Universidad de Antioquia
Instituto de Física
Facultad de Ciencias Exactas y Naturales
Grupo de Física Atómica y Molecular (GFAM)
Grupo de Física Teórica y Matemática Aplicada (GFTyMA)

Semiclassical Propagator of the Wigner Function for Open Quantum Systems

PhD Thesis

CARLOS ANDRÉS FLÓREZ ACOSTA

Advisor: Leonardo A. Pachón

Profesor Universidad de Antioquia

Medellín, 2018

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Approved by Date.

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Abstract

The concept of open quantum system is very broad and it is related to the ability of measuring only certain degree of freedoms of a particular system. Although this idea is relatively simple, the separation between the system of interest, the degree of freedoms that are accesible experimentally, and the reservoir, the degree of freedoms that are not accesible experimentally, is not always clear. For instance, in molecular systems, electronic spectroscopy has access only to electronic degree of freedoms so that the nuclear and vibrational degree of freedom become the reservoir, this makes its description not trivial. This scenario leads to have non-trivial and structured reservoirs and to develop powerful tools to analyze them. The hallmark of non-trivial and structured reservoirs is the non-Markovian dynamics. By translating the Feynman and Vernon influence functional approach into phase-space representation, we develop two theories of semiclassical evolution of the Wigner function of the system of interest that incorporate non-Markovian dynamics and highly non-trivial quantum effects such as non-locality of quantum mechanics: (i) We translate the Caldeira-Leggett model into phase-space representation of quantum mechanics and (ii) we consider the possibility of having non-linear baths and therefore, truly quantum reservoirs.

During the last forty years the study of energy loss and coherence in quantum systems has been based on the Ullersma-Caldeira-Leggett model, a model that describes the environment of quantum systems of interest as a collection of harmonic oscillators with classical evolution. We constructed this model in the Wigner-Weyl representation of quantum mechanics and discuss the classical nature of the evolution of the bath modes and the semiclassical evolution of the central system. As an application of the semiclassical Wigner propagator, the non-Markovian time evolution under the Morse potencial is analyzed. There, it is clear how decohering processes shrink the propagator to smaller regions of phase space implying that the dynamics become more local, i.e., more classical.

The current level of experimentation and control of physical systems have called into question the validity of the model in, one hand, molecular systems (e.g. photosynthetic complexes immersed in solvents, chemical systems in liquid phase or gas and manipulated with intense laser pulses) and, in the other hand, solid state systems (e.g. Josephson junctions, spins in quantum dots or "spinning ice"). Given the importance of these systems in the development of new quantum technologies and in the understanding of quantum phenomena in mesoscopic systems, it has become necessary to develop new models of the environment and efficient methodologies with quantitative prediction power. However, some of them are artificial modifications of the Ullersma-Caldeira-Leggett model without solid and clean physical support. Here we formulated a general framework that allows the study of quantum correlations in quantum systems in the presence of non-harmonic thermal baths (e.g. baths formed by strongly coupled diatomic molecules). This formulation will allow a more precise and quantitative description of processes such as the transport of excitons in photosynthetic complexes, the transfer of heat in solid state devices, among others. Results clearly show the non-classical time dynamics of the bath modes. The implementation of this particular theory remains, however, as a challenge.

Keywords

Wigner propagator, semiclassical physics, non-linearities, phase-space, non-locality.

Abbreviations and Notation

DOF	Degree(s) of Freedom.
PDF	Probability density function.
S	System.
B	Bath.
SB	System-Bath.
DO	Displacement operator.
$\mathbf{r}$,$\tilde{\mathbf{r}}$	vectors in a $2f$ dimensional phase-space for the central system.
$\mathbf{R}$,$\tilde{\mathbf{R}}$	vectors in a $2F$ dimensional phase-space for the bath modes.
$\mathcal{R}$,$\tilde{\mathcal{R}}$	vectors in a $2(f+F)$ dimensional phase-space for the universe.
$\breve{\mathbf{r}}$,$\breve{\mathbf{R}}$	Phase space points having units of $(\text{action})^{\frac{1}{2}}$.
J	Symplectic matrix.
M	Stability matrix.
E	Eigenvector matrix of M.
$\hat{\square}$	Operator acting on a Hilbert space.
$\square_{\mathrm{W}}$	Weyl symbol (transform) of an operator $\hat{\square}$.
$\hat{\rho}$	Density operator.
ρ_{W}	Wigner function associated to $\hat{\rho}$.
$G_{\mathrm{W}}(\mathbf{r}'', t; \mathbf{r}', 0)$	Wigner propagator from point $\mathbf{r}'$ at time 0 to point $\mathbf{r}''$ at time t.
$\widetilde{G}(\gamma, \gamma_0)$	Fourier transform of the Wigner propagator G_{W}.
γ, α, β	Dual Fourier variables associated to phase-space variables.
$\hat{U}, U_{\mathrm{W}}$	Unitary evolution operator and its associated Weyl symbol.
$K(\mathbf{q}'', t''; \mathbf{q}', t')$	Feynman propagator from point $\mathbf{q}'$ at time t' to point $\mathbf{q}''$ at time t''.
$J_{\mathrm{W}}(\mathbf{r}'', t; \mathbf{r}', 0)$	Propagating function acting on the Wigner function of S.
$\mathcal{F}_{\mathrm{W}}\left[\{\mathbf{r}\}, \{\tilde{\mathbf{r}}\}, t\right]$	Influence functional in phase-space.
$R_j(\mathbf{q}'', t''; \mathbf{q}', t')$	Hamilton principal function.
$\mathcal{S}$	Action functional.
$\mathcal{S}^{\mathrm{vV}}$	Action functional in the van Vleck approximation.
ϕ_n	Discrete-time action functional.
Φ	Action functional in the van Vleck approximation of U_{W}.
A_j	Symplectic area.
$\mathrm{Ai}(\mathbf{r})$	Airy function.
$H_j\left(\mathbf{r}_j\right)$	Energy of the classical trajectory j.
$\wedge$	Binary operation indicating a symplectic product among two phase-space vectors.
$\mathcal{D}\mathbf{r}$,$\mathcal{D}\mathbf{R}$	Measures in the path integral formalism.
$\gamma(t)$	Dissipation kernel.

$I(\omega)$	Spectral density associated to the bath.
$\alpha(t)$, $\alpha_{\rm R}(t)$, $\alpha_{\rm I}(t)$	Noise correlation kernel together with its real and imaginary parts.
$\hat{\xi}_{\pm}(t)$	Stochastic bath operators acting on the Hilbert spaces of B and SB.
$\hat{\zeta}_{\pm}(t)$	Stochastic bath operators acting on the Hilbert space of B.

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Chapter 1

Quantum mechanics in phase space

1.1 Introduction

The phase-space formulation of quantum mechanics has its roots in the classic work of E. Wigner, where he introduced the phase-space distribution function in the derivation of quantum corrections terms to classical thermodynamic averages [1]. H. Weyl, around the same time and independently, made decisive contributions to laid out the foundations of this remarkable picture of quantum mechanics [2]. Nonetheless, the full, self-standing theory was put together in a crowning achievement by H. Groenewold and J. Moyal independently of each other [3–5].

The main tool for this formulation of the quantum theory is the phase-space distribution function. Although there are several kind of distributions that enables this formulation of quantum mechanics, including those of Wigner, Glauber-Sudarshan, Husimi, Kirkwood, etc; from all them, the Wigner distribution function is the only fundamentally associated to the Lie algebra structure of quantum mechanics [2, 6, 7]. In this Wigner-Weyl formulation of the theory, every quantum observable $\hat{A}$ is represented by a real valued phase-space function $A(\mathbf{p}, \mathbf{q})$ via the Weyl transform. Conversely, every real phase-space function $A(\mathbf{p}, \mathbf{q})$ represents some quantum observable $\hat{A}$ via Weyl quantization. Moreover, this correspondence is bijective [8], i.e., quantum mechanics can be consistent and autonomously formulated in phase space, with c-number position and momentum variables simultaneously placed on an equal footing, in a way that fully respects Heisenberg's principle [5]. This framework is equivalent to the Hilbert space approach of the theory in configuration space. However, the phase-space version provides a great amount of connections to the formulation of statistical physics and, by extension, to classical mechanics. In this manner, it appeals naturally to one's intuition and can provide useful physical insights that cannot be easily gained from other approaches [6].

Wigner function behaves like a quasi-probability density, in the sense that the expectation values of the physical observables can be computed as in the classical case. However, the fact that the Wigner function can take on negative values put strong limits to this interpretation linked to probability. Nonetheless, the Wigner function satisfies a broad set of properties that makes it easy to handle in calculations. For instance, it is a real-valued function which naturally admits the mixed state representation which is not so better suited in standard wave mechanics. In Table 1.1 we can see some key conceptual differences between these two formulations of the quantum theory that arise basically from the fact that wave mechanics belong to the projective Hilbert space whereas the phase-space formulation does not.

	Wave mechanics	**Wigner p-s mechanics**
Initial condition	$\psi(\mathbf{q}, 0)$	$\rho_{\mathrm{W}}(\mathbf{p}, \mathbf{q}, 0)$
Dynamics	Feynman propagator	Wigner propagator
Final evolution	$\psi(\mathbf{q}, t)$	$\rho_{\mathrm{W}}(\mathbf{p}, \mathbf{q}, t)$
Mixed states	No	Yes

Table 1.1: *Wave mechanics vs. Wigner phase-space formulation*

Finally, the dynamical evolution of the Wigner distribution can be formulated in terms either of the Groenewold-Moyal equation [3, 4], or by a non-local integral kernel known as Wigner propagator [9]. It is precisely the latter framework the one which will be used throughout the present work.

In this chapter, we shortly review the formulation of the Wigner distribution function and the Weyl quantization scheme. A collection of properties fulfilled by this distribution and its associated Wigner propagator are summarized. For a detailed description of these topics there are several reviews available in the literature. Among them, see [6, 8, 10–13]

1.2 The Weyl-Wigner formalism

1.2.1 The ordering problem

The goal of the Wigner-Weyl formalism is to establish a bijective correspondence among phase-space functions $A_{\mathrm{W}}(\mathbf{r})$[1] and phase-space observables $\hat{A}(\hat{\mathbf{r}})$. The mathematical tool that satisfies this requirements is the Weyl-Wigner transform: It is an invertible map between functions in the quantum phase-space formulation and Hilbert space operators in the Schrödinger picture. Usually, when we are transforming phase-space functions into operator-valued functions, this transform is named Weyl transform and was introduced by Weyl [2]. On the other hand, when we are mapping operators into functions in phase-space, this transform is called the Wigner transform [1].

In the special case of moving from vectorial functions on phase-space to operator functions in Hilbert space, there must exist a mechanism that guarantees the correct ordering of the canonical operators. To achieve this, while keeping the correspondence of a unique operator associate to a fixed phase-space function, Weyl proposed in his celebrated paper [2], the following prescription: Write down the double Fourier transform of the phase space function as

$$A_{\mathrm{W}}(\mathbf{p}, \mathbf{q}) = \int \mathrm{d}\mathbf{u}\mathrm{d}\mathbf{v}\ \alpha(\mathbf{u}, \mathbf{v}) e^{\mathrm{i}(\mathbf{u}\cdot\mathbf{p}+\mathbf{v}\cdot\mathbf{q})}. \tag{1.1}$$

Then, the quantization appears as the replacement in the exponential of $\mathbf{p} \to \hat{\mathbf{p}}$ and $\mathbf{q} \to \hat{\mathbf{q}}$,

$$\hat{A}(\hat{\mathbf{p}}, \hat{\mathbf{q}}) = \int \mathrm{d}\mathbf{u}\mathrm{d}\mathbf{v}\ \alpha(\mathbf{u}, \mathbf{v}) e^{\mathrm{i}(\mathbf{u}\cdot\hat{\mathbf{p}}+\mathbf{v}\cdot\hat{\mathbf{q}})}. \tag{1.2}$$

The coefficients $\alpha(\mathbf{u}, \mathbf{v})$ of the Fourier expansion of $A_{\mathrm{W}}(\mathbf{p}, \mathbf{q})$ can be obtained by an inverse Fourier

[1] $\mathbf{r} = (\mathbf{p}, \mathbf{q})$ is a vector in a $2f$ dimensional phase-space.

transform as

$$\alpha(\mathbf{u},\mathbf{v}) = \frac{1}{(2\pi)^{2f}} \int \mathrm{d}\mathbf{p}\mathrm{d}\mathbf{q} A_{\mathrm{W}}(\mathbf{p},\mathbf{q}) e^{-\mathrm{i}(\mathbf{u}\cdot\mathbf{p}+\mathbf{v}\cdot\mathbf{q})}. \tag{1.3}$$

It is possible to show that the Weyl quantization procedure is just the inverse of the operation that goes from Hilbert space to phase-space and will be known as Wigner transform [8]. Nonetheless, there is a non-trivial question that should be addressed by the Weyl quantization scheme: Is there a unique way of mapping phase-space functions which are non-separable products of $\mathbf{p}$ and $\mathbf{q}$? For instance, since $\hat{\mathbf{p}}$ and $\hat{\mathbf{q}}$ do not commute, a classically well-defined product of the form $\mathbf{p}^n\mathbf{q}^m$ can be translated into a multitude of quantum operators that differ in the ordering of the factors of the canonical operators. The most unbiased choice would treat all possible orderings on equal footing by taking the average value of all the combinations. This special and important prescription is called Weyl ordering or Weyl quantization. For a product of operators $\hat{A}_1\hat{A}_2\ldots\hat{A}_n$, the Weyl ordering is defined as the sum over all permutations $P(i_1,\ldots,i_n)$ of the indices such that[2] [14]

$$\left(\hat{A}_1\hat{A}_2\ldots\hat{A}_n\right)_{\mathrm{O}} = \frac{1}{\text{number of permutations}} \sum_P \hat{A}_{i_1}\hat{A}_{i_2}\ldots\hat{A}_{i_n}. \tag{1.4}$$

There is an elegant method, for one single component operators, to construct the Weyl ordering. It is based on the identity [14]

$$(u\hat{p}+v\hat{q})^n = \sum_{k=0}^{n} \binom{n}{k} u^{n-k}v^k \left(\hat{p}^{n-k}\hat{q}^k\right)_{\mathrm{O}}. \tag{1.5}$$

Thus, the $(k+l)$th power of $u\hat{p}+v\hat{q}$ serves as the generating function for the Weyl product $\left(\hat{p}^k\hat{q}^l\right)_{\mathrm{O}}$, if one differentiates with respect to the formal parameters u, v

$$\left(\hat{p}^k\hat{q}^l\right)_{\mathrm{O}} = \frac{1}{(k+l)!}\left(\frac{\partial}{\partial u}\right)^k\left(\frac{\partial}{\partial v}\right)^l (u\hat{p}+v\hat{q})^{k+l}. \tag{1.6}$$

1.2.2 Weyl transform for products of canonical operators

As we have previously mentioned in the introduction, the Wigner-Weyl operations when going from Hilbert space to phase-space and viceversa constitutes a bijection. Meanwhile, in the last section we showed how to proceed from c-function into operator space by doing an appropriate ordering. In the present section we want to address the issue of how to transform products of the canonical quantum operators into phase-space. Taking advantage of the operator method developed in appendix B, we have found a quite interesting way to calculate Weyl transforms of products of pair of canonical operators in the form $\hat{p}^m\hat{q}^n$ and $\hat{q}^n\hat{p}^m$. Here we summarize these results and leave the main derivation of these expressions for Appendix D.

[2] The subindex "O" stands for Weyl ordered product of operators, whereas "W" stands for Weyl symbol of an operator.

$$(\hat{p}^m \hat{q}^n)_{\mathrm{W}} = \left(\frac{\hbar}{2\mathrm{i}}\right)^n \frac{\mathrm{d}^n}{\mathrm{d}P^n} \left[(p+P)^m \exp\left(\frac{2\mathrm{i}}{\hbar} qP\right)\right]_{P=0}$$
$$= \left(\frac{\hbar}{2\mathrm{i}}\right)^n \sum_{k=0}^{m} \binom{m}{k} p^{m-k} \frac{\mathrm{d}^n}{\mathrm{d}P^n} \left[P^k \exp\left(\frac{2\mathrm{i}}{\hbar} qP\right)\right]_{P=0}, \tag{1.7}$$

and

$$(\hat{q}^n \hat{p}^m)_{\mathrm{W}} = \left(-\frac{\hbar}{2\mathrm{i}}\right)^m \frac{\mathrm{d}^m}{\mathrm{d}Q^m} \left[(q+Q)^n \exp\left(-\frac{2\mathrm{i}}{\hbar} pQ\right)\right]_{Q=0}$$
$$= \left(-\frac{\hbar}{2\mathrm{i}}\right)^m \sum_{k=0}^{n} \binom{n}{k} q^{n-k} \frac{\mathrm{d}^n}{\mathrm{d}Q^m} \left[Q^k \exp\left(-\frac{2\mathrm{i}}{\hbar} pQ\right)\right]_{Q=0}. \tag{1.8}$$

1.2.3 The Weyl symbol of an operator

For an arbitrary operator $\hat{A}(\hat{\mathbf{p}}, \hat{\mathbf{q}})$, the Weyl symbol is formally defined as

$$A_{\mathrm{W}}(\mathbf{p}, \mathbf{q}) = T_{\mathrm{W}}[\hat{A}](\mathbf{p}, \mathbf{q}) = \mathrm{Tr}[\hat{A}(\hat{\mathbf{p}}, \hat{\mathbf{q}}) \hat{d}(\hat{\mathbf{p}}, \hat{\mathbf{q}})], \tag{1.9}$$

with $\mathbf{p} = (p_1, p_2, \ldots, p_f)$ and $\mathbf{q} = (q_1, q_2, \ldots, q_f)$. We are dealing with a general $2f$-dimensional multi-particle phase space in such a way that for each degree of freedom (DOF), we are considering pairs of conjugate variables. The $\hat{d}(\hat{\mathbf{p}}, \hat{\mathbf{q}})$ operator is defined, in terms of the displacement operator $\hat{T}(\mathbf{u}, \mathbf{v})$ that generates the polynomial algebra of observables in quantum mechanics [7], as

$$\hat{d}(\hat{\mathbf{p}}, \hat{\mathbf{q}}) = \frac{1}{(2\pi\hbar)^f} \int \mathrm{d}\mathbf{u} \mathrm{d}\mathbf{v} \exp\left\{\frac{\mathrm{i}}{\hbar}(\mathbf{u} \cdot \mathbf{p} + \mathbf{v} \cdot \mathbf{q}) \hat{T}(-\mathbf{u}, -\mathbf{v})\right\}. \tag{1.10}$$

See Appendix B for a set of properties fulfilled by these two operators [11].

If the operator $\hat{A}(\hat{\mathbf{p}}, \hat{\mathbf{q}})$ is written in a symmetrized form, its Weyl symbol will be obtained by the simple substitution $\hat{\mathbf{q}} \to q$ and $\hat{\mathbf{p}} \to p$. Particularly, this is true for all operators having the structure $\hat{M}(\hat{\mathbf{p}}) + \hat{N}(\hat{\mathbf{q}})$; being the separable standard Hamiltonians the most relevant example.

The definition of the Weyl symbol for the operator $\hat{A}(\hat{\mathbf{p}}, \hat{\mathbf{q}})$ in Eq. (1.9) is basis-independent. However, for practical calculations, it would be convenient to have it written in a basis-dependent form. By choosing the standard coordinate basis, we can write the Weyl symbol as

$$A_{\mathrm{W}}(\mathbf{p}, \mathbf{q}) = \int \mathrm{d}\mathbf{u} \exp\left\{-\frac{\mathrm{i}}{\hbar} \mathbf{p} \cdot \mathbf{u}\right\} \left\langle \mathbf{q} + \frac{\mathbf{u}}{2} \right| \hat{A} \left| \mathbf{q} - \frac{\mathbf{u}}{2} \right\rangle. \tag{1.11}$$

A similar expression can be written in terms of the momentum representation.

1.2.4 The Wigner distribution function

The quantum state of a physical system is completely determined by the density operator $\hat{\rho}$. For the general case of a mixed state, it takes the form

$$\hat{\rho} = \sum_i P_i \left|\psi_i\right\rangle \left\langle\psi_i\right|, \tag{1.12}$$

with $P_i > 0$ the set of probabilities that indicates the fraction of the statistical ensemble being described by a particular pure state present in the superposition. Therefore, $\sum_i P_i = 1$. As can be easily checked from its definition, the density operator satisfies the Hermicity property $\hat{\rho}^\dagger = \hat{\rho}$, which gives to it the status of a quantum observable. Additionally, the density operator satisfies $\hat{\rho}^2 \leq 1$, with the equality satisfied only by pure states. In this particular case, all but one of the probabilities P_i are zero, giving place to a pure quantum state described by $\hat{\rho} = |\psi\rangle\langle\psi|$.

As long as $\hat{\rho}$ completely describes the state of the system in the Schrödinger picture, the natural question that arises is: which physical quantity would be its equivalent in the phase-space version of the theory? The answer comes directly from Eq. (1.11). The Wigner function, i.e., the version of $\hat{\rho}$ in phase-space, is defined as the Weyl transform of the density operator

$$\rho_{\mathrm{W}}(\mathbf{p},\mathbf{q}) = \int \mathrm{d}\mathbf{u} \exp\left\{-\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{u}\right\} \left\langle \mathbf{q}+\frac{\mathbf{u}}{2}\right| \frac{\hat{\rho}}{(2\pi\hbar)^f} \left|\mathbf{q}-\frac{\mathbf{u}}{2}\right\rangle . \tag{1.13}$$

This distribution function satisfies some interesting properties in phase-space. In Table 1.1 there are summarized the most relevant of them, while in Appendix E they are formally proved.

The Wigner function takes on a very interesting form when the density operator $\hat{\rho}$ represents a general mixed state,

$$\rho_{\mathrm{W}}(\mathbf{p},\mathbf{q}) = \sum_i P_i \, \rho_{\mathrm{W},i}(\mathbf{p},\mathbf{q}), \tag{1.14}$$

showing that the Wigner transform of a mixed state corresponds to a mixed Wigner function in phase-space. On the other hand, when the system can be described by a pure state, the Wigner function can be written as

$$\rho_{\mathrm{W}}(\mathbf{p},\mathbf{q}) = \int \mathrm{d}\mathbf{u} \exp\left\{-\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{u}\right\} \psi(\mathbf{q}+\mathbf{u}/2)\psi^*(\mathbf{q}-\mathbf{u}/2). \tag{1.15}$$

This expression can be understood as an f-dimensional Fourier transform acting on the product of two wave functions separated in their arguments by $\mathbf{u}$ [11].

Contrary to what one might think about this distribution, it does not behaves like a probability density function (PDF) in phase-space. The concept of a joint probability at a $(\mathbf{p},\mathbf{q})$ phase-space point is not allowed in quantum mechanics due to the Heisenberg uncertainty principle. Even more, one of the more prominent characteristics of the Wigner function lies in the fact that it can take on negative values, completely ruling out its interpretation as a PDF. Nonetheless, as can be seen in Table 1.2, the Wigner distribution allows for calculating expectation values of physical observables just like the classical case where a proper PDF can be unambiguously defined. This seeming PDF behavior, together with its intrinsic negativities, which gives it its quantum characteristics, has put it into a pseudo-PDF status. With all of this in mind, the quantum phase-space distribution function should therefore be considered simply a mathematical tool that facilitates quantum calculations.

1.3 Properties of the Wigner function

The Wigner distribution function satisfies some interesting properties that can be proved from its definition in Eq. (1.13). In Table 1.2 we summarize the most relevant properties fulfilled by this function [15], whereas in Appendix E we present a complete derivation of them.

