tr(T) < \infty \right\}$$
(7.16)

Let us consider the couple (a, B) where $a \in \mathcal{H}$ and $B \in L_1^+(\mathcal{H})$ and denote by

$$\{e_k : k \ge 1\} \quad \text{resp.} \quad \{c_k : k \ge 1\}$$

a complete orthonormal basis for \mathcal{H} resp. a sequence of nonnegative numbers such that:

$$B \cdot e_k = c_k e_k \qquad \forall k \ge 1$$

Since we can identify \mathcal{H} with the set of all sequences of numbers which are square integrable, i.e. with:

$$l_2 \equiv \left\{ \{x_i\}_{i \ge 1} : x_i \in \mathbb{R} \ , \ \sum_{i \ge 1} | \ x_i |^2 < +\infty \right\}$$

we will use this identification in what follows. In the unidimensional case to any couple of numbers $(a, c) \in \mathbb{R} \times \mathbb{R}^+$ there is associated the following unidimensional Gaussian measure:

$$\mu_{a,c} \equiv \frac{1}{\sqrt{2\pi c}} e^{-\frac{(x-a)^2}{2c}} dx$$

We define the corresponding product measure $\mu_{a,B} \equiv \bigotimes_{k=1}^{\infty} \mu_{a_k,c_k}$ on the cartesian product $\mathbb{R}^{\infty} \equiv \times_{k=1}^{\infty} \mathbb{R}$, with the corresponding Borel σ – algebra, see e.g. [Hal50]. We call, in analogy with the unidimensional case, the above defined measure $\mu_{a,B}$ Gaussian measure of average a and Covariance matrix B. Besides the characteristic function of $\mu_{a,B}$ reads as follows:

$$\int_{\mathcal{H}} e^{i\langle \alpha, x \rangle} d\mu_{a,B}(x) = e^{i\langle a, \alpha \rangle} e^{-\frac{1}{2}\langle B\alpha, \alpha \rangle}$$

Let us consider the following type of infinite dimensional oscillatory integral:

$$\int_{\mathcal{H}\times\mathcal{H}} e^{i\langle(\gamma-\gamma'),(I-L)(\gamma+\gamma')\rangle} e^{-\frac{i}{2\hbar}(\gamma-\gamma'),B(\gamma-\gamma')\rangle} f(\gamma,\gamma') d\gamma d\gamma'$$
(7.17)

where $L : \mathcal{H} \to \mathcal{H}$ is a self adjoint trace-class operator, such that (I - L) is invertible, and $f : \mathcal{H} \times \mathcal{H} \to \mathbb{C}$ be the Fourier transform of a complex bounded variation measure μ_f on $\mathcal{H} \times \mathcal{H}$, while B is as before a positive definite operator on \mathcal{H} .

The oscillatory integral in (7.17) is well defined by means of finite dimensional approximations, see [AHK76] and Sec.(7.1) of this chapter and Sec.(2.2) in Ch.(2). Moreover since the function:

$$e^{-\frac{1}{2\hbar}(\gamma-\gamma'),B(\gamma-\gamma')}$$

is the characteristic function of a zero-mean Gaussian measure $\mu_{\frac{B}{\hbar}}$, on \mathcal{H} evaluated at $\gamma - \gamma'$, with covariance matrix $\hbar^{-1}B$ then for the previous integral an analogue of the Parseval formula obtained in(2.2.2) holds. Let us consider the following form for the function $f(\gamma, \gamma')$:

$$f(\gamma,\gamma') \equiv e^{-\frac{i}{\hbar}V(\gamma) + \frac{i}{\hbar}V(\gamma')} \cdot g(\gamma,\gamma')$$
(7.18)

where $g \in \mathcal{F}(\mathcal{H}, \mathcal{H})$ and $V \in \mathcal{F}(\mathcal{H})$. With suitable assumption on the operators I - L and B we have that the phase:

$$\phi(\gamma,\gamma') = \frac{i}{2} \left(\gamma - \gamma', (I - L) \cdot (\gamma + \gamma') - \frac{1}{2} \left(\gamma - \gamma', B \cdot (\gamma - \gamma')\right) - iV(\gamma) + iV(\gamma')$$
(7.19)

has a unique isolated stationary point. Let us indicate this point by (γ_c, γ'_c) , then, imposing regularity conditions on the potential V, we have that (γ_c, γ'_c) is non degenerate stationary point for the phase ϕ . By the application of the *Cameron-Martin* formula, we can translate the above mentioned point at the origin. Then we can perform the asymptotic expansion of (7.17) as $\hbar \to 0$ using tecniques developed in Sec.3 of [AB93], see also Sec.(7.1.1) of this chapter and [APM06b].

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Erklärung

Ich erkläre an Eides statt, dass ich die vorliegende Arbeit "Asymptotic Expansions of Integrals: Statistical Mechanics and Quantum Theory" selbständing verfasst und keine anderen als die angegebenen Hilfsmittel benutz habe.