Wigner function is real and normalized in phase space
$\rho_{\mathrm{W}}^{*}(\mathbf{p},\mathbf{q}) = \rho_{\mathrm{W}}(\mathbf{p},\mathbf{q}), \qquad \int \mathrm{d}\mathbf{p}\mathrm{d}\mathbf{q}\rho_{\mathrm{W}}(\mathbf{p},\mathbf{q}) = 1$
Marginals of the Wigner function
$\int \mathrm{d}\mathbf{q}\rho_{\mathrm{W}}(\mathbf{p},\mathbf{q}) = \sum_f P_f \lvert\psi_f(\mathbf{q})\rvert^2, \qquad \int \mathrm{d}\mathbf{p}\rho_{\mathrm{W}}(\mathbf{p},\mathbf{q}) = \sum_f P_f \lvert\psi_f(\mathbf{p})\rvert^2$
Wigner function is bounded for pure states
$\lvert\rho_{\mathrm{W}}(\mathbf{p},\mathbf{q})\rvert \leq \left(\frac{2}{\hbar}\right)^f$
Overlap of two Wigner functions
$\int \mathrm{d}^f p \mathrm{d}^f q \rho_{\mathrm{W},\psi}(\mathbf{p},\mathbf{q})\rho_{\mathrm{W},\phi}(\mathbf{p},\mathbf{q}) = h^{-f}\lvert\langle\psi\vert\phi\rangle\rvert^2$
Full overlap of a Wigner function with itself
If $\langle\psi\vert\psi\rangle = 1, \text{then} \int \mathrm{d}^f p \mathrm{d}^f q \rho_{\mathrm{W}}^2(\mathbf{p},\mathbf{q}) = h^{-f}$
Orthogonality of Wigner functions: they can be negative
If $\langle\psi\vert\phi\rangle = 0$, then $\int \mathrm{d}^f p \mathrm{d}^f q \rho_{\mathrm{W},\psi}(\mathbf{p},\mathbf{q})\rho_{\mathrm{W},\phi}(\mathbf{p},\mathbf{q}) = 0$
Translational properties of the Wigner function
If $\psi(\mathbf{q}) \to \psi(\mathbf{q}-\mathbf{q}') \implies \rho_{\mathrm{W}}(\mathbf{p},\mathbf{q}) \to \rho_{\mathrm{W}}(\mathbf{p},\mathbf{q}-\mathbf{q}')$ If $\psi(\mathbf{q}) \to \psi(\mathbf{q})\exp\left(\frac{\mathrm{i}}{\hbar}\mathbf{q}\cdot\mathbf{p}'\right) \implies \rho_{\mathrm{W}}(\mathbf{p},\mathbf{q}) \to \rho_{\mathrm{W}}(\mathbf{p}-\mathbf{p}',\mathbf{q})$
Reflection symmetries of the of the Wigner function
Time reflection: $\psi(\mathbf{q}) \to [\psi(\mathbf{q})]^* \implies \rho_{\mathrm{W}}(\mathbf{p},\mathbf{q}) \to \rho_{\mathrm{W}}(-\mathbf{p},\mathbf{q})$ Space reflection: $\psi(\mathbf{q}) \to \psi(-\mathbf{q}) \implies \rho_{\mathrm{W}}(\mathbf{p},\mathbf{q}) \to \rho_{\mathrm{W}}(-\mathbf{p},-\mathbf{q})$
Operator expectation values
$\langle f(\hat{\mathbf{q}})\rangle = \int \mathrm{d}\mathbf{q}\mathrm{d}\mathbf{p} f(\mathbf{q})\rho_{\mathrm{W}}(\mathbf{p},\mathbf{q})$ $\langle g(\hat{\mathbf{p}})\rangle = \int \mathrm{d}\mathbf{q}\mathrm{d}\mathbf{p} g(\mathbf{p})\rho_{\mathrm{W}}(\mathbf{p},\mathbf{q})$ If $\hat{H}(\hat{\mathbf{p}},\hat{\mathbf{q}}) = \hat{T}(\hat{\mathbf{p}}) + \hat{V}(\hat{\mathbf{q}}), \qquad \langle\hat{H}\rangle = \int \mathrm{d}\mathbf{q}\mathrm{d}\mathbf{p} H(\mathbf{p},\mathbf{q})\rho_{\mathrm{W}}(\mathbf{p},\mathbf{q})$
Linear superposition of Wigner functions for mixed states
If $\hat{\rho} = \sum_i P_i \lvert\psi_i\rangle\langle\psi_i\rvert, \qquad \rho_{\mathrm{W}}(\mathbf{p},\mathbf{q}) = \sum_i P_i \rho_{\mathrm{W},i}(\mathbf{p},\mathbf{q})$
Relation to the wave function in coordinate space
$\psi(\mathbf{q}) = \frac{1}{\psi^*(\mathbf{0})}\int \mathrm{d}^f p \exp\left\{\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{q}\right\}\rho_{\mathrm{W}}\left(\mathbf{p},\frac{\mathbf{q}}{2}\right)$

Table 1.2: *Mathematical properties of the Wigner distribution function*

1.4 Quantum dynamics in phase space

For an isolated system described by a time-independent Hamiltonian $\hat{H}_{\mathrm{S}}$, the time evolution of the operator $\hat{\rho}_{\mathrm{S}}(0)$ is determined by the Landau-von Neumann equation

$$\mathrm{i}\hbar\frac{\mathrm{d}\hat{\rho}_{\mathrm{S}}}{\mathrm{d}t} = [\hat{H}_{\mathrm{S}}, \hat{\rho}_{\mathrm{S}}]. \tag{1.16}$$

Its formal solution can be written as the standard operator product

$$\hat{\rho}_{\mathrm{S}}(t) = \hat{U}(t)\hat{\rho}_{\mathrm{S}}(0)\hat{U}^{\dagger}(t), \tag{1.17}$$

with $\hat{U}(t) = \exp\left(-\mathrm{i}t\hat{H}_{\mathrm{S}}/\hbar\right)$ the unitary evolution operator. Although $\hat{\rho}_{\mathrm{S}}(t)$ in Eq. (1.17) formally solves Eq. (1.16), it does not represent, at this stage, an explicit solution of the dynamics under study. With the purpose of finding the desirable solution to $\hat{\rho}_{\mathrm{S}}(t)$, different theoretical approaches has been formulated. Among these, we would like to highlight, on one hand, the Moyal equation and, on the other hand, the Wigner propagator method. In the first case, the evolution of the dynamics is studied by means of the equation [10]

$$\frac{\partial}{\partial t}\rho_{\mathrm{W}}(\mathbf{p},\mathbf{q},t) = -\frac{\partial H_{\mathrm{W}}}{\partial p}\frac{\partial \rho_{\mathrm{W}}}{\partial q} + \frac{\partial H_{\mathrm{W}}}{\partial q}\frac{\partial \rho_{\mathrm{W}}}{\partial p} + \sum_{n>2,\mathrm{odd}} \frac{1}{n!}\left(\frac{\hbar}{2\mathrm{i}}\right)^{n-1} \frac{\partial^n H_{\mathrm{W}}}{\partial q^n}\frac{\partial^n \rho_{\mathrm{W}}}{\partial p^n}, \tag{1.18}$$

where the first two terms correspond to the classical evolution of the PDF $\rho_{\mathrm{W}}(\mathbf{p},\mathbf{q},t)$, and the remaining terms provide the quantum corrections. This equation can be shortened by the introduction of the Moyal brackets [4],

$$\frac{\partial}{\partial t}\rho_{\mathrm{W}}(\mathbf{p},\mathbf{q},t) = \{H_{\mathrm{W}}, \rho_{\mathrm{W}}\}_{\mathrm{M}}\,. \tag{1.19}$$

In the second case, the propagation of the dynamics is formulated by means of an integral kernel. Its mathematical form and its interpretation depends upon the formal construct that supports the model. Thus, in configuration space is the Feynman propagator the integral kernel that evolves the system [16–18], whereas in phase-space the dynamical evolutions corresponds to the Wigner propagator. In the present work, we will be working under the latter approach. Therefore, we will start from Eq. (1.17) by projecting this operator product into the coordinate basis such that

$$\rho_{\mathrm{S}}(\mathbf{q}''_{+},\mathbf{q}''_{-},t) = \int \mathrm{d}\mathbf{q}'_{+}\mathrm{d}\mathbf{q}'_{-} J\left(\mathbf{q}''_{+},\mathbf{q}''_{-},t;\mathbf{q}'_{+},\mathbf{q}'_{-},0\right)\rho_{\mathrm{S}}(\mathbf{q}'_{+},\mathbf{q}'_{-},0), \tag{1.20}$$

where

$$J\left(\mathbf{q}''_{+},\mathbf{q}''_{-},t;\mathbf{q}'_{+},\mathbf{q}'_{-},0\right) = U\left(\mathbf{q}''_{+},\mathbf{q}'_{+},t\right)U^{*}\left(\mathbf{q}''_{-},\mathbf{q}'_{-},t\right), \tag{1.21}$$

defines the propagating function for the unitary case.

By applying the Weyl transform to Eq. (1.20), we are able to translate the dynamical evolution of the coordinate density matrix into the evolution of the Wigner function in phase-space. Thus,

$$\begin{aligned}\rho_{\mathrm{W}}(\mathbf{r}'',t) =& \frac{1}{(2\pi\hbar)^f}\int \mathrm{d}\mathbf{v}\mathrm{d}\mathbf{v}'\mathrm{d}\mathbf{r}' e^{\frac{\mathrm{i}}{\hbar}(\mathbf{p}'\cdot\mathbf{v}'-\mathbf{p}''\cdot\mathbf{v})} \\ &\times J\left(\mathbf{q}''+\frac{\mathbf{v}}{2},\mathbf{q}''-\frac{\mathbf{v}}{2},t;\mathbf{q}'+\frac{\mathbf{v}'}{2},q'-\frac{\mathbf{v}'}{2},0\right)\rho_{\mathrm{W}}(\mathbf{r}',0).\end{aligned} \tag{1.22}$$

By means of this equation, we can give a first definition of the Wigner integral kernel as

$$G_{\mathrm{W}}(\mathbf{r}'', t; \mathbf{r}', 0) = \frac{1}{(2\pi\hbar)^f} \int \mathrm{d}\mathbf{v}\mathrm{d}\mathbf{v}' e^{\frac{\mathrm{i}}{\hbar}(\mathbf{p}'\cdot\mathbf{v}' - \mathbf{p}''\cdot\mathbf{v})} \times U\left(\mathbf{q}'' + \frac{\mathbf{v}}{2}, \mathbf{q}' + \frac{\mathbf{v}'}{2}, t\right) U^*\left(\mathbf{q}'' - \frac{\mathbf{v}}{2}, \mathbf{q}' - \frac{\mathbf{v}'}{2}, t\right), \tag{1.23}$$

such that

$$\rho_{\mathrm{W}}(\mathbf{r}'', t) = \int \mathrm{d}\mathbf{r}' G_{\mathrm{W}}(\mathbf{r}'', t; \mathbf{r}', 0)\rho_{\mathrm{W}}(\mathbf{r}', 0). \tag{1.24}$$

As can be clearly seen from this expression, the Wigner integral kernel plays the role of a dynamical propagator for the quantum state in phase-space. Thus, the *Wigner propagator* plays in phase-space the same role that the Feynman propagator plays in configuration space, i.e., it determines how a quantum state is propagated in time. Consequently, as in the Feynman path integral theory, knowing the propagator will allows us to know the time evolution of a physical system in phase-space. This picture, in turn, represents the set up for an enhanced path integral version of quantum theory formulated completely in phase-space. Although there are different approaches to a phase-space quantum mechanics description [6, 19–22], the one we are interested in for the present work makes use of the path integral representation of the Wigner operator [9, 23, 24] to describe the time evolution of quantum states.

Considering again the propagator in Eq. (1.23), we can see that it is related to the propagating function by means of a double Fourier transform. Instead of taking the Fourier transform over the propagating function, there is an alternate way to go to phase space and once there, obtain the Wigner propagator. The key idea is to consider first the Weyl transform of the propagating function. As long as the system under consideration is closed, i.e., its DOF are not coupled to a heat bath, the propagating function can be written as a product of propagators in configuration space. Then, by applying to them, individually, the Weyl transform will give us the Weyl propagator as

$$U_{\mathrm{W}}(\mathbf{r}, t) = \int \mathrm{d}\mathbf{u} \exp\left(-\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{u}\right) U\left(\mathbf{q} + \frac{\mathbf{u}}{2}, \mathbf{q} - \frac{\mathbf{u}}{2}, t\right). \tag{1.25}$$

Consequently, we are now in position to apply the symplectic Fourier transform[3] to the product of the Weyl propagators to obtain the Wigner propagator as [25]

$$G_{\mathrm{W}}(\mathbf{r}'', t; \mathbf{r}', 0) = \int \frac{\mathrm{d}\tilde{r}}{(2\pi\hbar)^2} e^{\frac{\mathrm{i}}{\hbar}(\mathbf{r}' - \mathbf{r}'')\wedge\tilde{r}} U_{\mathrm{W}}\left(\frac{\tilde{\mathbf{r}}' + \tilde{\mathbf{r}}'' + \tilde{\mathbf{r}}}{2}, t\right) U_{\mathrm{W}}^*\left(\frac{\tilde{\mathbf{r}}' + \tilde{\mathbf{r}}'' - \tilde{\mathbf{r}}}{2}, t\right). \tag{1.26}$$

With the symplectic product defined, by means of the symplectic matrix J, as

$$\mathbf{r}_1 \wedge \mathbf{r}_2 = \mathbf{r}_1^{\mathrm{T}} \mathsf{J} \mathbf{r}_2, \qquad \mathsf{J} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{1.27}$$

It is relevant to point out the importance of the Weyl propagator as a tool from which is possible to build a semiclassical approximation. Thus, as we will see in the next chapter, it will be the starting point for the van Vleck semiclassical approximation of the propagator [26, 27].

[3]See Eq. 4.33

1.5 Properties of the Wigner propagator

Some useful properties of the Weyl propagator can be deduced and then applied to characterize the Wigner propagator (see appendix E). Also, the Wigner propagator itself satisfies some useful properties that are summarized in Table 1.2 [9].

Wigner propagator at initial time
$G_{\mathrm{W}}(\mathbf{r}'', 0; \mathbf{r}', 0) = \delta(\mathbf{r}'' - \mathbf{r})$
Composition Law
$G_{\mathrm{W}}(\mathbf{r}'', 0; \mathbf{r}', 0) = \int \mathrm{d}^{2f}\mathbf{r}''' G_{\mathrm{W}}(\mathbf{r}'', t; \mathbf{r}''', t''') G_{\mathrm{W}}(\mathbf{r}''', t'''; \mathbf{r}', 0)$
Backward time propagator
$G_{\mathrm{W}}(\mathbf{r}'', 0; \mathbf{r}', 0) = G_{\mathrm{W}}(\mathbf{r}', -t; \mathbf{r}'', 0) = G_{\mathrm{W}}(\mathbf{r}', 0; \mathbf{r}'', t)$
G_{W} is real
Since $\rho_{\mathrm{W}}(\mathbf{r}_1, \ldots, \mathbf{r}_f) \in \mathbb{R}$, then, $G_{\mathrm{W}}(\mathbf{r}'', 0; \mathbf{r}', 0) \in \mathbb{R}$
Orthogonality
$\int \mathrm{d}^{2f}\mathbf{r}''' G_{\mathrm{W}}(\mathbf{r}'', 0; \mathbf{r}', 0) G_{\mathrm{W}}(\mathbf{r}''', 0; \mathbf{r}', 0) = \delta(\mathbf{r}'' - \mathbf{r}')$
Aditional properties
★ For autonomous systems, G_{W} generates a group parametrized by t

Table 1.3: *Properties of the Wigner propagator*

1.6 Path integral representation of the Wigner propagator

Taking Eq. (1.17) as the staring point, we want to transform it into a product of c-functions depending upon the phase-space coordinates and momenta. Thus, the Weyl transform of the product of three operators allows us to write Eq. (1.17) as[4]

$$\begin{aligned}\rho_{\mathrm{W}}(\mathbf{r}, t) =& \frac{1}{(\pi\hbar)^{2f}} \int \mathrm{d}\mathbf{r}_1 \mathrm{d}\mathbf{r}_2 \mathrm{d}\mathbf{r}_3 U_{\mathrm{W}}(\mathbf{r}_1) \rho_{\mathrm{W}}(\mathbf{r}_2) U_{\mathrm{W}}^*(\mathbf{r}_3) \\ &\times \exp\left[\frac{2\mathrm{i}}{\hbar}(\mathbf{r} \wedge \mathbf{r}_3 + \mathbf{r}_2 \wedge \mathbf{r}_1)\right] \delta[\mathbf{r} + \mathbf{r}_2 - (\mathbf{r}_3 + \mathbf{r}_1)].\end{aligned} \tag{1.28}$$

In order to build the propagator, let us consider a homogeneous partition of the time-like interval of width $\Delta t = t/N$. In this way, we can write down a short-time evolution for the Wigner function in the interval $[n-1, n]\Delta t$ such that [23]

$$\begin{aligned}\rho_{\mathrm{W}}(\mathbf{r}_n, n\Delta t) =& \frac{1}{(\pi\hbar)^{2f}} \int \mathrm{d}\mathbf{r}_{n-1} \mathrm{d}\mathbf{r}'_n \mathrm{d}\mathbf{r}''_n U_{\mathrm{W}}(\mathbf{r}'_n) U_{\mathrm{W}}^*(\mathbf{r}''_n) \\ &\times \exp\left[\frac{2\mathrm{i}}{\hbar}(\mathbf{r}_n \wedge \mathbf{r}''_n + \mathbf{r}_{n-1} \wedge \mathbf{r}'_n)\right] \\ &\times \delta[\mathbf{r}_n + \mathbf{r}_{n-1} - (\mathbf{r}''_n + \mathbf{r}'_n)] \rho_{\mathrm{W}}(\mathbf{r}_{n-1}, (n-1)\Delta t).\end{aligned} \tag{1.29}$$

[4]See Appendix B.

The Weyl symbols of the evolution operator can be calculated in the short-time regime by a Taylor expansion up to first order in Δt. In that spirit,

$$\hat{U}(\Delta t) = \exp\left(-\frac{\mathrm{i}}{\hbar}\hat{H}\Delta t\right) = \sum_{n=0}^{\infty}\frac{1}{n!}\left(-\frac{\mathrm{i}}{\hbar}\Delta t\right)^n \hat{H}^n \approx \hat{1} - \frac{\mathrm{i}}{\hbar}\Delta t\hat{H} + \mathcal{O}(\Delta t^2). \tag{1.30}$$

Therefore,

$$U_{\mathrm{W}}(\Delta t) \approx \left[\hat{1} - \frac{\mathrm{i}}{\hbar}\Delta t\hat{H}\right]_{\mathrm{W}} = 1 - \frac{\mathrm{i}}{\hbar}\Delta t H_{\mathrm{W}} \approx \exp\left(-\frac{\mathrm{i}}{\hbar}\Delta t H_{\mathrm{W}}\right). \tag{1.31}$$

Using this result in Eq. (1.29),

$$\begin{aligned}\rho_{\mathrm{W}}(\mathbf{r}_n, n\Delta t) =& \frac{1}{(\pi\hbar)^{2f}}\int \mathrm{d}\mathbf{r}_{n-1}\mathrm{d}\mathbf{r}'_n\mathrm{d}\mathbf{r}''_n \exp\left(-\frac{\mathrm{i}}{\hbar}\Delta t H_{\mathrm{W}}(\mathbf{r}'_n)\right)\exp\left(\frac{\mathrm{i}}{\hbar}\Delta t H_{\mathrm{W}}(\mathbf{r}''_n)\right) \\ &\times \exp\left[\frac{2\mathrm{i}}{\hbar}(\mathbf{r}_n\wedge\mathbf{r}''_n + \mathbf{r}_{n-1}\wedge\mathbf{r}'_n)\right]\delta[\mathbf{r}_n + \mathbf{r}_{n-1} - (\mathbf{r}''_n + \mathbf{r}'_n)] \\ &\times \rho_{\mathrm{W}}(\mathbf{r}_{n-1}, (n-1)\Delta t) \\ =& \int \mathrm{d}\mathbf{r}_{n-1} G_{\mathrm{W}}(\mathbf{r}_n, n\Delta t; \mathbf{r}_{n-1}, (n-1)\Delta t)\rho_{\mathrm{W}}(\mathbf{r}_{n-1}, (n-1)\Delta t).\end{aligned} \tag{1.32}$$

Then, we can introduce the Wigner propagator $G_{\mathrm{W}}(\mathbf{r}_n, n\Delta t; \mathbf{r}_{n-1}, (n-1)\Delta t) \equiv G_{\mathrm{W}}^{n,n-1}$ as

$$\begin{aligned}G_{\mathrm{W}}^{n,n-1} =& \frac{1}{(\pi\hbar)^{2f}}\int \mathrm{d}\mathbf{r}'_n\mathrm{d}\mathbf{r}''_n \exp\left[\frac{\mathrm{i}}{\hbar}\left(2\mathbf{r}_n\wedge\mathbf{r}''_n + 2\mathbf{r}_{n-1}\wedge\mathbf{r}'_n\right)\right] \\ &\times \exp\left[-\frac{\mathrm{i}}{\hbar}\left(H_{\mathrm{W}}(\mathbf{r}'_n) - H_{\mathrm{W}}(\mathbf{r}''_n)\right)\Delta t\right] \\ &\times \delta[\mathbf{r}_n + \mathbf{r}_{n-1} - (\mathbf{r}''_n + \mathbf{r}'_n)].\end{aligned} \tag{1.33}$$

At this point it is convenient to introduce the semi-sum and difference variables in the following way: $\check{\mathbf{r}}_n = (\mathbf{r}'_n + \mathbf{r}''_n)/2$, and $\tilde{\mathbf{r}}_n = \mathbf{r}'_n - \mathbf{r}''_n$, such that the measure becomes $\mathrm{d}\mathbf{r}'_n\mathrm{d}\mathbf{r}''_n = \mathrm{d}\check{\mathbf{r}}_n\mathrm{d}\tilde{\mathbf{r}}_n$. Thus, by inverting the system defined by these expressions we obtain the relations $\mathbf{r}'_n = \check{\mathbf{r}}_n + \frac{\tilde{\mathbf{r}}_n}{2}$ and $\mathbf{r}''_n = \check{\mathbf{r}}_n - \frac{\tilde{\mathbf{r}}_n}{2}$. Therefore,

$$\begin{aligned}G_{\mathrm{W}}^{n,n-1} =& \frac{1}{(\pi\hbar)^{2f}}\int \mathrm{d}\check{\mathbf{r}}_n\mathrm{d}\tilde{\mathbf{r}}_n \exp\left(\frac{\mathrm{i}}{\hbar}\left[2(\mathbf{r}_{n-1} + \mathbf{r}_n)\wedge\check{\mathbf{r}}_n + (\mathbf{r}_{n-1} - \mathbf{r}_n)\wedge\tilde{\mathbf{r}}_n\right]\right) \\ &\times \exp\left(-\frac{\mathrm{i}}{\hbar}\left[H_{\mathrm{W}}\left(\check{\mathbf{r}}_n + \frac{\tilde{\mathbf{r}}_n}{2}\right) - H_{\mathrm{W}}\left(\check{\mathbf{r}}_n - \frac{\tilde{\mathbf{r}}_n}{2}\right)\right]\Delta t\right) \\ &\times \delta\left(\mathbf{r}_n + \mathbf{r}_{n-1} - 2\check{\mathbf{r}}_n\right).\end{aligned} \tag{1.34}$$

After the integration over the $\check{\mathbf{r}}_n$ variable by means of the delta, we arrive to

$$\begin{aligned}G_{\mathrm{W}}^{n,n-1} =& \frac{1}{(2\pi\hbar)^{2f}}\int \mathrm{d}\tilde{\mathbf{r}}_n \exp\left(\frac{\mathrm{i}}{\hbar}\left[(\mathbf{r}_{n-1} - \mathbf{r}_n)\wedge\tilde{\mathbf{r}}_n\right]\right) \\ &\times \exp\left(-\frac{\mathrm{i}}{\hbar}\left[H_{\mathrm{W}}\left(\frac{1}{2}(\mathbf{r}_n + \mathbf{r}_{n-1}) + \frac{\tilde{\mathbf{r}}_n}{2}\right) - H_{\mathrm{W}}\left(\frac{1}{2}(\mathbf{r}_n + \mathbf{r}_{n-1}) - \frac{\tilde{\mathbf{r}}_n}{2}\right)\right]\Delta t\right).\end{aligned} \tag{1.35}$$

Let us now consider the definitions

$$\bar{\mathbf{r}}_n = \frac{1}{2}(\mathbf{r}_n + \mathbf{r}_{n-1}), \qquad \Delta\mathbf{r}_n = \mathbf{r}_n - \mathbf{r}_{n-1}, \tag{1.36}$$

thus,

$$\begin{aligned} G_{\mathrm{W}}^{n,n-1} =& \frac{1}{(2\pi\hbar)^{2f}} \int \mathrm{d}\tilde{\mathbf{r}}_n \exp\left(-\frac{\mathrm{i}}{\hbar}\left[\Delta\mathbf{r}_n \wedge \tilde{\mathbf{r}}_n\right]\right) \\ & \times \exp\left(-\frac{\mathrm{i}}{\hbar}\left[H_{\mathrm{W}}\left(\bar{\mathbf{r}}_n + \frac{\tilde{\mathbf{r}}_n}{2}\right) - H_{\mathrm{W}}\left(\bar{\mathbf{r}}_n - \frac{\tilde{\mathbf{r}}_n}{2}\right)\right]\Delta t\right). \end{aligned} \tag{1.37}$$

This result applies only to the time interval Δt. In order to obtain the complete propagator over the interval $[0, t]$, we must do the composition over N intervals with $N-1$ integrations,

$$\begin{aligned} G_{N,0} = & \left(\prod_{n=1}^{N-1}\int \mathrm{d}\mathbf{r}_n\right)\left(\prod_{n=1}^{N}\int \frac{\mathrm{d}\tilde{\mathbf{r}}_n}{(2\pi\hbar)^{2f}}\right) \\ & \times \exp\left(-\frac{\mathrm{i}}{\hbar}\sum_{n=1}^{N}\left[\Delta\mathbf{r}_n \wedge \tilde{\mathbf{r}}_n + \left[H_{\mathrm{W}}\left(\bar{\mathbf{r}}_n + \frac{\tilde{\mathbf{r}}_n}{2}\right) - H_{\mathrm{W}}\left(\bar{\mathbf{r}}_n - \frac{\tilde{\mathbf{r}}_n}{2}\right)\right]\Delta t\right]\right). \end{aligned} \tag{1.38}$$

By taking the limit $N \to \infty$, the measures in the above expression becomes

$$\lim_{N\to\infty}\left(\prod_{n=1}^{N-1}\int \mathrm{d}\mathbf{r}_n\right)\lim_{N\to\infty}\left(\prod_{n=1}^{N}\int \frac{\mathrm{d}\tilde{\mathbf{r}}_n}{(2\pi\hbar)^{2f}}\right) = \frac{1}{(2\pi\hbar)^{f}}\int \mathcal{D}\mathbf{r}\int \mathcal{D}\tilde{\mathbf{r}}. \tag{1.39}$$

Meanwhile, the phase of the exponential function takes its continuum form as

$$-\frac{\mathrm{i}}{\hbar}\int_0^t \left[(\dot{\mathbf{r}} \wedge \tilde{\mathbf{r}}) + H_{\mathrm{W}}\left(\mathbf{r} + \frac{\tilde{\mathbf{r}}}{2}\right) - H_{\mathrm{W}}\left(\mathbf{r} - \frac{\tilde{\mathbf{r}}}{2}\right)\right]\mathrm{d}s.$$

Then, by setting up $\mathbf{r}(t) = \mathbf{r}''$ as the final point of propagation of the dynamics at time t, and $\mathbf{r}(0) = \mathbf{r}'$ as the initial point, we obtain the final form of the propagator as

$$G_{\mathrm{W}}(\mathbf{r}'', t; \mathbf{r}', 0) = \frac{1}{(2\pi\hbar)^{f}}\int \mathcal{D}\mathbf{r}\int \mathcal{D}\tilde{\mathbf{r}} \exp\left(-\frac{\mathrm{i}}{\hbar}\mathcal{S}[\{\mathbf{r}\}, \{\tilde{\mathbf{r}}\}, t]\right), \tag{1.40}$$

with

$$\mathcal{S}[\{\mathbf{r}\}, \{\tilde{\mathbf{r}}\}, t] = \int_0^t \left[\dot{\mathbf{r}} \wedge \tilde{\mathbf{r}} + H_{\mathrm{W}}\left(\mathbf{r} + \frac{\tilde{\mathbf{r}}}{2}\right) - H_{\mathrm{W}}\left(\mathbf{r} - \frac{\tilde{\mathbf{r}}}{2}\right)\right]\mathrm{d}s. \tag{1.41}$$

Here, $\mathbf{r}(s)$ represents a possible trajectory in phase-space subject to the boundary conditions $\mathbf{r}(0) = \mathbf{r}'$ and $\mathbf{r}(t) = \mathbf{r}''$. On the other hand, $\tilde{\mathbf{r}}$ represents the quantum fluctuations around the classical trajectories. However, since there are not boundary conditions for $\tilde{\mathbf{r}}$, we will say that all the $\tilde{\mathbf{r}}$ variables are unconstrained quantum fluctuations [23]. Regarding the physical meaning of the action in Eq. (1.41), we can get a more clearer physical insight of it by considering a Hamiltonian in the standard form $H_{\mathrm{W}}(\mathbf{p}, \mathbf{q}) = \frac{1}{2m}\mathbf{p}^2 + V(\mathbf{q})$. Thus, we obtain, by means of

Eq. (1.27) and the Hamilton equations of motion the following structure for the action

$$\mathcal{S}[\{\mathbf{r}\},\{\tilde{\mathbf{r}}\},t] = \int_0^t \left[V\left(\mathbf{q} + \frac{\tilde{\mathbf{q}}}{2}\right) - V\left(\mathbf{q} - \frac{\tilde{\mathbf{q}}}{2}\right) - \tilde{\mathbf{q}}\frac{\partial V(\mathbf{q})}{\partial \mathbf{q}} \right] \mathrm{d}s. \tag{1.42}$$

As can be seen from this expression, the propagator of the Wigner function, by means of the action, contains the non-local expression $V(\mathbf{q}+\tilde{\mathbf{q}}/2) - V(\mathbf{q}-\tilde{\mathbf{q}}/2)$, which clearly expresses the non-local character of the quantum evolution provided by the fact that it depends on the potential at two different positions. Then, this result can be linked to the scalar Aharonov-Bohm effect expressing the fact that the quantum dynamics is fundamentally no-local, which is in sharp contrast with the local evolution of the wave function governed by the Schrödinger equation [28–31]. Therefore, the dynamical quantum non-locality is imprinted in the very generator of the quantum dynamics. By going one step further, we can see what happens to the action when the system potential is the one of the harmonic oscillator. In this linear case, for the particular case of one DOF, we have $V_{\text{har}}(q+\tilde{q}/2) - V_{\text{har}}(q-\tilde{q}/2) = m\omega^2\tilde{q}q$. Additionally, $\tilde{q}dV/dq = m\omega^2\tilde{q}q$. Thus, for a harmonic oscillator the quantum and the classical dynamics coincide because the action becomes null and the Wigner propagator takes the mathematical structure of a Dirac delta along the classical trajectory. Thus, deviations from the classical evolution are only expected for non-harmonic cases as we will explore in the following chapters of the present work. Finally we can summarize the above ideas by saying that the physical interpretation of the Eq. (1.41) is that the dynamical non-local character of quantum mechanics, in this case within the phase-space, is provided by the degree of non-linearity of the system.

Chapter 2

Semiclassical description of the dynamics

2.1 Introduction

In this chapter we discuss the semiclassical limit of the quantum Wigner propagator by means of two different approaches: Firstly, we focus our attention on the path integral representation of the propagator found in section Sec. 1.6. By applying the stationary phase approximation we arrive to its semiclassical version. Secondly, we explore the perturbative expansion of the action up to third order and calculate the mathematical structure that acquires the propagator when we trace out over the quantum fluctuations around the classical trajectory. The main advantage of exploring these two frameworks for the propagator lies in the fact that, even though there is no a unique way to approach the semiclassical regime, all of the possible schemes offers different and complementary perspectives of how the dynamics behaves within this regime.

2.2 van Vleck and Weyl Semiclassical propagators

There is no a unique method to approach the quantum dynamics in the semiclassical realm. Historically, the starting point for a semiclassical analysis of the dynamics of a quantum system was the approximation of the Feynman propagator in configuration space

$$K(\mathbf{q}'', t''; \mathbf{q}', t') \equiv \left\langle \mathbf{q}'' \right| e^{-\frac{\mathrm{i}}{\hbar}\hat{H}t} \left| \mathbf{q}' \right\rangle . \tag{2.1}$$

In the quantum description of the time-evolution, this propagator represents a sum over all paths. However, in the semiclassical realm, the sum only takes into account the set of classical paths, labelled by j, starting from $\mathbf{q}'$ and ending at $\mathbf{q}''$ in time t. Such approximation was first derived by Van Vleck in 1928 [26]. However, Gutzwiller re-derived van Vleck's approximation from Feynman's path integral, arriving to the mathematical expression [32]

$$K(\mathbf{q}'', t''; \mathbf{q}', t') = \sum_j \sqrt{\frac{1}{h^f} \left| \det\left(\frac{\partial^2 R_j(\mathbf{q}'', t''; \mathbf{q}', t')}{\partial \mathbf{q}'' \partial \mathbf{q}'} \right) \right|} \exp\left\{ \frac{\mathrm{i}}{\hbar} R_j(\mathbf{q}'', t''; \mathbf{q}', t') - \mathrm{i}\mu_j \frac{\pi}{2} \right\} . \tag{2.2}$$

Here, $R_j(\mathbf{q}'', t''; \mathbf{q}', t')$ represents the Hamilton principal function along the j-th classical path [33],

$$R_j(\mathbf{q}'', t''; \mathbf{q}', t') = -H_j(\mathbf{r}_j)\, t + \int_{\mathbf{q}'}^{\mathbf{q}''} \mathrm{d}\mathbf{q} \cdot \mathbf{p}_j(\mathbf{q}), \tag{2.3}$$

whereas μ_j denotes the Maslov index of each trajectory [34, 35]. To obtain the semiclassical approximation in phase space we will consider the Weyl symbol of the unitary operator

$$U_{\mathrm{W}}(\mathbf{r},t) = \int \mathrm{d}^f u \exp\left(-\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{u}\right) K\left(\mathbf{q}+\frac{\mathbf{u}}{2},t;\mathbf{q}-\frac{\mathbf{u}}{2},0\right). \tag{2.4}$$

We note that from the coordinate propagator in Eq. (2.1) and its representation in the half-sum and difference coordinates we obtain the relations $\mathbf{q}'' = \mathbf{q}+\mathbf{u}/2$ and $\mathbf{q}' = \mathbf{q}-\mathbf{u}/2$. From these equations emerges a key property of the semiclassical propagation in the coordinate representation

$$\mathbf{q} = \frac{1}{2}\left(\mathbf{q}'+\mathbf{q}''\right). \tag{2.5}$$

Thus, the entry point for semiclassical analysis is an approximation for the coordinate propagator K, and correspondingly, for its Weyl symbol, as a sum over all classical paths, labelled by j, that start at $\mathbf{q}'$ and end up at $\mathbf{q}''$ in time t [27].

By using the van Vleck approximation given in Eq. (2.2) into in Eq. (2.4), we are moving from the semiclassical coordinate approximation to the phase-space description. With the purpose of finding an analytical solution to this integration, we will use the method of stationary phase [9,27]. This procedure is justified by the fact that when the propagator is composed, and therefore, integrated over a set of time intervals, the exponential function $\exp\left[(\mathrm{i}/\hbar)R_j\right]$ becomes highly oscillatory when $\hbar$ is small compared to R_j, which is particularly evident in the classical limit of the propagator. As a consequence, the contributions to the integral mostly cancel. The only paths along which the integrand varies slowly are the classical trajectories which makes the integral of R_j stationary according to Hamilton variational principle. Furthermore, since the equations of motion may have several solutions corresponding to distinct classical paths, one has to add the contributions from all allowed classical paths, hereby making use of the superposition principle [32, 36].

The phase

$$\Phi = R_j\left(\mathbf{q}+\frac{\mathbf{u}}{2},t;\mathbf{q}-\frac{\mathbf{u}}{2},0\right) - \mathbf{p}\cdot\mathbf{u}. \tag{2.6}$$

gives a contribution to the propagator along stationary trajectories that makes the action an extremal. This is the case when the phase fulfill the variational equations

$$\frac{d}{dt}\left(\frac{\partial\Phi}{\partial\dot{\mathbf{u}}}\right) - \frac{\partial\Phi}{\partial\mathbf{u}} = 0. \tag{2.7}$$

Thus, as long as Φ does not depend explicitly on $\dot{\mathbf{u}}$,

$$\frac{\partial\Phi}{\partial\mathbf{u}} = 0. \tag{2.8}$$

Thus, with $\Phi = R_j\left(\mathbf{q}+\frac{\mathbf{u}}{2},t;\mathbf{q}-\frac{\mathbf{u}}{2},0\right) - \mathbf{p}\cdot\mathbf{u} - \hbar\mu_j\frac{\pi}{2}$, and the initial and final points of propagation fixed by the coordinates $(\mathbf{q}',\mathbf{q}'')$ and its conjugate momenta $(\mathbf{p}',\mathbf{p}'')$, we obtain

$$\frac{\partial\Phi}{\partial\mathbf{u}} = -\frac{\partial}{\partial\mathbf{u}}\left[\hbar\mu_j\frac{\pi}{2} + H_j\left(\mathbf{r}_j\right)t + \mathbf{p}\cdot\mathbf{u} - \int_{\mathbf{q}'-\frac{\mathbf{u}}{2}}^{\mathbf{q}''+\frac{\mathbf{u}}{2}} \mathrm{d}\mathbf{Q}\cdot\mathbf{p}_j(\mathbf{Q},H_j)\right] = 0, \tag{2.9}$$

then,

$$\mathbf{p} = \frac{\partial}{\partial \mathbf{u}} \int_{\mathbf{q}'-\frac{\mathbf{u}}{2}}^{\mathbf{q}''+\frac{\mathbf{u}}{2}} \mathrm{d}\mathbf{Q} \cdot \mathbf{p}_j(\mathbf{Q}, H_j) \tag{2.10}$$
$$= \frac{\partial}{\partial \mathbf{u}} \left[\int_{\mathbf{Q}'}^{\mathbf{q}''+\frac{\mathbf{u}}{2}} \mathrm{d}\mathbf{Q} \cdot \mathbf{p}_j(\mathbf{Q}, H_j) - \int_{\mathbf{Q}'}^{\mathbf{q}'-\frac{\mathbf{u}}{2}} \mathrm{d}\mathbf{Q} \cdot \mathbf{p}_j(\mathbf{Q}, H_j) \right],$$

where $\mathbf{Q}'$ represents an arbitrary and fixed point. Thus,

$$\mathbf{p} = \frac{1}{2} \left[\mathbf{p}_j \left(\mathbf{q}'' + \frac{\mathbf{u}}{2}, H_j \right) + \mathbf{p}_j \left(\mathbf{q}' - \frac{\mathbf{u}}{2}, H_j \right) \right], \tag{2.11}$$

which represents the midpoint rule given, in short notation, by

$$\mathbf{p} = \frac{1}{2} \left[\mathbf{p}'' + \mathbf{p}' \right]. \tag{2.12}$$

Based on the symmetrical role of the coordinate and momentum in phase-space, this result was already expected as long as the coordinates in Eq. (2.5) satisfies the same property. Thus, by means of these two results, we have obtained the the celebrated midpoint rule: the semiclassical Weyl propagator at position $\mathbf{r}$ contains contributions from all the classical paths j that, in time t, link the phase-space points $\mathbf{r}'$ and $\mathbf{r}''$, having $\mathbf{r}$ as the center of the straight line linking them [27]. In this manner, the semiclassical propagation must always satisfy

$$\mathbf{r} = \frac{1}{2} \left[\mathbf{r}_j(t) + \mathbf{r}_j(0) \right] = \frac{1}{2} \left[\mathbf{r}_j'' + \mathbf{r}_j' \right]. \tag{2.13}$$

On the other hand, Almeida [11] describes the same relation from a deep and powerful cord construction in which, starting from a phase-space point, it is possible to go to another one either by a reflection around the center $\mathbf{r} = (\mathbf{r}'' + \mathbf{r}')/2$ or by a translation along the chord $\mathbf{u} = \mathbf{r}'' - \mathbf{r}'$. Even more, by means of compositions of these two operations, it is shown in this work how to link $\mathbf{r}$ to $\mathbf{u}$ by means of a combined transformation of the aforementioned operations. In this spirit, the theory developed in [11] establishes, by means of the transformation theory, the celebrated midpoint relations such that the determination of the the chord is possible once the center is known and conversely, by means of the representation of the canonical transformation involved.

Putting this midpoint rule into the phase of the propagator,

$$\Phi = - H_j \left(\mathbf{r}_j \right) t - \mathbf{p} \cdot \mathbf{u} + \int_{\mathbf{q}-\frac{\mathbf{u}}{2}}^{\mathbf{q}+\frac{\mathbf{u}}{2}} \mathrm{d}\mathbf{Q} \mathbf{p}_j(\mathbf{Q}) \tag{2.14}$$
$$= - \frac{1}{2} \left(\mathbf{p}_j'' + \mathbf{p}_j' \right) \cdot \left(\mathbf{q}_j'' - \mathbf{q}_j' \right) - H_j \left(\mathbf{r}_j \right) t + \int_{\mathbf{q}-\frac{\mathbf{u}}{2}}^{\mathbf{q}+\frac{\mathbf{u}}{2}} \mathrm{d}\mathbf{Q} \mathbf{p}_j(\mathbf{Q})$$
$$= A_j(\mathbf{r}, t) - H_j \left(\mathbf{r}_j \right) t,$$

with $H_j \left(\mathbf{r}_j \right)$ representing the energy of the path. As can be seen from this equation, the first term is a pure geometrical term

$$A_j(\mathbf{r}, t) = -\frac{1}{2} \left(\mathbf{p}_j'' + \mathbf{p}_j' \right) \cdot \left(\mathbf{q}_j'' - \mathbf{q}_j' \right) + \int_{\mathbf{q}-\frac{\mathbf{u}}{2}}^{\mathbf{q}+\frac{\mathbf{u}}{2}} \mathrm{d}\mathbf{Q} \mathbf{p}_j(\mathbf{Q}) \tag{2.15}$$

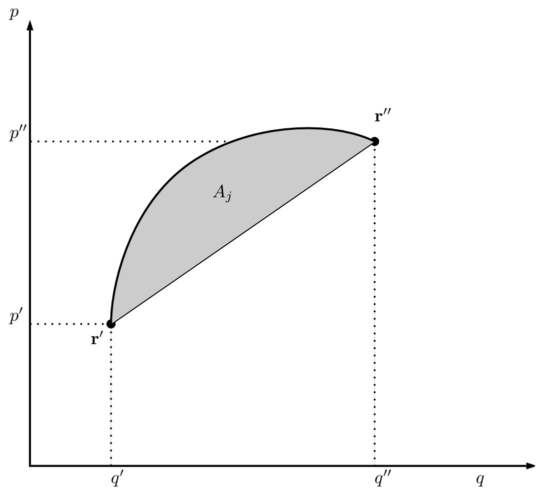

Figure 2.1: *Geometrical interpretation of the contribution of the symplectic area to the phase propagator.* $\mathbf{r}'$ *and* $\mathbf{r}''$ *represent the initial and final points of the propagation. The curved line represent the* j*-th classical trajectory linking the aforementioned phase-space points. The straight line linking* $\mathbf{r}'$ *and* $\mathbf{r}''$ *represents the chord, with its midpoint, known as the center, the point where we are evaluating the contribution of the classical trajectory to the propagator. The grey area represents, together with the energy of the path in time* t*, the main contribution to the phase propagator. See the main text for additional details.*

The integral corresponds to the area under the curve that represents the classical trajectory. This area is also bounded by the line $\mathbf{p} = 0$ and initial and final conditions $\mathbf{q}'_j$, $\mathbf{q}''_j$. The other term represents the area of a trapezium with height given by $\mathbf{q}''_j - \mathbf{q}'_j$, see Fig. 2.1. Then, as a result, the geometrical term $A_j(\mathbf{r}, t)$ corresponds to a symplectic area that follows the chord rule, i.e., the area formed by the circuit that goes from $\mathbf{r}'_j$ to $\mathbf{r}''_j$ along the classical path j and returns to the starting point following the straight line that connects those border points [27]. Furthermore, Eq. (2.14) represents the classical action contribution for the propagator made by every classical path labelled by j.

Once the phase of the propagator has been obtained by the stationary phase method, we would like to take a look to the prefactor in Eq. (2.2). Following Berry's ideas, it is possible to show that this term becomes [27]

$$\sqrt{\frac{1}{h^f}\left|\det\left(\frac{\partial^2 R_j(\mathbf{q}'', t''; \mathbf{q}', t')}{\partial \mathbf{q}'' \partial \mathbf{q}'}\right)\right|} = \sqrt{\frac{2^{2f}}{\det(\mathsf{M}_j + 1)}} \tag{2.16}$$

with M_j being the stability matrix of the trajectories. Therefore, the Weyl propagator in the van Vleck- Gutzwiller approximation takes the form

$$U_{\mathrm{W}}(\mathbf{r}, t) = 2^f \sum_j \frac{1}{\sqrt{\det(\mathsf{M}_j + 1)}} \exp\left\{\frac{\mathrm{i}}{\hbar}\left[A_j(\mathbf{r}, t) - H_j(\mathbf{r}_j)\, t\right] - \mathrm{i}\mu_j \frac{\pi}{2}\right\}. \tag{2.17}$$

There are some limits that can be explored out of this propagator. In particular, when $t \to$

0 the couple of trajectories tends to become one. Additionally, M_j gets close to the identity matrix, whereas the symplectic area goes to zero. In this way, the limit of the semiclassical Weyl propagator becomes $U_{\mathrm{W}}(\mathbf{r},t) \rightarrow \exp(-\mathrm{i}H(\mathbf{r})t/\hbar)$, which represents the appropriate short-time approximation of the dynamics.

From Eq. (2.17) it is possible to calculate, by means of a double Fourier transform in phase-space and some manipulations with the stability matrix [9], the Wigner propagator as

$$G_{\mathrm{W}}(\mathbf{r}'',t;\mathbf{r}',0) = \frac{2^f}{h^f}\sum_j \frac{2\cos\left(\frac{1}{\hbar}\mathcal{S}_j^{\mathrm{vV}}(\mathbf{r}'',\mathbf{r}',t) - \mu_j\frac{\pi}{4}\right)}{\left|\det\left(\mathsf{M}_{j_+} - \mathsf{M}_{j_-}\right)\right|^{1/2}}, \tag{2.18}$$

where $\mathcal{S}_j^{\mathrm{vV}}$ represents the action in the van Vleck approximation, whereas $M_{j\pm}$ are the stability matrices for the couple of trajectories $j_\pm$ satisfying the midpoint rule.

2.3 From Phase-Space Path-Integrals to Semiclassical Wigner Propagator

In this section we want to evaluate, under the semiclassical approximation, the path-integral expression for the Wigner propagator of a closed system given in Eq. (1.40). This semiclassical approximation is valid whenever the quantum fluctuations $\tilde{\mathbf{r}}$ are small, or equivalently, when the actions involved are large compared to Planck's constant so that the later may be considered to be small. Then, from a mathematical point of view, we have to evaluate the path integral over $\exp\left(-\mathrm{i}\mathcal{S}[\{\mathbf{r}\},\{\tilde{\mathbf{r}}\},t]/\hbar\right)$ for small $\hbar$. This can be done making use of the stationary-phase approximation where the exponent has to be expanded around the extrema of the action [37]. Therefore, to calculate this extrema solutions, we have to find all the possible trajectories that makes S stationary, identifying them as the classical solutions to the dynamics in phase space. Once they are known, we can proceed to expand the action around them.

Since the action $\mathcal{S}[\{\mathbf{r}\},\{\tilde{\mathbf{r}}\},t]$ is a functional, its extremal are calculated by means of the functional conditions

$$\frac{\delta\mathcal{S}}{\delta\mathbf{r}} = 0, \qquad \frac{\delta\mathcal{S}}{\delta\tilde{\mathbf{r}}} = 0. \tag{2.19}$$

From Eq. (1.41) we see that the action can be conveniently written as

$$\mathcal{S}[\{\mathbf{r}\},\{\tilde{\mathbf{r}}\},t] = \int_0^t \mathrm{d}s\phi\left(\{\mathbf{r}\},\{\tilde{\mathbf{r}}\},s\right), \tag{2.20}$$

with

$$\phi\left(\{\mathbf{r}\},\{\tilde{\mathbf{r}}\},s\right) = \dot{\mathbf{r}}\wedge\tilde{\mathbf{r}} + H_{\mathrm{W}}\left(\mathbf{r}+\frac{\tilde{\mathbf{r}}}{2}\right) - H_{\mathrm{W}}\left(\mathbf{r}-\frac{\tilde{\mathbf{r}}}{2}\right). \tag{2.21}$$

Thus, the variational derivatives in Eq (2.19) becomes the Euler-Lagrange equations over the integral kernel ϕ as

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial\phi}{\partial\dot{\mathbf{r}}}\right) - \frac{\partial\phi}{\partial\mathbf{r}} = 0, \qquad \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial\phi}{\partial\dot{\tilde{\mathbf{r}}}}\right) - \frac{\partial\phi}{\partial\tilde{\mathbf{r}}} = 0, \tag{2.22}$$

which, in turn, can be simplified to

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \phi}{\partial \dot{\mathbf{r}}}\right) - \frac{\partial \phi}{\partial \mathbf{r}} = 0, \qquad \frac{\partial \phi}{\partial \tilde{\mathbf{r}}} = 0. \tag{2.23}$$

This set of four differential equations can be written explicitly as

$$\begin{aligned}
\dot{\mathbf{p}} =& -\frac{\partial}{\partial \tilde{\mathbf{q}}}\left[H_{\mathrm{W}}\left(\mathbf{r}+\frac{\tilde{\mathbf{r}}}{2}\right) - H_{\mathrm{W}}\left(\mathbf{r}-\frac{\tilde{\mathbf{r}}}{2}\right)\right], \\
\dot{\mathbf{q}} =& \frac{\partial}{\partial \tilde{\mathbf{p}}}\left[H_{\mathrm{W}}\left(\mathbf{r}+\frac{\tilde{\mathbf{r}}}{2}\right) - H_{\mathrm{W}}\left(\mathbf{r}-\frac{\tilde{\mathbf{r}}}{2}\right)\right], \\
\dot{\tilde{\mathbf{p}}} =& -\frac{\partial}{\partial \mathbf{q}}\left[H_{\mathrm{W}}\left(\mathbf{r}+\frac{\tilde{\mathbf{r}}}{2}\right) - H_{\mathrm{W}}\left(\mathbf{r}-\frac{\tilde{\mathbf{r}}}{2}\right)\right], \\
\dot{\tilde{\mathbf{q}}} =& \frac{\partial}{\partial \mathbf{p}}\left[H_{\mathrm{W}}\left(\mathbf{r}+\frac{\tilde{\mathbf{r}}}{2}\right) - H_{\mathrm{W}}\left(\mathbf{r}-\frac{\tilde{\mathbf{r}}}{2}\right)\right].
\end{aligned} \tag{2.24}$$

We can go one step further in the simplification of this set of equations by means of the change of variables $\mathbf{r}_{\pm} = \mathbf{r} \pm \frac{\tilde{\mathbf{r}}}{2}$. Inverting this system gives us $\mathbf{r} = (\mathbf{r}_{+} + \mathbf{r}_{-})/2$ and $\tilde{\mathbf{r}} = \mathbf{r}_{+} - \mathbf{r}_{-}$. Then, by means of the chain rule $\frac{\partial}{\partial \mathbf{r}_{\pm}} = \frac{1}{2}\frac{\partial}{\partial \mathbf{r}} \pm \frac{\partial}{\partial \tilde{\mathbf{r}}}$, we obtain, from Eq. (2.24)

$$\begin{aligned}
\dot{\mathbf{p}}_{\pm} =& -\frac{\partial}{\partial \mathbf{q}_{\pm}} H_{\mathrm{W}}\left(\mathbf{r}_{\pm}\right), \\
\dot{\mathbf{q}}_{\pm} =& \frac{\partial}{\partial \mathbf{p}_{\pm}} H_{\mathrm{W}}\left(\mathbf{r}_{\pm}\right).
\end{aligned} \tag{2.25}$$

Following [23], let us consider the "symplectic gradient" operator $\nabla_k = (\mathsf{J}^{\mathrm{T}})_{kl}\partial/\partial \mathbf{r}_l$, with $k, l = 1, 2, \ldots, 2f$; and summation over the repeated indices. In terms of this gradient, the above set of equations in the $\mathbf{r}_{\pm}$ variables takes the form

$$\dot{\mathbf{r}}_{\pm} = \nabla H_{\mathrm{W}}(\mathbf{r}_{\pm}). \tag{2.26}$$

Under this notation, the semiclassical approximation given by the equation set in Eq. (2.24) can be compactly written as

$$\begin{aligned}
\dot{\mathbf{r}} =& \frac{1}{2}\left[\nabla H_{\mathrm{W}}\left(\mathbf{r}+\frac{\tilde{\mathbf{r}}}{2}\right) + \nabla H_{\mathrm{W}}\left(\mathbf{r}-\frac{\tilde{\mathbf{r}}}{2}\right)\right] \\
\dot{\tilde{\mathbf{r}}} =& \left[\nabla H_{\mathrm{W}}\left(\mathbf{r}+\frac{\tilde{\mathbf{r}}}{2}\right) - \nabla H_{\mathrm{W}}\left(\mathbf{r}-\frac{\tilde{\mathbf{r}}}{2}\right)\right].
\end{aligned} \tag{2.27}$$

Remarkably, $\hbar$ does not at all appear in this approximation. However this is a general expected result irrespective of the method used to arrive at the semiclassical version of the dynamics [23].

The set found in Eq. (2.27) consist of $2f$ first-order differential equations for $2f$ functions with $2f$ boundary conditions given by $\mathbf{r}(0) = \mathbf{r}'$, and $\mathbf{r}(t) = \mathbf{r}''$. Unlike the initial value problem, the question whether a solution does exist, or is unique, cannot be answerd readily, as usual in the semiclassical approximation [23].

As can be seen from Eq. (2.27), the trajectory connecting the boundary points under the trivial solution $\tilde{\mathbf{r}} = 0$, is precisely a classical one. Indeed, if we put this solution into Eq. (2.27), we obtain

$$\dot{\mathbf{r}} = \nabla H_{\mathrm{W}}(\mathbf{r}), \tag{2.28}$$

which represents the classical Hamilton equations of motion. This, in turn, implies that the set of trajectories $\mathbf{r}_{\pm}$ in Eq. (2.26), not only determine the propagation in phase space, but also are solutions of the classical equations of motion. This is a special feature of the restricted picture we are working on: as long as the system under study is closed, its dynamical evolution is unitary. This will no longer be the case when we move into an open system dynamics with the introduction of dissipation as in Chapter 4. In that more realistic case, the $\mathbf{r}_{\pm}$ trajectories will behave quite differently from the one we are discussing here. Specifically, in the special case of Ohmic damping, the $\mathbf{r}_{\pm}$ trajectories grow exponentially whereas the semi-sum behaves classically [25].

It is worth to mention that if the action possesses more than one extremum, one has to sum over the contributions of all extrema unless one extremum can be shown to be dominant [37]. Thus, if the index j labels all the possible classical trajectories, Eq. (2.28) must be written as

$$\dot{\mathbf{r}}_j = \nabla H_j(\mathbf{r}_j), \tag{2.29}$$

with $H_j(\mathbf{r}_j)$ representing the energy of the path. Then, by knowing the stationary trajectories, the action should be expanded around the classical trajectories $\mathbf{r}_j$ up to the first order contribution in the fluctuations $\tilde{\mathbf{r}}$. Moreover, the since the action is stationary at classical paths, we are obliged to express the general path as [37]

$$\mathbf{r}_j(s) = \mathbf{r}_j^{\mathrm{cl}}(s) + \tilde{\mathbf{r}}_j(s). \tag{2.30}$$

Then, in this approximation, the path-integral expressions are replaced by summation over these trajectories and weighted by the second derivatives of the action along these trajectories. It turns out that those second-derivatives, written in a matrix array, can be related to the subtraction of the stability matrices of $\mathbf{r}_+$ and $\mathbf{r}_-$ as [9, 27]

$$\det\begin{pmatrix} \frac{\partial^2 S}{\partial \tilde{\mathbf{q}}^2} & \frac{\partial^2 S}{\partial \tilde{\mathbf{p}}^2} \\ \frac{\partial^2 S}{\partial \mathbf{q}^2} & \frac{\partial^2 S}{\partial \mathbf{p}^2} \end{pmatrix} = \frac{1}{4^f}\det\begin{pmatrix} \frac{\partial \mathbf{q}''_+}{\partial \mathbf{q}'_+} - \frac{\partial \mathbf{q}''_-}{\partial \mathbf{q}'_-} & \frac{\partial \mathbf{q}''_+}{\partial \mathbf{p}'_+} - \frac{\partial \mathbf{q}''_-}{\partial \mathbf{p}'_-} \\ \frac{\partial \mathbf{p}''_+}{\partial \mathbf{q}'_+} - \frac{\partial \mathbf{p}''_-}{\partial \mathbf{q}'_-} & \frac{\partial \mathbf{p}''_+}{\partial \mathbf{p}'_+} - \frac{\partial \mathbf{p}''_-}{\partial \mathbf{p}'_-} \end{pmatrix} = \frac{1}{4^f}\det(\mathsf{M}_+ - \mathsf{M}_-). \tag{2.31}$$

Since the summation over trajectories contains terms j_+j_- and j_-j_+ we can guarantee that the propagator is real and takes the final form as

$$G_{\mathrm{W}}(\mathbf{r}'', t; \mathbf{r}', 0) = \frac{4^f}{h^f}\sum_j \frac{2\cos\left(\frac{1}{\hbar}\mathcal{S}_j^{\mathrm{vV}}(\mathbf{r}'', \mathbf{r}', t) - \mu_j\frac{\pi}{4}\right)}{\left|\det\left(\mathsf{M}_{j_+} - \mathsf{M}_{j_-}\right)\right|^{1/2}}, \tag{2.32}$$

with μ_j representing the "index of inertia" associated to the matrix $\mathsf{M}_{j_{+-}} = \mathsf{M}_{j_+} - \mathsf{M}_{j_-}$. It can be calculated by finding the eigenvalues of those matrices and computing the subtraction among the number of positive and negative eigenvalues for each matrix. [24]. On the other hand, the action

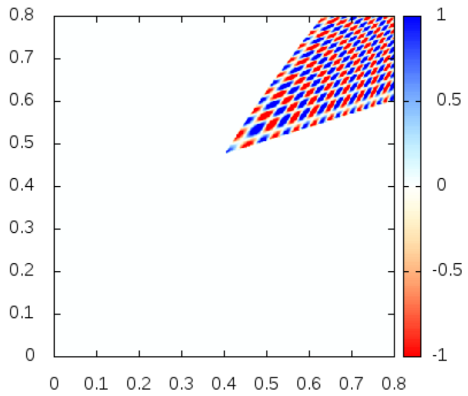

Figure 2.2: *Phase-space propagating function for unitary evolution under the Morse potential at time $t = 0,63s$. Parameter values are $m = 0.5$, $\hbar\omega_{min} = 0.0125$, $D = 1$, $a = 0.125$. ω_{min} denotes the frequency in the harmonic approximation, $\omega_{min} = \sqrt{2a^2D/m}$.*

in the above phase is given by

$$\mathcal{S}_j^{\mathrm{vV}}(\mathbf{r}'', \mathbf{r}', t) = \int_0^t \mathrm{d}s \left\{ \dot{\bar{\mathbf{r}}}_j \wedge \tilde{\mathbf{r}}_j - \left[H_{j+}(\mathbf{r}_{j+}) - H_{j-}(\mathbf{r}_{j-}) \right] \right\}, \tag{2.33}$$

where $\bar{\mathbf{r}}_j \equiv \left(\mathbf{r}_{j_+} + \mathbf{r}_{j_-}\right)/2$ and $\tilde{\mathbf{r}}_j \equiv \mathbf{r}_{j_+} - \mathbf{r}_{j_-}$.

2.4 Semiclassical Wigner propagator from path integrals

2.4.1 Discrete Wigner propagator

Let us consider a physical system in a two-dimensional phase space completely isolated from its surroundings and under the influence of a time-independent potential $V(q)$. This closed system dynamics is governed by a Weyl-transformed Hamiltonian $H_{\mathrm{W}} = T(p) + V(q)$. Our main interest is to find the mathematical structure of the Wigner propagator of this system when the potential becomes anharmonic due to the inclusion of non-linear terms in its Taylor expansion.

To begin with, we will use the discrete version of the Wigner propagator previously studied in Sec. 1.6 (See Eq. 1.37)

$$G_{\mathrm{W}}(\mathbf{r}_n, n\Delta t; \mathbf{r}_{n-1}, (n-1)\Delta t) \equiv G_{n,n-1} = \frac{1}{(2\pi\hbar)^2} \int \mathrm{d}\tilde{\mathbf{r}}_n \exp\left(-\frac{\mathrm{i}}{\hbar}\phi_n\right), \tag{2.34}$$

with $\tilde{\mathbf{r}}_n = (\tilde{p}_n, \tilde{q}_n)$ the quantum fluctuations associated with the trajectory $\mathbf{r}_n$. The discrete action

ϕ_n is given by

$$\begin{aligned}\phi_n =& \Delta\mathbf{r}_n \wedge \tilde{\mathbf{r}}_n + \left[H_\mathrm{W}\left(\bar{\mathbf{r}}_n + \frac{\tilde{\mathbf{r}}_n}{2}\right) - H_\mathrm{W}\left(\bar{\mathbf{r}}_n - \frac{\tilde{\mathbf{r}}_n}{2}\right)\right]\Delta t \\ =& \Delta p_n \tilde{q}_n - \left(\Delta q_n - \frac{\Delta t}{m}\bar{p}_n\right)\tilde{p}_n + \left[V\left(\bar{q}_n + \frac{\tilde{q}_n}{2}\right) - V\left(\bar{q}_n - \frac{\tilde{q}_n}{2}\right)\right]\Delta t.\end{aligned} \tag{2.35}$$

Under the shift $\mathbf{r}_n \to \mathbf{r}_n + \hat{\mathbf{r}}_n$, and a Taylor expansion of the potential up to third order, we obtain

$$\begin{aligned}\phi_n =& \left(\Delta p_n + \Delta\hat{p}_n + V^{(1)}(\hat{\bar{q}}_n)\Delta t + V^{(2)}(\hat{\bar{q}}_n)\bar{q}_n\Delta t + \frac{1}{2}V^{(3)}(\hat{\bar{q}}_n)\bar{q}_n^2\Delta t\right)\tilde{q}_n \\ & - \left(\Delta q_n + \Delta\hat{q}_n - \frac{\Delta t}{m}(\bar{p}_n + \hat{\bar{p}}_n)\right)\tilde{p}_n + \frac{1}{24}V^{(3)}(\hat{\bar{q}}_n)\Delta t\tilde{q}_n^3.\end{aligned} \tag{2.36}$$

By means of the classical equations,

$$\Delta\hat{p}_n + V^{(1)}(\hat{\bar{q}}_n)\Delta t \to 0, \qquad \Delta\hat{q}_n - \frac{\Delta t}{m}\hat{\bar{p}}_n \to 0, \tag{2.37}$$

the Wigner propagator in Eq. (2.34) takes the form

$$\begin{aligned}G_{n,n-1} =& \frac{1}{(2\pi\hbar)}\int \mathrm{d}\tilde{p}_n \exp\left(\frac{\mathrm{i}}{\hbar}\left[\Delta q_n - \frac{\Delta t}{m}\bar{p}_n\right]\tilde{p}_n\right) \\ & \times \frac{1}{(2\pi\hbar)}\int \mathrm{d}\tilde{q}_n \exp\left(-\frac{\mathrm{i}}{\hbar}\left[\Delta p_n + V^{(2)}(q_n^\mathrm{cl})\bar{q}_n\Delta t + \frac{1}{2}V^{(3)}(q_n^\mathrm{cl})\bar{q}_n^2\Delta t\right]\tilde{q}_n\right) \\ & \times \exp\left(-\frac{\mathrm{i}}{\hbar}\left[\frac{1}{24}V^{(3)}(q_n^\mathrm{cl})\Delta t\tilde{q}_n^3\right]\right).\end{aligned} \tag{2.38}$$

If we introduce the change of variable

$$q_n' = \left[\frac{V^{(3)}(q_n^\mathrm{cl})}{8\hbar}\Delta t\right]^{\frac{1}{3}}\tilde{q}_n = \alpha^{\frac{1}{3}}\tilde{q}_n,$$

and the definitions

$$\breve{p}_n = \left[mV^{(2)}(q_n^\mathrm{cl})\right]^{-\frac{1}{4}}p_n, \quad \breve{q}_n = \left[mV^{(2)}(q_n^\mathrm{cl})\right]^{\frac{1}{4}}q_n, \quad \breve{\tau}_n^{-\frac{1}{3}} = \frac{\alpha^{-\frac{1}{3}}}{\hbar}\left[mV^{(2)}(q_n^\mathrm{cl})\right]^{\frac{1}{4}}, \tag{2.39}$$

we can write the Wigner propagator as

$$G_{n,n-1} = \breve{\tau}_n^{-\frac{1}{3}}\delta\left(\Delta\breve{q}_n - \sqrt{\frac{V^{(2)}(q_n^\mathrm{cl})}{m}}\Delta t\breve{\bar{p}}_n\right)\mathrm{Ai}\left(\breve{\tau}_n^{-\frac{1}{3}}\left[\Delta\breve{p}_n + \sqrt{\frac{V^{(2)}(q_n^\mathrm{cl})}{m}}\Delta t\breve{\bar{q}}_n\right]\right). \tag{2.40}$$

From this propagator, we can write down the following system of equations

$$\begin{aligned}\breve{p}_n &= \breve{p}_{n-1} - \theta_n\breve{\bar{q}}_n \\ \breve{q}_n &= \breve{q}_{n-1} + \theta_n\breve{\bar{p}}_n,\end{aligned} \tag{2.41}$$

where we have used the notational simplification $\theta_n = \sqrt{\frac{V^{(2)}(q_n^\mathrm{cl})}{m}}\Delta t$. After solving it, we found the solution

$$\begin{pmatrix} \breve{p}_n \\ \breve{q}_n \end{pmatrix} = \frac{1}{4+\theta_n^2} \begin{pmatrix} 4-\theta_n^2 & -4\theta_n \\ 4\theta_n & 4-\theta_n^2 \end{pmatrix} \begin{pmatrix} \breve{p}_{n-1} \\ \breve{q}_{n-1} \end{pmatrix}. \tag{2.42}$$

Consequently, the propagator in Eq. (2.40) takes the time-linearized form [38]

$$G_{n,n-1} = \breve{\tau}_n^{-\frac{1}{3}} \delta\left(\breve{q}_n - (\mathsf{M}_n \breve{\mathbf{r}}_{n-1})_{\breve{q}}\right) \mathrm{Ai}\left(\breve{\tau}_n^{-\frac{1}{3}} \left[\breve{p}_n - (\mathsf{M}_n \breve{\mathbf{r}}_{n-1})_{\breve{p}}\right]\right). \tag{2.43}$$

2.4.2 Propagator composition in Fourier space

Let $\gamma_n = (\alpha_n, \beta_n)$ and $\gamma_{n-1} = (\alpha_{n-1}, \beta_{n-1})$. Then

$$\widetilde{G}_{n,n-1}(\gamma_n, \gamma_{n-1}) = \frac{1}{(2\pi)^2} \int \mathrm{d}\breve{\mathbf{r}}_n \mathrm{d}\breve{\mathbf{r}}_{n-1} G_{n,n-1}(\breve{\mathbf{r}}_n, \breve{\mathbf{r}}_{n-1}) \exp\left(\mathrm{i}\left[\gamma_n \wedge \breve{\mathbf{r}}_n - \gamma_{n-1} \wedge \breve{\mathbf{r}}_{n-1}\right]\right). \tag{2.44}$$

By using the propagator in Eq. (2.40), we can perform all the integrations such that the propagator in Fourier space takes the form

$$\begin{aligned} \widetilde{G}_{n,n-1} =& \frac{4}{4+\theta_n^2} \exp\left(-\frac{\mathrm{i}}{3}\breve{\tau}_n \left[\frac{2\alpha_n\theta_n - 4\beta_n}{(4+\theta_n^2)}\right]^3\right) \delta\left(\alpha_n - \alpha_{n-1} - \frac{2\theta_n}{4+\theta_n^2}\left[\alpha_n\theta_n - 2\beta_n\right]\right) \\ & \times \delta\left(\beta_{n-1} + \frac{1}{4+\theta_n^2}\left[4\alpha_n\theta_n - 4\beta_n + \theta_n^2\beta_n\right]\right). \end{aligned} \tag{2.45}$$

As we had reasoned before, in the limit $\Delta t \to 0$, $\theta_n^2 \ll 1$. Thus we can approach this propagator to its simplest version

$$\widetilde{G}_{n,n-1}(\gamma_n, \gamma_{n-1}) = \exp\left(\frac{\mathrm{i}}{3}\breve{\tau}_n \beta_n^3\right) \delta(\gamma_n - M_n \gamma_{n-1}). \tag{2.46}$$

In order to compute the composition of propagators, we make use of the Chapman-Kolmogorov relation in Fourier space

$$\widetilde{G}_{n+1,n-1} = \int \mathrm{d}\gamma_n \widetilde{G}_{n+1,n} \widetilde{G}_{n,n-1}, \tag{2.47}$$

such that

$$\widetilde{G}_{N,0} = \left(\prod_{n=1}^{N-1} \int \mathrm{d}\gamma_n\right) \exp\left(\frac{\mathrm{i}}{3}\sum_{n=1}^{N} \breve{\tau}_n \beta_n^3\right) \prod_{n=1}^{N} \delta(\gamma_n - \mathsf{M}_n \gamma_{n-1}). \tag{2.48}$$

By integrating out over the γ_n variables, and considering the limit $\Delta t \to 0$ we obtain the following structure for the propagator

$$\widetilde{G}(\gamma, \gamma_0) = \lim_{N\to\infty} \exp\left(\frac{\mathrm{i}}{3}\sum_{n=1}^{N} \breve{\tau}_n \left(\left[\prod_{j=0}^{n-1} \mathsf{M}_{n-j}\right] \gamma_0\right)_\beta^3\right) \delta\left(\gamma_N - \left[\prod_{j=0}^{N-1} \mathsf{M}_{N-j}\right] \gamma_0\right), \tag{2.49}$$

After some manipulations, the matrix M_n, in the limit, takes the form

$$\mathsf{M}(t) = \begin{pmatrix} \cos\theta(t) & -\sin\theta(t) \\ \sin\theta(t) & \cos\theta(t) \end{pmatrix}, \tag{2.50}$$

where

$$\theta(t) = \int_0^t \sqrt{\frac{V^{(2)}(q_{\rm cl}(s))}{m}} \mathrm{d}s. \tag{2.51}$$

With this result and the definition $\sigma = \breve{\tau}_n/\Delta t$, the composite Wigner propagator takes the form

$$\widetilde{G}(\gamma,\gamma_0) = \exp\left(\frac{\mathrm{i}}{3}\int_0^t \mathrm{d}t' \left([\mathsf{M}(t')\gamma_0]_\beta\right)^3 \sigma(t')\right)\delta\left(\gamma - \mathsf{M}(t)\gamma_0\right). \tag{2.52}$$

Explicitly, after an expansion of the above phase and by using the auxiliary equations defined in Eq. (G.1) of Appendix G, we obtain

$$\begin{aligned} G(\breve{\mathbf{r}}'',t;\breve{\mathbf{r}}',0) =& \int \frac{\mathrm{d}\gamma_0}{(2\pi)^2} \exp\left(\mathrm{i}[a\alpha_0^3 + b\alpha_0^2\beta_0 + c\alpha_0\beta_0^2 + d\beta_0^3 + \left[\mathsf{M}^{-1}\breve{\mathbf{r}}'' - \breve{\mathbf{r}}'\right]\wedge\gamma_0]\right) \\ =& \frac{1}{(2\pi)^2}\int \mathrm{d}\alpha_0\mathrm{d}\beta_0 \exp\left(\mathrm{i}\left[a\alpha_0^3 + d\beta_0^3 + \beta_0\left(b\alpha_0^2 + \left[\mathsf{M}^{-1}\breve{\mathbf{r}}''\right]_{\breve{p}''} - \breve{p}'\right)\right]\right) \\ &\times \exp\left(\mathrm{i}\left[\alpha_0\left(c\beta_0^2 - \left[\mathsf{M}^{-1}\breve{\mathbf{r}}''\right]_{\breve{q}''} + \breve{q}'\right)\right]\right), \end{aligned} \tag{2.53}$$

with the notation $\left[\mathsf{M}^{-1}\breve{\mathbf{r}}''\right]_{\breve{p}''}$, $\left[\mathsf{M}^{-1}\breve{\mathbf{r}}''\right]_{\breve{q}''}$ indicating the first and second components, respectively, of the matrix product $\mathsf{M}^{-1}\breve{\mathbf{r}}''$.

2.4.3 Recovering the Airy functions

Our next goal is to obtain a mathematical expression for the Wigner propagator in Eq. (2.53) in terms of Airy functions. To start with, let's write the phase of the propagator in the following way

$$\begin{aligned} \phi(t) =& a\alpha_0^3 + b\alpha_0^2\beta_0 + c\alpha_0\beta_0^2 + d\beta_0^3 - \alpha_0\left(\left[\mathsf{M}^{-1}\breve{\mathbf{r}}''\right]_{\breve{q}''} - \breve{q}'\right) + \beta_0\left(\left[\mathsf{M}^{-1}\breve{\mathbf{r}}''\right]_{\breve{p}''} - \breve{p}'\right) \\ =& a\alpha_0^3 + b\alpha_0^2\beta_0 + c\alpha_0\beta_0^2 + d\beta_0^3 - \alpha_0 Q + \beta_0 P, \end{aligned} \tag{2.54}$$

where we have use the short and simple notation $Q = \left[\mathsf{M}^{-1}\breve{\mathbf{r}}''\right]_{\breve{q}''} - \breve{q}'$, $P = \left[\mathsf{M}^{-1}\breve{\mathbf{r}}''\right]_{\breve{p}''} - \breve{p}'$. In Appendix F we develop the details of a set of four successive linear transformations applied to the above phase with the purpose of writing it in terms of Airy function. Subsequently, the propagator takes the form

$$G(\breve{\mathbf{r}}'',t;\breve{\mathbf{r}}',0) = \frac{1}{2\lambda_4(2\pi)^2}\int \mathrm{d}\mu_4\mathrm{d}\nu_4 \exp\left(\mathrm{i}\left[\rho\mu_4^3 + (\chi+\xi)\,\mu_4 + \rho\nu_4^3 + (\chi-\xi)\,\nu_4\right]\right). \tag{2.55}$$

Thus, having successfully decoupled the multivariate cubic polynomial in Eq. (2.54), we obtain the final version of the propagator as

$$
\begin{aligned}
G(\check{\mathbf{r}}'', t; \check{\mathbf{r}}', 0) =& \frac{1}{2\lambda_3(t)} \frac{1}{\sqrt[3]{(3\rho(t))^2}} \mathrm{Ai}\left(\frac{\chi(\check{\mathbf{r}}'', \check{\mathbf{r}}', t) + \xi(\check{\mathbf{r}}'', \check{\mathbf{r}}', t)}{\sqrt[3]{3\rho(t)}} \right) \\
& \times \mathrm{Ai}\left(\frac{\chi(\check{\mathbf{r}}'', \check{\mathbf{r}}', t) - \xi(\check{\mathbf{r}}'', \check{\mathbf{r}}', t)}{\sqrt[3]{3\rho(t)}} \right).
\end{aligned}
\tag{2.56}
$$

This is a quite interesting result. It states that for a closed system subject to a non-linear potential, its dynamics in phase-space is governed by an explicitly non-local propagator in the coordinates and the momentum. This aspect of the propagator has been acquired once we have introduced a non-linear dynamics throughout the potential $V(q)$. Fig. 2.2 shows the non-local structure of the integral kernel for the Wigner function of the system, described as a single degree of freedom under the Morse potential. As can be seen, there is an interference pattern over significant regions of phase-space that shows how different regions contributes to the propagation of the dynamics. Specially important has been the midpoint rule of Eq. (2.13) in the numerical study of this propagator.

Chapter 3

Open quantum systems in phase-space

3.1 Introduction

In this chapter we construct the theory of quantum open systems in phase space. To achieve this, we first make use of Marinov's path integrals in phase-space to translate the Feynman and Vernon approach into phase-space language to obtain the propagating function in phase-space assuming a Ullersma-Caldeira-Leggett model for the bath. Moreover, starting from these results, we will be able to calculate the dissipative version of the Wigner propagator presented in Sec. 1.6. Finally, starting from this propagator, we will proceed to evaluate the path integrals by means of semiclassical approximations.

3.2 Composite system propagator

We have already calculated the Wigner propagator for a quantum system evolving unitarily. In this chapter we will be more interested on the study of composite interacting systems. Specifically we will configure the composite system, from now on named the universe, in such a way that we can define at initial time $t = 0$, on one hand, a central system (S) with f DOF and, on the other hand, a bath reservoir (B) constituted by F non-interacting harmonic oscillators. At a later time $t > 0$, the universe will consist not only of S and B, but all the interactions and correlations created by the interaction among them as well.

The approach we will follow on this thesis will be to consider a position-position coupling among S and the bath DOF. In this way, we will be extending the Ullersma-Caldeira-Leggett model [39, 40] from configuration space into phase-space, preserving the physical setup rooted in the study of the dissipation of the energy from the system to the bath and in the process of decoherence while these correlations are translated into the reservoir in a mechanism widely studied in the literature [41, 42].

Let us define the physical structure of our universe[1] by means the Hamiltonian

$$H_{\mathrm{W}}(\mathbf{r},\mathbf{R}) = H_{\mathrm{W,S}}(\mathbf{r}) + H_{\mathrm{W,B}}(\mathbf{R}) + H_{\mathrm{W,SB}}(\mathbf{r},\mathbf{R}). \tag{3.1}$$

As we can see from this expression, we have split the dynamics into three parts: the system dynamics alone, described by $H_{\mathrm{W,S}}(\mathbf{r})$; the bath mode dynamics, given by $H_{\mathrm{W,B}}(\mathbf{r})$, and, finally,

[1] We will be considering directly the Weyl symbols of the Hamiltonian operators involved in the universe dynamics. See [15] for details.

the interaction among S and B determined by $H_{\mathrm{W,SB}}(\mathbf{r},\mathbf{R})$. On the other hand, the points $\mathbf{r},\mathbf{R}$ are defined as $\mathbf{r}=(p_1,p_2,\cdots,p_f,q_1,q_2,\cdots,q_f)$ and $\mathbf{R}=(P_1,P_2,\cdots,P_F,Q_1,Q_2,\cdots,Q_F)$ respectively. Before giving a mathematical form to the aforementioned Hamiltonians, which will be done within the next section, we will focus completely in the construction of a path integral representation of the Wigner function for S and its propagating function. For this purpose, we will use the already developed theory of open systems in the path integral formalism developed in the configuration space [39, 43, 44].

As long as the universe described by Eq. (3.1) is closed, its dynamical evolution will be unitary. Therefore, by means of the Wigner propagator already calculated in Eq. (1.40) we can write down a universe propagator. For this purpose, we proceed to introduce the notation that we will be using throughout the text. Let $\mathcal{R}=(\mathbf{r},\mathbf{R})$ be a vector in the composite phase-space. Explicitly, $\mathcal{R}=(p_1,p_2,\cdots,p_f,P_1,P_2,\cdots,P_F,q_1,q_2,\cdots,q_f,Q_1,Q_2,\cdots,Q_F)$. Thus, by means of Eq. (1.40), we can write the Wigner propagator for the universe as

$$G_{\mathrm{W}}(\mathcal{R}'',t;\mathcal{R}',0)=\frac{1}{(2\pi\hbar)^{(f+F)}}\int\mathcal{D}\mathcal{R}\int\mathcal{D}\tilde{\mathcal{R}}\exp\left\{-\frac{\mathrm{i}}{\hbar}\mathcal{S}\left[\{\mathcal{R}\},\{\tilde{\mathcal{R}}\},t\right]\right\},\tag{3.2}$$

where we have set the boundary conditions as $\mathcal{R}(0)=\mathcal{R}'$ and $\mathcal{R}(t)=\mathcal{R}''$. The variable $\tilde{\mathcal{R}}$ represents the whole set of quantum fluctuations around $\mathcal{R}(s)$, and, as in the single system case, they do not have boundary restrictions [23] . In addition, $\mathcal{D}\mathcal{R}$ and $\mathcal{D}\tilde{\mathcal{R}}$ denote an infinity product of measures in the composite phase-space; whereas $\mathcal{S}[\{\mathcal{R}\},\{\tilde{\mathcal{R}}\},t]$ represents the action of the universe. Being an extensive quantity, it can be written as $\mathcal{S}[\{\mathcal{R}\},\{\tilde{\mathcal{R}}\},t]=\mathcal{S}_{\mathrm{S}}[\{\mathbf{r}\},\{\tilde{\mathbf{r}}\},t]+\mathcal{S}_{\mathrm{B}}[\{\mathbf{R}\},\{\tilde{\mathbf{R}}\},t]+\mathcal{S}_{\mathrm{SB}}[\{\mathbf{r}\},\{\tilde{\mathbf{r}}\},\{\mathbf{R}\},\{\tilde{\mathbf{R}}\},t]$. Meanwhile, as a single quantity, it takes the mathematical form

$$\mathcal{S}[\{\mathcal{R}\},\{\tilde{\mathcal{R}}\},t]=\int_0^t\mathrm{d}s\left[\dot{\mathcal{R}}\wedge\tilde{\mathcal{R}}+H_{\mathrm{W}}\left(\mathcal{R}+\frac{1}{2}\tilde{\mathcal{R}}\right)-H_{\mathrm{W}}\left(\mathcal{R}-\frac{1}{2}\tilde{\mathcal{R}}\right)\right].\tag{3.3}$$

Since we are mainly interested in the dynamics of the central system S under the influence of the bath, we would like to find a mathematical description, in terms of path integrals, of S alone. Thus, from this perspective, the propagator in Eq. (3.2) will not be the central object of our discussion. Instead, as we will see below, once we integrate the bath DOF, we will obtain the path integral representation of the Wigner function for S and its kernel of propagation, known as the propagating function.

Let us begin by writing the Wigner function evolution for the universe. From Eq. (1.24) and Eq. (3.2) we obtain

$$\begin{aligned}\rho_{\mathrm{W}}(\mathbf{R}'',\mathbf{r}'',t)=&\int\frac{\mathrm{d}\mathbf{R}'}{(2\pi\hbar)^F}\frac{\mathrm{d}\mathbf{r}'}{(2\pi\hbar)^f}\int\mathcal{D}\mathbf{r}\int\mathcal{D}\tilde{\mathbf{r}}\int\mathcal{D}\mathbf{R}\int\mathcal{D}\tilde{\mathbf{R}}\\&\times\exp\left\{-\frac{\mathrm{i}}{\hbar}\left[\mathcal{S}_{\mathrm{S}}\left[\{\mathbf{r}\},\{\tilde{\mathbf{r}}\},t\right]+\mathcal{S}_{\mathrm{B}}\left[\{\mathbf{R}\},\{\tilde{\mathbf{R}}\},t\right]+\mathcal{S}_{\mathrm{SB}}\left[\{\mathbf{r}\},\{\tilde{\mathbf{r}}\},\{\mathbf{R}\},\{\tilde{\mathbf{R}}\},t\right]\right]\right\}\\&\times\rho_{\mathrm{W}}(\mathbf{R}',\mathbf{r}',0).\end{aligned}\tag{3.4}$$

Here and in the following, we shall take $t=0$ to correspond to the time at which the interaction is switched on. For times $t<0$ the system and environment are usually assumed to be completely uncorrelated[2] and the Wigner function of the universe can be written as $\rho_{\rm W}(\mathbf{R}', \mathbf{r}', 0) = \rho_{\rm W,S}(\mathbf{r}', 0)\rho_{\rm W,B}(\mathbf{R}', 0)$ [9,42,44]. Thus, by using this factorization of the S+B state and after some manipulations, Eq. (3.4) takes the compact form

$$\rho_{\rm W,S}(\mathbf{r}'', t) = \int \mathrm{d}\mathbf{r}' J_{\rm W}(\mathbf{r}'', t; \mathbf{r}', 0)\, \rho_{\rm W,S}(\mathbf{r}', 0). \tag{3.5}$$

On the left-hand side, $\rho_{\rm W,S}(\mathbf{r}'', t)$ stands for the Wigner function characterizing the state of S; while on the right-hand side, the quantity $J_{\rm W}(\mathbf{r}'', t; \mathbf{r}', 0)$ represents the propagating function that allow us to evolve in time the Wigner function of the central system. In this way, J represents to the dynamics of the state of S, what the Wigner propagator in Eq. (3.2) to the dynamics of the universe.

The mathematical form of $J_{\rm W}(\mathbf{r}'', t; \mathbf{r}', 0)$ can be extracted from the last two equations such that

$$J_{\rm W}(\mathbf{r}'', t; \mathbf{r}', 0) = \frac{1}{h^f} \int \mathcal{D}\mathbf{r} \int \mathcal{D}\tilde{\mathbf{r}} \exp\left\{-\frac{\mathrm{i}}{\hbar}\mathcal{S}_{\rm S}\left[\{\mathbf{r}\}, \{\tilde{\mathbf{r}}\}, t\right]\right\} \mathcal{F}_{\rm W}\left[\{\mathbf{r}\}, \{\tilde{\mathbf{r}}\}, t\right], \tag{3.6}$$

where

$$\begin{aligned}\mathcal{F}_{\rm W}\left[\{\mathbf{r}\}, \{\tilde{\mathbf{r}}\}, t\right] =& \frac{1}{h^F} \int \mathrm{d}\mathbf{R}'' \int \mathrm{d}\mathbf{R}'\, \rho_{\rm W,B}(\mathbf{R}', 0) \int \mathcal{D}\mathbf{R} \int \mathcal{D}\tilde{\mathbf{R}} \\ &\times \exp\left\{-\frac{\mathrm{i}}{\hbar}\left[\mathcal{S}_{\rm B}\left[\{\mathbf{R}\}, \{\tilde{\mathbf{R}}\}, t\right] + \mathcal{S}_{\rm SB}\left[\{\mathbf{r}\}, \{\tilde{\mathbf{r}}\}, \{\mathbf{R}\}, \{\tilde{\mathbf{R}}\}, t\right]\right]\right\},\end{aligned} \tag{3.7}$$

represents the influence functional in phase-space . This object comprises all the information of the bath and the influence that it exerts on the central system. Thus, it plays a major role in the description of open system dynamics and was originally formulated in configuration space [43].

The influence functional has been analytically calculated for baths having, at most, quadratic potentials [44]. Moreover, there are scenarios where the coupling among the central system and the bath modes is non-linear. In this scenario, there are models where approximations schemes like a perturbation expansion of the action in the influence functional are mandatory [45].

Although, at this point we could be tempted to introduce semiclassical approximations for the evolution of the dissipative system, *e.g.* considering stationary-phase approximation for the influence functional $J_{\rm W}(\mathbf{r}'', t; \mathbf{r}', 0)$ or the total Wigner propagator $G_{\rm W}(\mathcal{R}'', t; \mathcal{R}', 0)$, it is very premature because dissipation is achieved just when the number of DOF of the bath tends to infinity. Otherwise what we will find again is the result for Hamiltonian systems derived in Ref. [46]. For this reason, semiclassical limit will be discussed later in Sec. 3.4.3.

[2]Whenever the total density matrix of the universe factorizes into subsystem density matrices $\hat{\rho} = \hat{\rho}_{\rm S} \otimes \hat{\rho}_{\rm B}$, there exist no quantum correlations between these subsystems [42]. This statement retains its validity when going from Hilbert space to phase-space quantum mechanics. Specifically, after the Weyl transformation, the total density operator of the universe at times $t < 0$ becomes the factor product of the two Wigner functions of S and B. The prove of this statement is a straightforward application of the Weyl transform definition and the fact that both operators belong to different Hilbert spaces.

3.3 Ullersma-Caldeira-Leggett Model in Phase Space

3.3.1 Hamiltonian for the model

Following Ullersma's ideas [40], we couple linearly a single DOF, $\mathbf{r} = (\mathbf{p}, \mathbf{q})$, to a thermal bath modeled as a collection of F independent harmonic oscillators. Their Hamiltonians read[3]

$$H_{\mathrm{S}}(\mathbf{r}) = \frac{p^2}{2m} + V(q), \tag{3.8}$$

$$H_{\mathrm{B}}(\mathbf{R}) = \sum_{j=1}^{F} \frac{1}{2m_j} {P_j}^2 + \frac{1}{2} m_j \omega_j^2 Q_j^2, \tag{3.9}$$

$$H_{\mathrm{SB}}(\mathbf{r}, \mathbf{R}) = -q \sum_{j=1}^{F} c_j Q_j + q^2 \sum_{j=1}^{F} \frac{c_j^2}{2m_j \omega_j^2}. \tag{3.10}$$

A special mention has to be made about the second term of the interaction Hamiltonian $H_{\mathrm{SB}}(\mathbf{r}, \mathbf{R})$. The physical reason for the inclusion of this term lies in a potential renormalization introduced by the the bilinear coupling in the same Hamiltonian. Then, the inclusion of the second term guarantees that the minimum of the Hamiltonian of the universe respect to the system coordinate is completely determined by the bare potential $V(q)$ [37].

The next step towards the construction of the Wigner propagator within this model corresponds to the derivation of the equations of motion for the set of DOF $\mathbf{r}, \mathbf{R}$. In this regard, there are different ways to proceed. One possibility is to calculate, in the Hilbert space of the universe, the Heisenberg equations of motion for the observables $\hat{p}, \hat{q}, \hat{P}_j$ and $\hat{Q}_j$. Then, by means of the Weyl transform, the equations of motion in phase-space are obtained. This procedure is straightforward due to the fact that the operator differential equations are linear and the observables of S and B commutes. Other straightforward alternative is to transform directly the Hamiltonians operators into their Weyl symbols and then, to obtain the differential equations by means of the classical Poisson brackets or its equivalent, the Hamilton equations of motion.[4] In the present work we use the latter approach to the dynamical equations which take the form

$$\dot{P}_j = -m_j \omega_j^2 Q_j + c_j q, \qquad \dot{Q}_j = \frac{P_j}{m_j}, \tag{3.11}$$

for the bath DOF. On the other hand, the canonical equations for the central system take the form

$$\dot{p} = -\frac{\partial V}{\partial q} + \sum_{j=1}^{F} c_j Q_j - q \sum_{j=1}^{F} \frac{c_j^2}{m_j \omega_j^2}, \qquad \dot{q} = \frac{p}{m}. \tag{3.12}$$

The solution for the set in Eq. (3.11) has been explicitly calculated in [37] within the configuration space framework. Despite of this, the solution set is the same because the equations take the same mathematical form. Once the bath equations has been solved, it is possible to construct a

[3] We are removing the label W from this point. It should be clear throughout this chapter that we are working with the Weyl symbols of the Hamiltonian operators.

[4] See section D.3 in Appendix D and reference [15] to see procedure to obtain the Weyl symbols of some important observables.

Langevin-like equation from which we can define the dissipation kernel, the history dependence of the damping and, most importantly, the construction of the spectral density to characterize the bath phenomenology. Instead of repeat these steps in the present framework, we want to explore an alternate way to obtain the same results. Thus, we will focus our discussion on the structure of the Wigner propagator for the Ullersma-Caldeira-Leggett model. From it, we will obtain the dynamical equations that makes the action functional an extremal and, from then, we will discuss the transition into the continuos regime for the bath modes.

3.3.2 Wigner propagator for the Ullersma-Caldeira-Leggett model

The discussion of the state evolution in phase-space, within the integral approach, requires the knowledge of the propagator that evolves states in time. To know the propagator is equivalent to have solved completely the dynamics. Nonetheless, even in the simplest case, the final goal does not correspond to the complete calculation of the path integral that represents the propagator. Instead, we just want to analyze the action functional to find, by means of the variational calculus, the classical allowed trajectories.

The Wigner propagator for the Ullersma-Caldeira-Leggett model takes the form[5]

$$
\begin{aligned}
G_{\mathrm{W}}(\mathbf{r}'', \mathbf{R}_j'', t; \mathbf{r}', \mathbf{R}_j', 0) = \frac{1}{2\pi\hbar} \int \mathcal{D}\mathbf{r} \int \mathcal{D}\tilde{\mathbf{r}} \exp\left(-\frac{\mathrm{i}}{\hbar} \mathcal{S}_{\mathrm{S}}[\{\mathbf{r}\}, \{\tilde{\mathbf{r}}\}, t] \right) \\
\times \prod_{j=1}^{F} \delta\left(P_j'' - P_j^{\mathrm{cl}}(P_j', Q_j', t) \right) \delta\left(Q_j'' - Q_j^{\mathrm{cl}}(P_j', Q_j', t) \right) \\
\times \exp\left\{ \frac{\mathrm{i}}{\hbar} \left[c_j \int_0^t \mathrm{d}s Q_j^{\mathrm{cl}}(P_j', Q_j', s) \tilde{q}(s) - \frac{c_j^2}{m_j \omega_j^2} \int_0^t \mathrm{d}s q(s) \tilde{q}(s) \right] \right\}.
\end{aligned}
\tag{3.13}
$$

In the first line we have the path integral representation of the Wigner propagator of the central system, with the action taking the form

$$
\mathcal{S}_{\mathrm{S}}[\{\mathbf{r}\}, \{\tilde{\mathbf{r}}\}, t] = \int_0^t \mathrm{d}s \left[\dot{\mathbf{r}} \wedge \tilde{\mathbf{r}} + H_{\mathrm{S}}\left(\mathbf{r} + \frac{1}{2}\tilde{\mathbf{r}} \right) - H_{\mathrm{S}}\left(\mathbf{r} - \frac{1}{2}\tilde{\mathbf{r}} \right) \right]. \tag{3.14}
$$

In the second line, $P_j^{\mathrm{cl}}(P_j', Q_j', t)$ and $Q_j^{\mathrm{cl}}(P_j', Q_j', t)$ represent the solution to the classical equations of motion for the bath DOF in Eq. (3.11). Thus, the Wigner propagator is a δ-function along the classical trajectory in the phase-space components of the bath. This in turn shows unambiguously the classical nature of the dynamics of thermal baths described by collections of harmonic modes. These classical dynamics prevent the system-bath interaction to exhibit non-trivial quantum effects in phase-space. An approximation that incorporates quantum aspects of the bath dynamics will be developed in Chap. 4. Finally, The third line of the propagator provides, on one hand, the bilinear interaction term among the system and the bath DOF. On the other hand, the last term represents the renormalization term for the system potential. As can be seen from the propagator in Eq. (3.13), the decoupled case ($c_j = 0$) directly implies an isolated system dynamics evolving uniquely under the $\mathcal{S}_{\mathrm{S}}$, whereas all the bath modes becomes independent harmonic

[5] A more general propagator will be constructed in chapter 4. Particularly, The special case of the propagator for the Ullersma-Caldeira-Leggett model used in this chapter will be deduced, as a particular case of Eq. (4.53), in Appendix A.

oscillators evolving along the classical trajectory defined by their bare frequencies ω_j.

3.3.3 Propagating function for the Ullersma-Caldeira-Leggett model

In this section, we shall assume that initial Wigner function of the total system can be written as $\rho_{\mathrm{W,S}}(\mathbf{r}', 0)\rho_{\mathrm{W,B}}(\mathbf{R}'_1, \mathbf{R}'_2, \ldots \mathbf{R}'_F, 0)$. Additionally, as in the last case, we assume that the environment is initially at constant temperature T. Since the bath modes are independent of each other, then, the Wigner function of the bath can be written as

$$\rho_{\mathrm{W,B}}(\mathbf{R}'_1, \mathbf{R}'_2, \ldots \mathbf{R}'_F, 0) = \prod_{j=1}^{F} \rho_{\mathrm{W},j}(P'_j, Q'_j, 0), \tag{3.15}$$

where the j-th bath mode Wigner function takes the form

$$\rho_{\mathrm{W},j}(P'_j, Q'_j, 0) = \frac{1}{\pi\hbar} \tanh\left(\hbar\beta\omega_j/2\right) \exp\left[-\frac{\tanh\left(\hbar\beta\omega_j/2\right)}{m_j\omega_j\hbar}(P'^2_j + m_j^2\omega_j^2 Q'^2_j)\right]. \tag{3.16}$$

This result allow us to characterize completely the initial state of the bath Additionally, it is a key ingredient to include in the calculation of the influence functional given in Eq. (3.7). Once one includes the action functionals and the bath initial state into $\mathcal{F}_{\mathrm{W}}$, the calculation can be done due to the linearity of the bath potentials. Thus, after a lenghty calculation, it is possible to shown that the initial factorizing conditions lead us to the influence given by [44]

$$\begin{aligned}\mathcal{F}_{\mathrm{W}}[\{\mathbf{r}\}, \{\tilde{\mathbf{r}}\}, t] = \exp\Bigg\{&-\mathrm{i}\frac{2\mu}{\hbar}\int_0^t \mathrm{d}s q(s)\tilde{q}(s) - \mathrm{i}\frac{2}{\hbar}\int_0^t \mathrm{d}s \int_0^s \mathrm{d}u \alpha_{\mathrm{I}}(s-u) q(u)\tilde{q}(s) \\ &- \frac{1}{\hbar}\int_0^t \mathrm{d}s \int_0^s \mathrm{d}u \alpha_{\mathrm{R}}(s-u)\tilde{q}(u)\tilde{q}(s)\Bigg\},\end{aligned} \tag{3.17}$$

where

$$\mu = \sum_{j=1}^{F} \frac{c_j^2}{2m_j\omega_j^2}, \qquad \alpha_{\mathrm{I}}(s-u) = -\sum_{j=1}^{F} \frac{c_j^2}{2m_j\omega_j} \sin\omega_j(s-u), \tag{3.18}$$

and

$$\alpha_{\mathrm{R}}(s-u) = \sum_{j=1}^{F} \frac{c_j^2}{2m_j\omega_j} \coth\left(\frac{\hbar\omega_j\beta}{2}\right) \cos\omega_j(s-u). \tag{3.19}$$

Expression (3.17), in appropriate coordinates of difference and half-sum, coincides with the standard result [47, 48]. At this point we cannot talk about dissipation yet because an important step is left, the evaluation of $F \to \infty$. To achieve that, let us describe the continuum of harmonic oscillators, as in the previous approach, by the spectral distribution $I(\omega)$. In this framework, the integral kernel

$$\alpha(s) = \alpha_{\mathrm{R}}(s) + \mathrm{i}\alpha_{\mathrm{I}}(s) = \frac{1}{\pi}\int_0^\infty \mathrm{d}\omega I(\omega)\left[\coth\left(\frac{\hbar\omega\beta}{2}\right)\cos\omega s - \mathrm{i}\sin\omega s\right] = \frac{1}{\hbar}K(s), \tag{3.20}$$

plays a predominant role in the description of the bath behavior and the influence it exerts on the central system. It can be shown that this kernel defines completely the structure of the phase of the influence functional, and therefore, the dynamics of the system [44, 49]. The imaginary part $\alpha_{\rm I}(t)$ of the Feynman-Vernon kernel is related to the damping kernel $\gamma(s)$ of the classical equation of motion of this model,

$$\alpha_{\rm I}(s) = \frac{m}{2}\frac{{\rm d}\gamma(s)}{{\rm d}s}, \tag{3.21}$$

Thus, the propagating function of the Wigner function for non-Markovian dissipative system within the Caldeira-Leggett approach can be written as

$$\begin{aligned} J_{\rm W}(\mathbf{r}'', \mathbf{r}', t) = \frac{1}{h}\int \mathcal{D}\mathbf{r} \int \mathcal{D}\tilde{\mathbf{r}} \exp\left(-\frac{\rm i}{\hbar} S_{\rm S}[\{\mathbf{r}\}, \{\tilde{\mathbf{r}}\}, t]\right) \\ \exp\left\{-{\rm i}\frac{2\mu}{\hbar}\int_0^t {\rm d}s q(s)\tilde{q}(s) - {\rm i}\frac{m}{\hbar}\int_0^t {\rm d}s \int_0^s {\rm d}u \frac{{\rm d}\gamma(s-u)}{{\rm d}(s-u)} q(u)\tilde{q}(s) \right. \\ \left. - \frac{1}{\hbar}\int_0^t {\rm d}s \int_0^s {\rm d}u \alpha_R(s-u)\tilde{q}(u)\tilde{q}(s)\right\}, \end{aligned} \tag{3.22}$$

3.4 Stochastic Non-Markovian Dissipative Propagator of the Wigner Function

3.4.1 Stochastic Propagating Function for the Density Matrix

Let us a consider the time evolution of the central system S under the standard Hamiltonian $H_{\rm S} = \frac{p^2}{2m} + V(q)$ and the external influence of the bath by means of an stochastic force $\zeta(t)$ with a first statistical moment $\langle\zeta(t)\rangle = 0$, and characterized by the two-time correlation function [37]

$$\langle\zeta_\pm(t)\zeta_\pm(0)\rangle = \hbar\int_0^\infty \frac{{\rm d}\omega}{\pi} I(\omega)\left[\coth\left(\frac{\hbar\omega\beta}{2}\right)\cos(\omega t) \mp {\rm i}\sin(\omega t)\right]. \tag{3.23}$$

Assuming the dipolar coupling approximation to the fluctuating force, the Feynman-propagator matrix elements will be given by

$$\langle q''_+|\hat{U}(t)|q'_+\rangle = \int \mathcal{D}q_+ \exp\left\{\frac{\rm i}{\hbar}\int_0^t {\rm d}s \left[\frac{1}{2}m\dot{q}_+^2 - V(q_+) + q_+\zeta_+(s) + \frac{m}{2}\gamma(0)q_+^2\right]\right\}. \tag{3.24}$$

The first two terms in the square brackets represent the unitary standard Lagrangian function for the q_+ DOF. The third one represents the aforementioned dipolar coupling between the system DOF and the bath stochastic force. The final term, a renormalization factor, has been introduced for later convenience.

For the propagator of the density matrix of S and knowing that

$$J(q''_+, q''_-, t; q'_+, q'_-) = \langle q''_+|\hat{U}(t)|q'_+\rangle\langle q''_-|\hat{U}^\dagger(t)|q'_-\rangle, \tag{3.25}$$

we have

$$
\begin{aligned}
&J(q''_+, q''_-, t; q'_+, q'_-) = \\
&\int \mathcal{D}q_+ \exp\left\{\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}s \left[\frac{1}{2}m\dot{q}_+^2 - V(q_+) + \frac{m}{2}\gamma(0)q_+^2 + q_+\zeta_+(s)\right]\right\} \\
&\times \int \mathcal{D}q_- \exp\left\{-\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}s \left[\frac{1}{2}m\dot{q}_-^2 - V(q_-) + \frac{m}{2}\gamma(0)q_-^2 + q_-\zeta_-(s)\right]\right\}.
\end{aligned} \tag{3.26}
$$

Note that in the latter expression we have introduced independent stochastic forces for each $\hat{U}$ according to Eq. (3.23). The presence of two independent noises was already reported in [50, 51] in the context of the stochastic master equation. Then, from Eq. (3.26) we have

$$
\begin{aligned}
\langle J(q''_+, q''_-, t; q'_+, q'_-)\rangle &= \int \mathcal{D}q_+ \int \mathcal{D}q_- \left\langle \exp\left\{\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}s\, [q_+\zeta_+(s) - q_-\zeta_-(s)]\right\}\right\rangle \\
&\times \exp\left\{\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}s \left[\frac{1}{2}m\dot{q}_+^2 - \frac{1}{2}m\dot{q}_-^2 - V(q_+) + V(q_-) + \frac{m}{2}\gamma(0)q_+^2 - \frac{m}{2}\gamma(0)q_-^2\right]\right\}.
\end{aligned} \tag{3.27}
$$

Since we are assuming Gaussian stochastic processes, the average over the fluctuating forces $\zeta_\pm(s)$ can be carried out analytically[6], such that

$$
\left\langle \exp\left\{\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}s\, [q_+\zeta_+(s) - q_-\zeta_-(s)]\right\}\right\rangle = \tag{3.28}
$$

$$
\begin{aligned}
&\exp\left\{-\frac{1}{\hbar^2}\int_0^t \mathrm{d}s \int_0^s \mathrm{d}u\, [q_+(s)q_+(u)\langle\zeta_+(s)\zeta_+(u)\rangle - q_+(s)q_-(u)\langle\zeta_+(s)\zeta_-(u)\rangle]\right\} \\
&\times \exp\left\{-\frac{1}{\hbar^2}\int_0^t \mathrm{d}s \int_0^s \mathrm{d}u\, [q_-(s)q_-(u)\langle\zeta_-(s)\zeta_-(u)\rangle - q_-(s)q_+(u)\langle\zeta_-(s)\zeta_+(u)\rangle]\right\}.
\end{aligned} \tag{3.29}
$$

Since $\langle\zeta_\pm(s)\zeta_\mp(0)\rangle = \langle\zeta_\mp(s)\zeta_\mp(0)\rangle$, we finally have

$$
\begin{aligned}
&\langle J(q''_+, q''_-, t; q'_+, q'_-)\rangle = \\
&\int \mathcal{D}q_+ \int \mathcal{D}q_- \exp\left\{\frac{\mathrm{i}}{\hbar}\left[S_{\mathrm{S}}[q_+] - S_{\mathrm{S}}[q_-] + \frac{\mu}{2}\int_0^t \mathrm{d}s(q_+^2(s) - q_-^2(s))\right]\right\} \\
&\times \exp\left\{-\frac{1}{\hbar}\int_0^t \mathrm{d}s \int_0^s \mathrm{d}u[q_+(s) - q_-(s)]\,[q_+(u)\alpha(s-u) - q_-(s)\alpha^*(s-u)]\right\},
\end{aligned} \tag{3.30}
$$

where we have used, by means of Eq. (**??**) and Eq. (3.18), the relation $m\gamma(0) = \mu$. Additionally, we have used the relation, given by Eq (3.20), among the noise correlation function and the Feynman-Vernon kernel. Finally, it is worth mentioning that as it stands, Eq. (3.30) reproduces the usual form of the propagating function of the Caldeira-Leggett model, cf. p.110 in [49]. Additionally, semiclassical approaches are accessible from Eq. (3.26).

[6] Take the average over ζ_+ and ζ_- in Eq. (3.27) as a given function $G[\zeta_+, \zeta_-]$. Expand $G[\zeta_+, \zeta_+]$ in terms of ζ_+ and ζ_- and use the fact that the random forces are Gaussian (cf. Ref. [52])

3.4.2 Stochastic Propagating Function for the Wigner Function

For this case we have

$$\begin{aligned}
&G_{\mathrm{W}}(\mathbf{r}'',t;\mathbf{r}',0;\zeta_{\pm}) \\
&=\frac{1}{2\pi\hbar}\int\mathcal{D}\mathbf{r}\int\mathcal{D}\tilde{\mathbf{r}}\exp\left\{-\frac{\mathrm{i}}{\hbar}\int_0^t\mathrm{d}s\left[\dot{\mathbf{r}}\wedge\tilde{\mathbf{r}}+H_{\mathrm{S}}\left(\mathbf{r}+\frac{1}{2}\tilde{\mathbf{r}}\right)-H_{\mathrm{S}}\left(\mathbf{r}-\frac{1}{2}\tilde{\mathbf{r}}\right)\right]\right\} \\
&\times\exp\left\{\frac{\mathrm{i}}{\hbar}\int_0^t\mathrm{d}s\left[m\gamma(0)q\tilde{q}+\tilde{q}(\zeta_+-\zeta_-)\right]\right\}
\end{aligned} \tag{3.31}$$

with $\zeta_{\pm}$ as in Eq. (3.23). By defining $G_{\mathrm{W}}(\mathbf{r}'',t;\mathbf{r}',0)=\langle G_{\mathrm{W}}(\mathbf{r}'',t;\mathbf{r}',0;\zeta_{\pm})\rangle$, we can write

$$\begin{aligned}
&G_{\mathrm{W}}(\mathbf{r}'',t;\mathbf{r}',0)= \\
&\int\mathcal{D}\mathbf{r}\int\mathcal{D}\tilde{\mathbf{r}}\exp\left\{-\frac{\mathrm{i}}{\hbar}\int_0^t\mathrm{d}s\left[\dot{\mathbf{r}}\wedge\tilde{\mathbf{r}}+H_{\mathrm{S}}\left(\mathbf{r}+\frac{1}{2}\tilde{\mathbf{r}}\right)-H_{\mathrm{S}}\left(\mathbf{r}-\frac{1}{2}\tilde{\mathbf{r}}\right)-m\gamma(0)q(s)\tilde{q}(s)\right]\right\} \\
&\times\left\langle\exp\left\{\frac{\mathrm{i}}{\hbar}\int_0^t\mathrm{d}s\left[q(s)(\zeta_+-\zeta_-)+\frac{1}{2}\tilde{q}(s)(\zeta_++\zeta_-)\right]\right\}\right\rangle.
\end{aligned} \tag{3.32}$$

Proceeding as we did in the last section, we obtain

$$\begin{aligned}
&\left\langle\exp\left\{\frac{\mathrm{i}}{\hbar}\int_0^t\mathrm{d}s\left[q(s)(\zeta_+-\zeta_-)+\frac{1}{2}\tilde{q}(s)(\zeta_++\zeta_-)\right]\right\}\right\rangle= \\
&\exp\left[-2\frac{\mathrm{i}}{\hbar}\int_0^t\mathrm{d}s\int_0^s\mathrm{d}u\tilde{q}(s)q(u)\alpha_{\mathrm{I}}(s-u)-\frac{1}{\hbar}\int_0^t\mathrm{d}s\int_0^s\mathrm{d}u\tilde{q}(s)\tilde{q}(u)\alpha_{\mathrm{R}}(s-u)\right],
\end{aligned} \tag{3.33}$$

Finally, by putting this result into Eq. (3.32) we obtain

$$\begin{aligned}
&G_{\mathrm{W}}(\mathbf{r}'',t;\mathbf{r}',0) \\
&=\int\mathcal{D}\mathbf{r}\int\mathcal{D}\tilde{\mathbf{r}}\exp\left\{-\frac{\mathrm{i}}{\hbar}\int_0^t\mathrm{d}s\left[\dot{\mathbf{r}}\wedge\tilde{\mathbf{r}}+H_{\mathrm{S}}\left(\mathbf{r}+\frac{1}{2}\tilde{\mathbf{r}}\right)-H_{\mathrm{S}}\left(\mathbf{r}-\frac{1}{2}\tilde{\mathbf{r}}\right)-2\mu q(s)\tilde{q}(s)\right]\right\} \\
&\times\exp\left[-2\frac{\mathrm{i}}{\hbar}\int_0^t\mathrm{d}s\int_0^s\mathrm{d}u\tilde{q}(s)q(u)\alpha_{\mathrm{I}}(s-u)-\frac{1}{\hbar}\int_0^t\mathrm{d}s\int_0^s\mathrm{d}u\tilde{q}(s)\tilde{q}(u)\alpha_{\mathrm{R}}(s-u)\right].
\end{aligned} \tag{3.34}$$

3.4.3 Semiclassical General Approximation in the Ullersma-Caldeira-Leggett model

In this section we will derive the general expression for the semiclassical propagating function of the Wigner function. In this general scenario and for real time, the action $\mathcal{S}[\{\mathbf{r}\},\{\tilde{\mathbf{r}}\},t]$ containing the dynamical information reads[7] [44, 49]

$$\begin{aligned}
\mathcal{S}[\{\mathbf{r}\},\{\tilde{\mathbf{r}}\},t]&=\mathcal{S}_{\mathrm{S}}[\{\mathbf{r}\},\{\tilde{\mathbf{r}}\},t]+mq(0)\int_0^t\mathrm{d}s\tilde{q}(s)\gamma(s) \\
&+m\int_0^t\mathrm{d}s\int_0^s\mathrm{d}u\gamma(s-u)\dot{q}(u)\tilde{q}(s)-\frac{\mathrm{i}}{2}\int_0^t\mathrm{d}s\int_0^t\mathrm{d}u\;\alpha_{\mathrm{R}}(s-u)\tilde{q}(u)\tilde{q}(s),
\end{aligned} \tag{3.35}$$

[7] We are using, in the last term of the action, the property $\int_0^t\mathrm{d}s\int_0^t\mathrm{d}u(\cdot)=2\int_0^t\mathrm{d}s\int_0^s\mathrm{d}u(\cdot)$

where $\mathcal{S}_{\rm S}[\{\mathbf{r}\},\{\tilde{\mathbf{r}}\},t]$ has the form

$$\mathcal{S}_{\rm S}[\{\mathbf{r}\},\{\tilde{\mathbf{r}}\},t] = \int_0^t \mathrm{d}s \left[\dot{\mathbf{r}} \wedge \tilde{\mathbf{r}} + H_{\rm S}\left(\mathbf{r} + \frac{1}{2}\tilde{\mathbf{r}}\right) - H_{\rm S}\left(\mathbf{r} - \frac{1}{2}\tilde{\mathbf{r}}\right)\right]. \tag{3.36}$$

The additional non-unitary terms in Ec. (3.35) comes from the analytical calculation of the influence functional in configuration space. From those terms can be seen that the symplectic symmetry is broken. This can be explained by the choice we have made for the coupling term: the central system is coupled to the bath just in the position, i.e., a qQ type of coupling. To recover the symmetry, one should introduce a similar coupling in the momenta, i.e., a general coupling term of the form $\sum_{j=1}^{F} \mathbf{r} \wedge \mathsf{C}_j \mathbf{R}_j$, with

$$\mathsf{C}_j = \begin{pmatrix} 0 & C_{j,qQ} \\ C_{j,pP} & 0 \end{pmatrix}. \tag{3.37}$$

However, in this case the behavior is qualitative very similar to the one in absence of p-coupling [53,54]. If we would introduce independent baths for q and p-couplings, we have to deal with some extra phenomena, e.g., a kind of semiclassical frustration of dissipation which is characterized by underdamped oscillations and longer relaxation times in the strong coupling regime which is generated because of the canonically conjugate character of position and momentum [53,54]. We have omitted the mixed coupling terms $C_{j,qP}$, and $C_{j,pQ}$ because, by means of canonicals transformations, they can be seen as couplings in positions and momenta, respectively, plus a harmonic shift of the potential [39]. So, the breaking of the symplectic geometry is well justified and we can guarantee that the basic features of quantum dissipation are encoded in Ec. (3.35) and, off course, the propagating function obtained from it.

We find convenient to express $\mathcal{S}[\{\mathbf{r}\},\{\tilde{\mathbf{r}}\},t]$ as

$$\mathcal{S}[\{\mathbf{r}\},\{\tilde{\mathbf{r}}\},t] = \int_0^t \mathrm{d}s \phi(\{\mathbf{r}\},\{\tilde{\mathbf{r}}\},s), \tag{3.38}$$

with

$$\begin{aligned} \phi(\{\mathbf{r}\},\{\tilde{\mathbf{r}}\},s) =& \dot{\mathbf{r}} \wedge \tilde{\mathbf{r}} + H_{\rm S}\left(\mathbf{r} + \frac{1}{2}\tilde{\mathbf{r}}\right) - H_{\rm S}\left(\mathbf{r} - \frac{1}{2}\tilde{\mathbf{r}}\right) + mq(0)\tilde{q}(s)\gamma(s) \\ &+ m\tilde{q}(s)\int_0^s \mathrm{d}u \gamma(s-u)\dot{q}(u) - \frac{\mathrm{i}}{2}\tilde{q}(s)\int_0^t \mathrm{d}u\ \alpha_{\rm R}(s-u)\tilde{q}(u). \end{aligned} \tag{3.39}$$

Thus, the stationary paths which make the action $\mathcal{S}$ an extremum are those that satisfy the variational conditions

$$\frac{\delta \mathcal{S}}{\delta \mathbf{r}} = 0, \qquad \frac{\delta \mathcal{S}}{\delta \tilde{\mathbf{r}}} = 0, \tag{3.40}$$

which, in turn, implies the that ϕ must satisfy the equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \phi}{\partial \dot{\mathbf{r}}}\right) - \frac{\partial \phi}{\partial \mathbf{r}} = 0, \qquad \frac{\partial \Phi}{\partial \tilde{\mathbf{r}}} = 0, \tag{3.41}$$

or equivalently,

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial\phi}{\partial\dot{p}}\right)-\frac{\partial\phi}{\partial p}=0, \qquad \frac{\partial\phi}{\partial\tilde{p}}=0,$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial\phi}{\partial\dot{q}}\right)-\frac{\partial\phi}{\partial q}=0, \qquad \frac{\partial\phi}{\partial\tilde{q}}=0. \tag{3.42}$$

Then, after the explicit calculation, but keeping in mind that the system potential V has not been yet specified, we obtain the following set of four equations

$$\begin{aligned}
\dot{p} &= -\frac{\partial}{\partial\tilde{q}}\left[H_{\mathrm{S}}\left(\mathbf{r}+\frac{1}{2}\tilde{\mathbf{r}}\right)-H_{\mathrm{S}}\left(\mathbf{r}-\frac{1}{2}\tilde{\mathbf{r}}\right)\right]-m\frac{\mathrm{d}}{\mathrm{d}s}\int_0^s \mathrm{d}u\gamma(s-u)q(u)\\
&+\mathrm{i}\int_0^t \mathrm{d}u\ \alpha_{\mathrm{R}}(s-u)\tilde{q}(u),\\
\dot{q} &= \frac{\partial}{\partial\tilde{p}}\left[H_{\mathrm{S}}\left(\mathbf{r}+\frac{1}{2}\tilde{\mathbf{r}}\right)-H_{\mathrm{S}}\left(\mathbf{r}-\frac{1}{2}\tilde{\mathbf{r}}\right)\right],\\
\dot{\tilde{p}} &= -\frac{\partial}{\partial q}\left[H_{\mathrm{S}}\left(\mathbf{r}+\frac{1}{2}\tilde{\mathbf{r}}\right)-H_{\mathrm{S}}\left(\mathbf{r}-\frac{1}{2}\tilde{\mathbf{r}}\right)\right]+m\frac{\mathrm{d}}{\mathrm{d}s}\int_s^t \mathrm{d}u\gamma(u-s)\tilde{q}(u)=0\\
\dot{\tilde{q}} &= \frac{\partial}{\partial p}\left[H_{\mathrm{S}}\left(\mathbf{r}+\frac{1}{2}\tilde{\mathbf{r}}\right)-H_{\mathrm{S}}\left(\mathbf{r}-\frac{1}{2}\tilde{\mathbf{r}}\right)\right].
\end{aligned} \tag{3.43}$$

It seem worth mentioning that an equivalent set of equations were previously derived by Grabert, Schramm and Ingold working in configuration space [55]. The classical limit in this case reduces to the Langevin equation without noise term and with an extra term, $-mq'\gamma(s)$, showing that even classical processes depend on the initial state (see [55] and reference therein). It is also important to emphasize the fact that this set of equations has as limit case the set found in Eq. (2.24) when we were discussing the semiclassical regime from the unitary dynamics. Clearly, as long as we decouple the central system from the bath, i.e., once we have set the condition $c_j=0$, the dissipation stops and the extremal equations in Eq. (3.43) becomes those of Eq. (2.24). Following the same procedure of that section, by a change of variables from $(\mathbf{r},\tilde{\mathbf{r}})$ to $(\mathbf{r}_+,\mathbf{r}_-)$ we can write the above set of equations as

$$\begin{aligned}
\dot{p}_\pm &= -\frac{\partial}{\partial q_\pm}H_{\mathrm{S}}\left(\mathbf{r}_+\right)-\frac{m}{2}\frac{\mathrm{d}}{\mathrm{d}s}\int_0^s \mathrm{d}u\gamma(s-u)\left(q_+(u)+q_-(u)\right)\\
&\pm\frac{m}{2}\frac{\mathrm{d}}{\mathrm{d}s}\int_s^t \mathrm{d}u\gamma(u-s)\left(q_+(u)-q_-(u)\right)+\mathrm{i}\int_0^t \mathrm{d}u\ \alpha_{\mathrm{R}}(s-u)\left(q_+(u)-q_-(u)\right),\\
\dot{q}_\pm &= \frac{\partial}{\partial p_\pm}H_{\mathrm{S}}\left(\mathbf{r}_\pm\right).
\end{aligned} \tag{3.44}$$

Considering that $\gamma(u-s)=\gamma(s-u)$, we can see that in this case the symmetry between the tips is broken. Although the dissipative kernel $\gamma(s)$ appears in a cumbersome way, we here see some additional effects like a kind of enhancement (or suppression) of dissipation for $\mathbf{r}_-$ and a contrary effect for $\mathbf{r}_+$ by the real integral term involving $(q_+(u)-q_-(u))$.

Having found the extremal equations directly from the more general phase functional within the Ullersma-Caldeira-Leggett model, we would like to write the mathematical expression for the propagating function. In this regard, we make use of the general expression defining this quantity in Eq. (3.6). Once the influence functional is known, we can put it into this equation and, from it, to implement the semiclassical approximation. Thus, if we take use the results in Eq. (2.18), Eq. (3.5) and Eq. (3.35), we can arrive at the following form of the propagating function at the semiclassical level in the van Vleck approximation within the phase-space description of the dynamics

$$
\begin{aligned}
J_{\mathrm{W}}(\mathbf{r}'', t; \mathbf{r}', 0) = \frac{4}{h} \sum_{j_+, j_-} \frac{1}{\sqrt{|\det(\mathsf{M}_{j_+, j_-})|}} \exp \Bigg\{ & -\frac{\mathrm{i}}{\hbar} \mathcal{S}_{\mathrm{S}} \left[\{\mathbf{r}_+\}, \{\mathbf{r}_-\}, t \right] \\
& + \frac{\mathrm{i}}{2} \pi \nu_{j_+, j_-} - \frac{\mathrm{i}}{\hbar} \frac{m}{2} \left(q_+(0) + q_-(0) \right) \int_0^t \mathrm{d}s \left(q_+(s) - q_-(s) \right) \gamma(s) \\
& - \frac{\mathrm{i}}{\hbar} \frac{m}{2} \int_0^t \mathrm{d}s \int_0^s \mathrm{d}u \; \gamma(s-u) \left(\dot{q}_+(u) + \dot{q}_-(u) \right) \left(q_+(s) - q_-(s) \right) \\
& - \frac{1}{2\hbar} \int_0^t \mathrm{d}s \int_0^t \mathrm{d}u \; \alpha_{\mathrm{R}}(s-u) \left(q_+(u) - q_-(u) \right) \left(q_+(s) - q_-(s) \right) \Bigg\} .
\end{aligned}
\tag{3.45}
$$

Here, ν_{j_+, j_-} represent the Maslov index for the pair of trajectories j_+, j_-. Similarly, $\mathsf{M}^{\alpha\beta}_{j_+, j_-} = \partial^2 \mathcal{S}_j / \partial r_\alpha \partial r_\beta$ represent the pair of stability matrices associated to the aforementioned trajectories. Regarding the additional terms in the above equation, we clearly interpret the ones related to the damping kernel $\gamma(s)$ as related to the dissipation process. On the other hand, the unique real term above represents the decoherence kernel. Thus, as is expected from the standard theory of decoherence, we see that this term depends only on the distance of the tips chords, q_+, q_-.

3.5 Numerical Results

In order to provide an insight of the performance of the semiclassical propagating function of the Wigner function in the presence of non-Markovian effects, we coupled a Morse oscillator to a collection of harmonic oscillators and calculate the propagating function at different times for a particular initial condition. Thus, the figures show our results using an Ohmic spectral density and a cutoff $\omega_{\mathrm{D}} = 4\omega_{\mathrm{min}}$. Since the damping rate, γ, and thermal energy, $k_{\mathrm{B}}T$, are lower than the typical time and energy scale of the system, respectively, we observe that the pattern of the propagator is similar in both cases. However, in the dissipative case we can observe how the probability is concentrated in a smaller region than in the unitary case. In particular, it is clear how contributions from large chords are suppressed in the damped case by the effect of decoherence.

3.5.1 Semiclassical unitary evolution

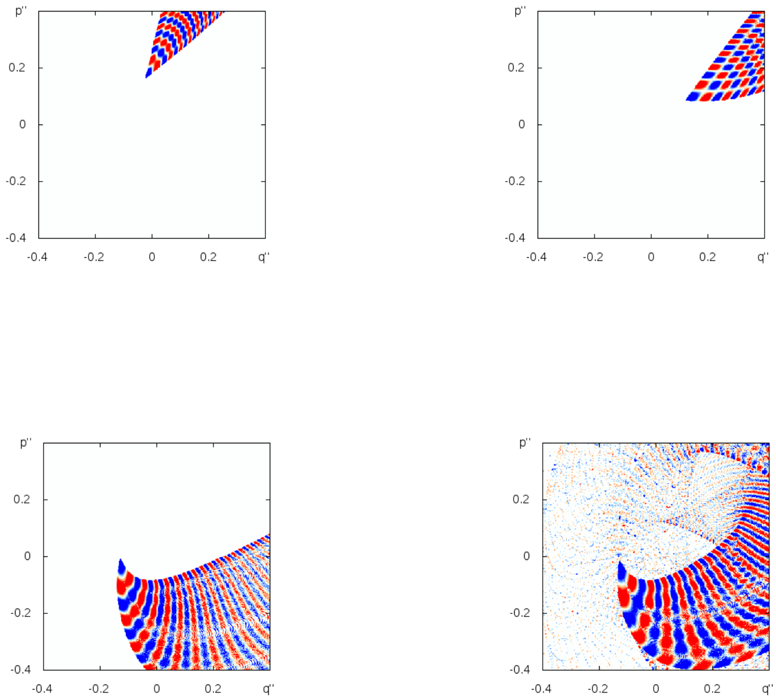

Figure 3.1: *Semiclassical unitary evolution at times* $t = 0.5072s$*,* $t = 1.0144s$*,* $t = 6.0864s$*, and* $t = 12.1728s$*; with initial phase-space point* $(p', q') = (0, -1)$*. Parameter values are* $m = 0.5$*,* $\omega_{min} = 0.0125$*,* $D = 1$*,* $a = 1.25$*,* $k_B T = 0.04\omega_{min}$*,* $\gamma = 0.04\omega_{min}$ *and* $\omega_D = 4\omega_{min}$*. Finally,* ω_{min} *denotes the frequency in the harmonic approximation,* $\omega_{min} = \sqrt{2a^2 D/m}$*.*

3.5.2 Semiclassical disipative evolution

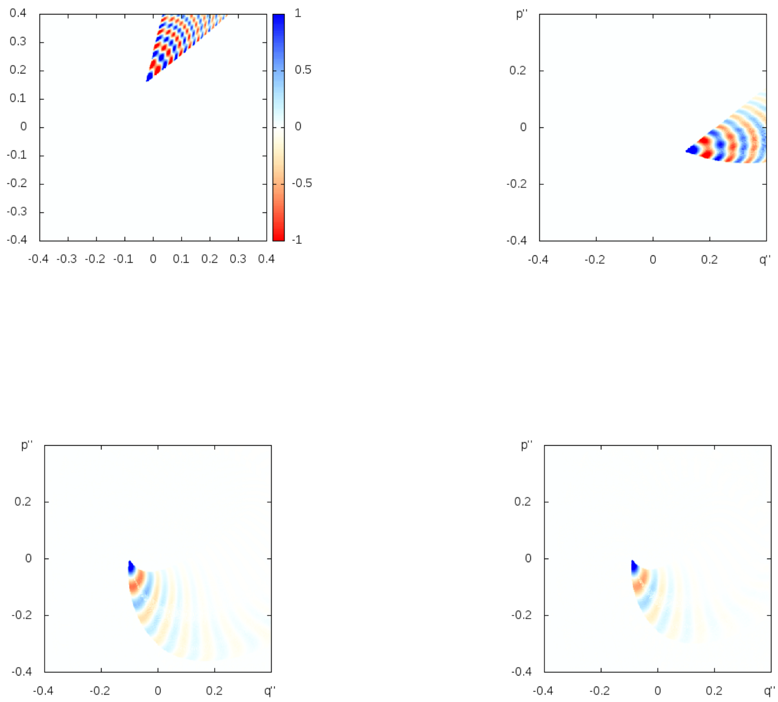

Figure 3.2: *Semiclassical dissipative evolution at times* $t = 0.5072s$, $t = 1.0144s$, $t = 6.0864s$, *and* $t = 12.1728s$; *with initial phase-space point* $(p', q') = (0, -1)$. *Parameter values are* $m = 0.5$, $\omega_{min} = 0.0125$, $D = 1$, $a = 1.25$, $k_BT = 0.04\omega_{min}$, $\gamma = 0.04\omega_{min}$ *and* $\omega_D = 4\omega_{min}$. *Finally,* ω_{min} *denotes the frequency in the harmonic approximation,* $\omega_{min} = \sqrt{2a^2D/m}$.

Chapter 4

Semiclassical open dynamics from path integrals

4.1 Introduction

On this chapter we will study a more realistic physical situation. We will consider the coupling among a quantum DOF and a set of F harmonic bath modes. The interaction potential will be considered non-linear, which in turn implies a more rich structure for the propagator. The mathematical framework will be, as in the unitary non-linear case, the path integral formulation in phase-space.

4.2 Semiclassical Wigner propagator for an open system

To begin with, let us consider the Hamiltonian of the universe as

$$\begin{aligned}\hat{H} =&\hat{H}_{\mathrm{S}}(\mathbf{r}) + \hat{H}_{\mathrm{B}}(\mathbf{R}) + \hat{H}_{\mathrm{SB}}(\mathbf{r},\mathbf{R}) \\ =&\frac{\hat{p}^2}{2m} + V_{\mathrm{S}}(\hat{q}) + \sum_{j=1}^{F}\left[\frac{\hat{P}_j^2}{2m_j} + V_{\mathrm{B}}(\hat{Q}_j)\right] + \sum_{j=1}^{F} V_{\mathrm{SB}}(\hat{q},\hat{Q}_j) \\ =&\frac{\hat{p}^2}{2m} + \sum_{j=1}^{F}\frac{\hat{P}_j^2}{2m_j} + W\left(\hat{q},\{\hat{Q}_j\}\right),\end{aligned} \tag{4.1}$$

where W represents the total contribution to the potential energy for the composite system. The Weyl symbol of the Hamiltonian is given by

$$H = \frac{p^2}{2m} + \sum_{j=1}^{F}\frac{P_j^2}{2m_j} + W\left(q,\{Q_j\}\right), \tag{4.2}$$

whereas the path integral representation of the Wigner propagator takes the form

$$G_{\mathrm{W}}(\mathcal{R}'',t;\mathcal{R}',0) = \frac{1}{(2\pi\hbar)^{F+1}}\int\mathcal{D}\mathcal{R}\int\mathcal{D}\widetilde{\mathcal{R}}\exp\left(-\frac{\mathrm{i}}{\hbar}S[\{\mathcal{R}\},\{\widetilde{\mathcal{R}}\},t]\right). \tag{4.3}$$

In order to calculate the propagator for the Hamiltonian in Eq. (4.2), we will consider the discrete version of this propagator

$$G_{\mathrm{W}}(\mathcal{R}_n,n\Delta t;\mathcal{R}_{n-1},(n-1)\Delta t) = \frac{1}{(2\pi\hbar)^{2(F+1)}}\int d^{2(F+1)}\widetilde{\mathcal{R}}_n\exp\left(-\frac{\mathrm{i}}{\hbar}\phi_n\right). \tag{4.4}$$

Here ϕ_n represents the discrete version of the action in phase space. Its mathematical form is given by

$$\phi_n = \Delta\mathcal{R}_n \wedge \widetilde{\mathcal{R}}_n + \left[H\left(\bar{\mathcal{R}}_n + \frac{\tilde{\mathcal{R}}_n}{2}\right) - H\left(\bar{\mathcal{R}}_n - \frac{\tilde{\mathcal{R}}_n}{2}\right)\right]\Delta t, \tag{4.5}$$

with $\mathcal{R}_0 = \mathcal{R}'$, $\mathcal{R}_N = \mathcal{R}''$, $\Delta\mathcal{R}_n = \mathcal{R}_n - \mathcal{R}_{n-1}$ and $\bar{\mathcal{R}}_n = \frac{\mathcal{R}_n + \mathcal{R}_{n-1}}{2}$. Regarding the first term of the phase, it corresponds to a purely geometrical term that involves a bilinear symplectic form that can be explicitly written as [9]

$$\Delta\mathcal{R}_n \wedge \tilde{\mathcal{R}}_n = \mathbf{\Delta r}_n \wedge \tilde{\mathbf{r}}_n + \sum_{j=1}^{F} \mathbf{\Delta R}_{jn} \wedge \tilde{\mathbf{R}}_{jn}, \tag{4.6}$$

where $\tilde{\mathbf{r}}_n$ and $\tilde{\mathbf{R}}_n$ represent the quantum fluctuations over the trajectories $\mathbf{r}_n, \mathbf{R}_n$ respectively. In relation to the terms in brackets in Eq. (4.5), they can be explicitly written as

$$\begin{aligned} \Delta H_n = &\frac{\bar{p}_n\tilde{p}_n}{m} + \sum_{j=1}^{F}\frac{\bar{P}_{jn}\tilde{P}_{jn}}{m_j} + V_{\mathrm{S}}\left(\bar{q}_n + \frac{\tilde{q}_n}{2}\right) - V_{\mathrm{S}}\left(\bar{q}_n - \frac{\tilde{q}_n}{2}\right) \\ &+ U\left(\bar{q}_n + \frac{\tilde{q}_n}{2}, \left\{\bar{Q}_{jn} + \frac{\tilde{Q}_{jn}}{2}\right\}\right) - U\left(\bar{q}_n - \frac{\tilde{q}_n}{2}, \left\{\bar{Q}_{jn} - \frac{\tilde{Q}_{jn}}{2}\right\}\right). \end{aligned} \tag{4.7}$$

Since the phase of the propagator includes all the relevant information about the physical state of the universe, we are mainly concerned with the mathematical form it will take once we have assigned a functional form for the potential. In this respect, we consider that, without limiting the generality of the discussion, the interaction potential can be put into a central potential form [37]

$$U\left(q, Q_j\right) \to U\left(Q_j - \frac{c_j}{m_j\omega_j^2}q\right), \tag{4.8}$$

with c_j playing the role of a coupling constant between the central system and the j-th bath mode. This choice is by no means arbitrary and allows, in turn, to characterize the potential as an invariant under coordinate translations. In terms of the dimensionless quantity $c_j/m_j\omega_j^2$, and for the sake of simplicity in the notation, we define the quantity

$$\mathsf{q}_{jn} = \frac{c_j}{m_j\omega_j^2}q_n, \tag{4.9}$$

which carries information about the intensity of the coupling of the central system with every individual bath mode. The natural question that arises at this point is: what will be the mathematical form of the U potential?, even more, how are we going to include a semiclassical description of the dynamics at this level in the formalism? In relation to the first question, we have decided not to specify the mathematical form of the potential but writing it in a Taylor series expansion up to the third term which, in turn, becomes the first non-linear correction to linear potential.On the other hand, for the last question the natural answer comes from the fact that within the semiclassical approximation it is decisive to expand around the path leading to the dominant contribution, i.e. the classical path [37]. Therefore, the decomposition of a general path into the classical path and fluctuations around it turns to be more a necessity than a convenience. Since the action is stationary at classical paths, we are obliged to express a general path for the central system as $\mathbf{r}_n = \mathbf{r}_n^{\text{cl}} + \tilde{\mathbf{r}}_n$. Here, $\hat{\mathbf{r}}_n$, $\hat{\mathbf{R}}_{jn}$ are the coordinates that represents the classical trajectories in n-th time interval. Then, from Eq. (4.7)

$$\Delta U_n = \sum_{j=1}^{F} \left[U_n \left(\bar{\mathcal{Q}}_{jn} + \hat{\bar{\mathcal{Q}}}_{jn} + \frac{\tilde{\mathcal{Q}}_{jn}}{2} \right) - U_n \left(\bar{\mathcal{Q}}_{jn} + \hat{\bar{\mathcal{Q}}}_{jn} - \frac{\tilde{\mathcal{Q}}_{jn}}{2} \right) \right], \tag{4.10}$$

where we have defined the quantity $\mathcal{Q}_{jn} = Q_{jn} - \mathsf{q}_{jn}$. In terms of this quantity we can Taylor expand both U_n as

$$U_n \left(\bar{\mathcal{Q}}_{jn} + \hat{\bar{\mathcal{Q}}}_{jn} \pm \frac{\tilde{\mathcal{Q}}_{jn}}{2} \right) \approx U^{(0)}(\hat{\bar{\mathcal{Q}}}_{jn}) + U^{(1)}(\hat{\bar{\mathcal{Q}}}_{jn}) \left[\bar{\mathcal{Q}}_{jn} \pm \frac{\tilde{\mathcal{Q}}_{jn}}{2} \right] \\ + \frac{1}{2!} U^{(2)}(\hat{\bar{\mathcal{Q}}}_{jn}) \left[\bar{\mathcal{Q}}_{jn} \pm \frac{\tilde{\mathcal{Q}}_{jn}}{2} \right]^2 + \frac{1}{3!} U^{(3)}(\hat{\bar{\mathcal{Q}}}_{jn}) \left[\bar{\mathcal{Q}}_{jn} \pm \frac{\tilde{\mathcal{Q}}_{jn}}{2} \right]^3, \tag{4.11}$$

giving place to

$$\Delta U_n = \sum_{j=1}^{F} \left[U^{(1)}(\hat{\bar{\mathcal{Q}}}_{jn}) \tilde{\mathcal{Q}}_{jn} + U^{(2)}(\hat{\bar{\mathcal{Q}}}_{jn}) \bar{\mathcal{Q}}_{jn} \tilde{\mathcal{Q}}_{jn} + \frac{1}{3!} U^{(3)}(\hat{\bar{\mathcal{Q}}}_{jn}) \left(3 \bar{\mathcal{Q}}_{jn}^2 \tilde{\mathcal{Q}}_{jn} + \frac{\tilde{\mathcal{Q}}_{jn}^3}{4} \right) \right]. \tag{4.12}$$

Following the same steps, this time for the system potential, allow us to write

$$\Delta V_n = V^{(1)}(\hat{\bar{q}}_n) \tilde{q}_n + V^{(2)}(\hat{\bar{q}}_n) \bar{q}_n \tilde{q}_n + \frac{1}{3!} V^{(3)}(\hat{\bar{q}}_n) \left(3 \bar{q}_n^2 \tilde{q}_n + \frac{\tilde{q}_n^3}{4} \right). \tag{4.13}$$

With the purpose of simplifying the writing in the system-bath sector of the potential, we find convenient to define the quantities

$$A_{jn} = \frac{\partial^2 U}{\partial \bar{\mathcal{Q}}_{jn}^2} \left(\bar{Q}_{jn} - \bar{\mathsf{q}}_{jn} \right) + \frac{1}{2} \frac{\partial^3 U}{\partial \bar{\mathcal{Q}}_{jn}^3} \left(\bar{Q}_{jn} - \bar{\mathsf{q}}_{jn} \right)^2, \qquad B_{jn} = \frac{\partial^3 U}{\partial \bar{\mathcal{Q}}_{jn}^3}, \tag{4.14}$$

such that the argument of the sum in Eq. (4.12) can be written as

$$\Delta U_{jn} = \frac{\partial U}{\partial \bar{\mathcal{Q}}_{jn}} \tilde{\mathcal{Q}}_{jn} + \Delta U_{jn}' = \frac{\partial U}{\partial \bar{\mathcal{Q}}_{jn}} \tilde{\mathcal{Q}}_{jn} + A_{jn} \tilde{\mathcal{Q}}_{jn} + \frac{B_{jn}}{24} \tilde{\mathcal{Q}}_{jn}^3. \tag{4.15}$$

By putting all of this into the action, we obtain

$$\phi_n = \left(\Delta p_n + \Delta \hat{p}_n \right) \tilde{q}_n - \left(\Delta q_n + \Delta \hat{q}_n \right) \tilde{p}_n + \frac{\left(\bar{p}_n + \hat{\bar{p}}_n \right) \tilde{p}_n}{m} \Delta t + \Delta V_n \Delta t \\ + \sum_{j=1}^{F} (\Delta P_{jn} + \Delta \hat{P}_{jn}) \tilde{Q}_{jn} - \sum_{j=1}^{F} (\Delta Q_{jn} + \Delta \hat{Q}_{jn}) \tilde{P}_{jn} \\ + \sum_{j=1}^{F} \frac{(\bar{P}_{jn} + \hat{\bar{P}}_{jn}) \tilde{P}_{jn}}{m_j} \Delta t + \sum_{j=1}^{F} \Delta U_{jn} \Delta t. \tag{4.16}$$

At this point, and anticipating the limit process we will face in the composition of the propagator, we can extract from the above phase the classical equations of motion. Thus, in the $\Delta t \to 0$ limit we will have

$$\begin{aligned} \Delta \hat{q}_n - \frac{\Delta t}{m} \hat{\bar{p}}_n &\to 0 \\ \Delta \hat{Q}_{jn} - \frac{\Delta t}{m_j} \hat{\bar{P}}_{jn} &\to 0 \\ \Delta \hat{p}_n + \frac{\partial V(\hat{\bar{q}}_n)}{\partial \bar{q}_n} \Delta t - \Delta t \sum_{j=1}^{F} \frac{c_j}{m_j \omega_j^2} \frac{\partial U(\hat{\bar{Q}}_{jn})}{\partial \bar{Q}_{jn}} &\to 0 \\ \Delta \hat{P}_{jn} + \frac{\partial U(\hat{\bar{Q}}_{jn})}{\partial \bar{Q}_{jn}} \Delta t &\to 0. \end{aligned} \tag{4.17}$$

Then, we take advantage of this simplification in the action phase, despite the fact we have not taken formally the limit over the propagator which, by now, is under construction. In this way, regardless the absence of the limit, we will write the simplified form of the phase as

$$\phi_n = \phi_n^{\mathrm{S}} + \sum_{j=1}^{F} \Delta P_{jn} (\mathfrak{q}_{jn} + \tilde{Q}_{jn}) - \sum_{j=1}^{F} \Delta Q_{jn} \tilde{P}_{jn} + \sum_{j=1}^{F} \frac{\bar{P}_{jn} \tilde{P}_{jn}}{m_j} \Delta t + \sum_{j=1}^{F} \Delta U'_{jn} \Delta t. \tag{4.18}$$

If we consider the SB sector of the above phase and take into account the integrals over the bath fluctuations in Eq. (4.4), we see that we are in position to integrate over $\tilde{Q}_{jn}, \tilde{P}_{jn}$. Thus, by means of the definition

$$\tilde{Q}'_{jn} = \left(\frac{B_{jn} \Delta t}{8\hbar} \right)^{\frac{1}{3}} \tilde{Q}_{jn} = \alpha_{jn}^{\frac{1}{3}} \tilde{Q}_{jn}, \tag{4.19}$$

we obtain the following structure for the propagator

$$\begin{aligned} G_{n,n-1} = \int \frac{\mathrm{d}\tilde{p}_n}{2\pi\hbar} \frac{\mathrm{d}\tilde{q}_n}{2\pi\hbar} \exp\left(-\frac{\mathrm{i}}{\hbar} \phi_n^{\mathrm{S}} \right) \prod_{j=1}^{F} \frac{\alpha_{jn}^{-\frac{1}{3}}}{\hbar} \delta\left(\Delta Q_{jn} - \frac{\bar{P}_{jn}}{m_j} \Delta t \right) \\ \times \mathrm{Ai}\left(\frac{\alpha_{jn}^{-\frac{1}{3}}}{\hbar} \left[U^{(2)}(Q_{jn}^{\mathrm{cl}}) \left(\bar{Q}_{jn} - \bar{\mathfrak{q}}_{jn} \right) \Delta t + \Delta P_{jn} \right] \right) \exp\left(-\frac{\mathrm{i}}{\hbar} \Delta P_{jn} \tilde{\mathfrak{q}}_{jn} \right). \end{aligned} \tag{4.20}$$

where

$$\phi_n^{\mathrm{S}} = \Delta p_n \tilde{q}_n - \left(\Delta q_n - \frac{\bar{p}_n}{m} \Delta t \right) \tilde{p}_n + \Delta V'_n \Delta t. \tag{4.21}$$

The factor $\alpha_{jn}^{-\frac{1}{3}}$, which depends upon the third derivative of the SB potential, determines how extended is the Airy function. Its oscillatory character will be determined by direct comparison between the discrete version of the action ϕ_n and $\hbar$. In a quantum regime, those quantities are of roughly of the same order of magnitude. Thus the oscillatory pattern is less pronounced that in the semiclassical regime, where $\phi_n \gg \hbar$, giving place to a highly oscillatory phase in the propagator. This, in turn, implies that the regions in phase-space where there oscillations are strong enough, the amplitude will rapidly decay to zero, whereas the non-trivial contribution will come from regions near to the stationary solutions, i.e., the classical trajectories.

To simplify the propagator in Eq. (4.20), we introduce, on one hand, the change of variables

$$\breve{P}_{jn} = \left[m_j U^{(2)}(Q^{\mathrm{cl}}_{jn})\right]^{-\frac{1}{4}} P_{jn}, \quad \breve{Q}_{jn} = \left[m_j U^{(2)}(Q^{\mathrm{cl}}_{jn})\right]^{\frac{1}{4}} Q_{jn}, \quad \breve{\mathsf{q}}_{jn} = \left[m_j U^{(2)}(Q^{\mathrm{cl}}_{jn})\right]^{\frac{1}{4}} \mathsf{q}_{jn}, \tag{4.22}$$

and, on the other hand, the definition

$$\breve{\tau}_{jn}^{-\frac{1}{3}} = \frac{\alpha_{jn}^{-\frac{1}{3}}}{\hbar}\left[m_j U^{(2)}(Q^{\mathrm{cl}}_{jn})\right]^{\frac{1}{4}}. \tag{4.23}$$

By doing so, we obtain the propagator

$$\begin{aligned} G_{n,n-1} = \int \frac{\mathrm{d}\tilde{p}_n}{2\pi\hbar}\frac{\mathrm{d}\tilde{q}_n}{2\pi\hbar} \exp\left(-\frac{\mathrm{i}}{\hbar}\phi^{\mathrm{S}}_n\right) \prod_{j=1}^{F} \breve{\tau}_{jn}^{-\frac{1}{3}} \delta\left(\Delta\breve{Q}_{jn} - \theta_{jn}\breve{\bar{P}}_{jn}\right) \\ \mathrm{Ai}\left(\breve{\tau}_{jn}^{-\frac{1}{3}}\left[\Delta\breve{P}_{jn} + \theta_{jn}\left(\breve{\bar{Q}}_{jn} - \breve{\bar{\mathsf{q}}}_{jn}\right)\right]\right) \exp\left(-\frac{\mathrm{i}}{\hbar}\Delta\breve{P}_{jn}\breve{\bar{\mathsf{q}}}_{jn}\right). \end{aligned} \tag{4.24}$$

where we have made use of the definition $\theta_{jn} = \sqrt{\frac{U^{(2)}(Q^{\mathrm{cl}}_{jn})}{m_j}}\Delta t$. This Wigner propagator will be trivially null unless

$$\breve{Q}_{jn} = \breve{Q}_{jn-1} + \theta_{jn}\breve{\bar{P}}_{jn}. \tag{4.25}$$

This equation establishes a concatenation among the $\breve{Q}_{jn}$ coordinates which, after taking the limit $\Delta t \to 0$, will imply a relation between the final and initial coordinates. However, and regardless its importance, the above equation cannot support the connection among the momenta at different times. This, off course, happens since we have considered couplings among coordinates exclusively in our formulation of the problem. Nevertheless, this apparent asymmetry in the treatment of the phase-space DOFs can be easily overcome by a canonical transformation. Effectively, an important feature of the above relation emerges once it is noticed that the distinction between $\breve{Q}_{jn}$ and $\breve{P}_{jn}$ is basically one of nomenclature. Under canonical transformation theory, the change $\breve{Q}_{jn} \to \breve{P}_{jn}$, $\breve{P}_{jn} \to -\breve{Q}_{jn}$ accounts for the same dynamics, leaving the Hamiltonian as a canonical invariant. In this sense, we are in position to raise the question about the consequences of expand the above relation into a system of equations taking the form

$$\begin{aligned} \breve{Q}_{jn} =& \breve{Q}_{jn-1} + \theta_{jn}\breve{\bar{P}}_{jn} \\ \breve{P}_{jn} =& \breve{P}_{jn-1} - \theta_{jn}\breve{\bar{Q}}_{jn}. \end{aligned} \tag{4.26}$$

Its solution will shade light on the connection between the initial and final state of the bath dynamics and will give help us to calculate the composition of the set of N discrete propagators before considering the continuum limit. Having pondered this special issue, we can take a look into the solution of this equation system as the matrix equation $\breve{\mathsf{R}}_{jn} = \mathsf{M}_{jn}\breve{\mathsf{R}}_{jn-1}$. Explicitly,

$$\begin{pmatrix} \breve{P}_{jn} \\ \breve{Q}_{jn} \end{pmatrix} = \frac{1}{4+\theta_{jn}^2}\begin{pmatrix} 4-\theta_{jn}^2 & -4\theta_{jn} \\ 4\theta_{jn} & 4-\theta_{jn}^2 \end{pmatrix}\begin{pmatrix} \breve{P}_{jn-1} \\ \breve{Q}_{jn-1} \end{pmatrix}. \tag{4.27}$$

Starting from this equation, we can establish the already metioned relation among the $\breve{P}_{jN}, \breve{Q}_{jN}$ and the $\breve{P}_{j0}, \breve{Q}_{j0}$ bath DOFs. To accomplish that, firstly we note that we will obtain a matrix product of N matrices having all the same mathematical structure. Then we want to calculate the matrix product $\mathsf{M}_{jN}\mathsf{M}_{jN-1}\cdots\mathsf{M}_{jn}\mathsf{M}_{jn-1}\cdots\mathsf{M}_{j2}\mathsf{M}_{j1}$. This can be done by diagonalizing every matrix in this product such that

$$\mathsf{M}_{jN}\mathsf{M}_{jN-1}\cdots\mathsf{M}_{j2}\mathsf{M}_{j1} = \mathsf{E}_j\mathsf{M}_{jN}^{\text{diag}}\mathsf{M}_{jN-1}^{\text{diag}}\cdots\mathsf{M}_{j2}^{\text{diag}}\mathsf{M}_{j1}^{\text{diag}}\mathsf{E}_j^{-1}, \tag{4.28}$$

where we have used the same eigenvector matrix E_j due to the fact that all the M_{jn} matrices have the same structure and only changes the time interval where they are studied. Nonetheless, as long as the time is a smooth parameter in non-relativistic quantum mechanics, i.e., time is homogeneous, the time evolution given by the matices M_{jn} is essentially the same, and therefore, we can safely consider that the eigensystem solution for M_{jn} applies equally for every value of n; allowing us to conclude that the eigenvector matrix E_j diagonalize them all. Then, after some manipulations of Eq. (4.28) and by taking the limit $\Delta t \to 0$, we obtain the matrix

$$\mathsf{M}_j(t) = \begin{pmatrix} \cos\theta_j(t) & -\sin\theta_j(t) \\ \sin\theta_j(t) & \cos\theta_j(t) \end{pmatrix}, \tag{4.29}$$

which represents precisely the stability matrix for the classical trajectory over the complete time-interval of propagation of the dynamics.

To get a physical insight into the meaning of the angle in the above result, we make use of the short-time approximation, which is valid as long as we are interested in the limit $\Delta t \to 0$ where $\Delta t^2 \ll 1$. Then, by using the notation $\theta_{jn} = \Theta_{jn}\Delta t$, we can write, after some manipulations, the Eq. (4.28) as

$$\mathsf{E}_j\left(\prod_{n=1}^{N}\mathsf{M}_{jn}^{\text{diag}}\right)\mathsf{E}_j^{-1} = \begin{pmatrix} 1 & -\sum_{n=1}^{N}\Theta_{jn}\Delta t \\ \sum_{n=1}^{N}\Theta_{jn}\Delta t & 1 \end{pmatrix}, \tag{4.30}$$

which in the limit $\Delta t \to 0$, i.e., $N \to \infty$, becomes

$$\mathsf{M}_j(t) = \begin{pmatrix} 1 & \theta_j(t) \\ \theta_j(t) & 1 \end{pmatrix}. \tag{4.31}$$

We see clearly from this result how the mathematical form of θ_j emerges as

$$\theta_j(t) = \int_0^t \mathrm{d}s\sqrt{\frac{U^{(2)}(Q_j^{\text{cl}}(s))}{m_j}}. \tag{4.32}$$

Even more, this procedure shows that the matrix found in Eq. (4.31) is the right approximation of its complete version in Eq. (4.29) when the argument is small enough to replace the entries with the first term of its series expansion.

Although we have successfully found the limit for the stability matrix of the trajectories for the bath modes, we have not yet accomplished the main purpose of the entire calculation, namely, the composition of the Wigner propagators along the whole time interval. With the aim of doing this, we must go back to Eq. (4.24) and work out the composition. However, as it stands, the composition of this propagator by direct use of the Airy functions becomes a cumbersome task. Hence, if we want to execute a simpler composition, we must get rid of the Airy function momentarily. How can this be possibly done? By means of one of the most valuable tool the scientist has at disposal: the Fourier transform.

Fourier Transform of $G_{n,n-1}$

Let us consider the formal definition of the symplectic Fourier transform of a phase space function $g(\mathbf{r})$ as [12]

$$\tilde{g}(\gamma) \equiv \frac{1}{2\pi} \int \mathrm{d}\mathbf{r} g(\mathbf{r}) \exp\left(\mathrm{i}\gamma \wedge \mathbf{r}\right), \tag{4.33}$$

where $\gamma = (\alpha, \beta)$ is the variable "dual" to $\mathbf{r}$. The usual Fourier transform of the function $g(\mathbf{r})$ is given by

$$\left(\mathcal{F}g\right)(\sigma, \tau) = \int \mathrm{d}p\mathrm{d}q \; g(p,q) \exp\left(\mathrm{i}[q\sigma + p\tau]\right). \tag{4.34}$$

This couple of Fourier transforms are simply related in the following way: $\tilde{g}(\alpha, \beta) = \left(\mathcal{F}g\right)(-\alpha, \beta)$. This relation enable us to use the traditional Fourier methods to recover the $g(\mathbf{r})$ function from $\tilde{g}(\gamma)$ as

$$g(\mathbf{r}) = \frac{1}{2\pi} \int \mathrm{d}\gamma \; \tilde{g}(\gamma) \exp\left(-\mathrm{i}\gamma \wedge \mathbf{r}\right). \tag{4.35}$$

Let $\gamma_{jn} = (\alpha_{jn}, \beta_{jn})$ and $\gamma_{jn-1} = (\alpha_{jn-1}, \beta_{jn-1})$ be the associated dynamical variables in the Fourier space[1]. Then, to transform the propagator in Eq. (4.24), we must calculate $5F$ integrals to transform the bath variables within the time interval $[n-1, n]\Delta t$. To do this, we will split the propagator in Eq. (4.24) into two parts: The central system piece of the propagator that does not depend on the index j, and the bath-system part (SB) that explicitly depend on this index; being this later part the one we need to work with at the moment.

If we write Eq. (4.24) as $G_{n,n-1} = G^{\mathrm{S}}_{n,n-1} G^{\mathrm{SB}}_{n,n-1}$, we are facing the task of calculating the symplectic Fourier transform of the $G^{\mathrm{SB}}_{n,n-1}$ sector of the whole propagator. Hence,

$$\begin{aligned}
\widetilde{G}^{\mathrm{SB}}_{n,n-1} &= \prod_{j=1}^{F} \frac{1}{(2\pi)^2} \int \mathrm{d}\breve{\mathbf{R}}_{jn} \mathrm{d}\breve{\mathbf{R}}_{jn-1} \exp\left(\mathrm{i}\left[\gamma_{jn} \wedge \breve{\mathbf{R}}_{jn} - \gamma_{jn-1} \wedge \breve{\mathbf{R}}_{jn-1}\right]\right) \breve{\tau}_{jn}^{-\frac{1}{3}} \\
&\quad \times \delta\left(\breve{Q}_{jn} - (M_{jn}\breve{\mathbf{R}}_{jn-1})_{\breve{Q}}\right) \mathrm{Ai}\left(\breve{\tau}_{jn}^{-\frac{1}{3}}\left[\breve{P}_{jn} - (M_{jn}\breve{\mathbf{R}}_{jn-1})_{\breve{P}}\right] - \breve{\tau}_{jn}^{-\frac{1}{3}} \theta_{jn} \breve{\mathfrak{q}}_{jn}\right) \\
&\quad \times \exp\left(-\frac{\mathrm{i}}{\hbar} \Delta \breve{P}_{jn} \breve{\mathfrak{q}}_{jn}\right) \\
&= \prod_{j=1}^{F} \widetilde{G}^{\mathrm{SB}}_{j;n,n-1}
\end{aligned} \tag{4.36}$$

As can be seen from this expression, we just need to complete the calculation for the j-th term of the above expression thanks to the non-interacting nature of the bath modes. Let Γ_{jn} be the

[1] The dimensions of the γ_{jn} variables are $(\text{action})^{-1/2}$

phase in $\widetilde{G}^{\mathrm{SB}}_{j;n,n-1}$ Then,

$$\Gamma_{jn} = \alpha_{jn}\breve{Q}_{jn} - \beta_{jn}\breve{P}_{jn} - \alpha_{jn-1}\breve{Q}_{jn-1} + \beta_{jn-1}\breve{P}_{jn-1} + \frac{1}{3}\left(\tilde{\mathcal{Q}}'_{jn}\right)^3 + \breve{\tau}_{jn}^{-\frac{1}{3}}\left[\Delta\breve{P}_{jn} + \theta_{jn}(\breve{Q}_{jn} - \breve{\mathsf{q}}_{jn})\right]\tilde{\mathcal{Q}}'_{jn} - \frac{\breve{\breve{\mathsf{q}}}_{jn}}{\hbar}\Delta\breve{P}_{jn}. \tag{4.37}$$

After some manipulations, we find the following structure for $\widetilde{G}^{\mathrm{SB}}_{j;n,n-1}$

$$\begin{aligned}\widetilde{G}^{\mathrm{SB}}_{j;n,n-1} =& \frac{4}{4+\theta^2_{jn}} \exp\left(\frac{64\mathrm{i}}{3}\breve{\tau}_{jn}\left[\frac{\beta_{jn} - \frac{1}{2}\alpha_{jn}\theta_{jn} + \breve{\breve{\mathsf{q}}}_n/\hbar}{(4+\theta^2_{jn})}\right]^3\right) \\ &\times \exp\left(-\frac{4\mathrm{i}\theta_{jn}}{4+\theta^2_{jn}}\left[\beta_{jn} - \frac{1}{2}\alpha_{jn}\theta_{jn} + \frac{\breve{\breve{\mathsf{q}}}_{jn}}{\hbar}\right]\breve{\mathsf{q}}_{jn}\right) \\ &\times \delta\left(\gamma_{jn} - \mathsf{M}_{jn}\gamma_{jn-1} - \mathsf{V}_{jn}\right).\end{aligned} \tag{4.38}$$

In fact, the delta in this propagator amounts to the product of two Dirac deltas in a more extended notation. The matrix M_{jn} is exactly the one the have found in Eq. (4.27), whereas the term V_{jn} represents a two column vector having the mathematical form

$$\mathsf{V}_{jn} = -\frac{4\theta_{jn}}{4+\theta^2_{jn}}\frac{\breve{\breve{\mathsf{q}}}_{jn}}{\hbar}\begin{pmatrix}1\\ \frac{\theta_{jn}}{2}\end{pmatrix}. \tag{4.39}$$

Although we can proceed from this point to the composition of the propagator, it is not yet convenient since the implementation of the composition will become a difficult task at the moment. To avoid the more than secure complexities arising out of the composition, we take the advantage, again, of the ultra-short time range for the propagation of the dynamics in each interval. This idea simplifies considerably the propagator shaping its form into the following expression for the whole set of bath modes

$$\widetilde{G}^{\mathrm{SB}}_{n,n-1} = \prod_{j=1}^{F}\exp\left(\frac{\mathrm{i}}{3}\breve{\tau}_{jn}\left[\beta_{jn} + \frac{\breve{\breve{\mathsf{q}}}_{jn}}{\hbar}\right]^3 - \mathrm{i}\theta_{jn}\left[\beta_{jn} + \frac{\breve{\breve{\mathsf{q}}}_{jn}}{\hbar}\right]\breve{\breve{\mathsf{q}}}_{jn}\right)\delta\left(\gamma_{jn} - \mathsf{M}_{jn}\gamma_{jn-1} - \mathsf{V}_{jn}\right). \tag{4.40}$$

Now that we have paved the way, we can proceed with the composition. This will be done simultaneously for the two sectors of the propagator. To proceed in this direction, we need to specify the way two and more propagators should be composed. Luckily, the propagator satisfies the Chapman-Kolmogorov relation, such that

$$\widetilde{G}^{\mathrm{SB}}_{n+1,n-1} = \left(\prod_{j=1}^{F}\int \mathrm{d}\gamma_{jn}\right)\widetilde{G}^{\mathrm{SB}}_{n+1,n}\widetilde{G}^{\mathrm{SB}}_{n,n-1}, \qquad G^{\mathrm{S}}_{n+1,n-1} = \int \mathrm{d}\mathbf{r}_n G^{\mathrm{S}}_{n+1,n}G^{\mathrm{S}}_{n,n-1}. \tag{4.41}$$

Then, for the whole set of finite time-intervals, the above pair of equations becomes

$$\widetilde{G}^{\mathrm{SB}}_{N,0} = \left(\prod_{n=1}^{N-1}\prod_{j=1}^{F}\int \mathrm{d}\gamma_{jn}\right)\prod_{n=1}^{N}\widetilde{G}^{\mathrm{SB}}_{n,n-1}, \qquad G^{\mathrm{S}}_{N,0} = \left(\prod_{n=1}^{N-1}\int \mathrm{d}\mathbf{r}_n\right)\prod_{n=1}^{N} G^{\mathrm{S}}_{n,n-1}. \tag{4.42}$$

Let us consider initially the first expression. We can write this propagator as

$$\widetilde{G}^{\mathrm{SB}}_{N,0} = \prod_{j=1}^{F}\left(\prod_{n=1}^{N-1}\int \mathrm{d}\gamma_{jn}\widetilde{G}^{\mathrm{SB}}_{j;n,n-1}\right)\widetilde{G}^{\mathrm{SB}}_{N,N-1}, \tag{4.43}$$

By means of the Dirac deltas in $\widetilde{G}^{\mathrm{SB}}_{j;n,n-1}$ we can integrate out the γ_{jn} variables to obtain

$$\begin{aligned}\widetilde{G}^{\mathrm{SB}}_{N,0} = &\prod_{j=1}^{F}\exp\sum_{n=1}^{N}\left(\frac{\mathrm{i}}{3}\breve{\tau}_{jn}\left[[\mathsf{M}_{jn}\gamma_{jn-1}+\mathsf{V}_{jn}]_{\beta}+\frac{\breve{\mathsf{q}}_{jn}}{\hbar}\right]^{3}\right)\\ &\times\exp\sum_{n=1}^{N}\left(-\mathrm{i}\theta_{jn}\left[[\mathsf{M}_{jn}\gamma_{jn-1}+\mathsf{V}_{jn}]_{\beta}+\frac{\breve{\mathsf{q}}_{jn}}{\hbar}\right]\breve{\mathsf{q}}_{jn}\right)\\ &\times\delta\left(\gamma_{jN}-\mathsf{M}_{jN}\gamma_{jN-1}-\mathsf{V}_{jN}\right).\end{aligned} \tag{4.44}$$

Additionally, from this set of integrations, we have collected the following inductive set of matrix equations

$$\begin{aligned}\gamma_{j1} &= \mathsf{M}_{j1}\gamma_{j0}+\mathsf{V}_{j1}\\ \gamma_{j2} &= \mathsf{M}_{j2}\gamma_{j1}+\mathsf{V}_{j2} = \mathsf{M}_{j2}\mathsf{M}_{j1}\gamma_{j0}+\mathsf{M}_{j2}\mathsf{V}_{j1}+\mathsf{V}_{j2}\\ &\vdots \qquad\quad \vdots \qquad\quad \vdots\\ \gamma_{jN} &= \mathsf{M}_{jN}\mathsf{M}_{jN-1}\cdots\mathsf{M}_{j1}\gamma_{j0}+\mathsf{M}_{jN}\mathsf{M}_{jN-1}\cdots\mathsf{M}_{j2}\mathsf{V}_{j1}+\cdots+\mathsf{M}_{jN}\mathsf{V}_{jN-1}+\mathsf{V}_{jN}.\end{aligned} \tag{4.45}$$

The process of taking the limit to the continuum requires that we specify how this matrix set behaves in that limit case. A careful manipulation of this matrix expression brings us to the expression

$$\begin{pmatrix}\alpha''_j\\ \beta''_j\end{pmatrix} = \begin{pmatrix}\cos\theta_j(t) & -\sin\theta_j(t)\\ \sin\theta_j(t) & \cos\theta_j(t)\end{pmatrix}\begin{pmatrix}\alpha'_j\\ \beta'_j\end{pmatrix} - \frac{1}{\hbar}\begin{pmatrix}\int_0^t \mathrm{d}s\Theta_j(s)\cos\left[\theta_j(t)-\theta_j(s)\right]\breve{\mathsf{q}}_j(s)\\ \int_0^t \mathrm{d}s\Theta_j(s)\sin\left[\theta_j(t)-\theta_j(s)\right]\breve{\mathsf{q}}_j(s)\end{pmatrix}. \tag{4.46}$$

Where $\alpha_j(t)=\alpha''_j$, $\alpha_j(0)=\alpha'_j$, $\beta_j(t)=\beta''_j$ and $\beta_j(0)=\beta'_j$. Thus, in a more compact notation, the above expression becomes $\gamma''_j = \mathsf{M}_j\gamma'_j+\mathsf{V}_j$.

Continuing with the implementation of the composition and limiting process over $\widetilde{G}^{\mathrm{SB}}_{N,0}$, we now take care of the phase in Eq. (4.44). From Eq. (4.23) we have

$$\breve{\tau}_{jn} = \frac{U^{(3)}(Q^{\mathrm{cl}}_{jn})\Delta t}{8\hbar^2}\left[m_j U^{(2)}(Q^{\mathrm{cl}}_{jn})\right]^{-\frac{3}{4}}. \tag{4.47}$$

Then, we define

$$\sigma_{jn} = \frac{\breve{\tau}_{jn}}{\Delta t} = \frac{U^{(3)}(Q^{\mathrm{cl}}_{jn})}{8\hbar^2}\left[m_j U^{(2)}(Q^{\mathrm{cl}}_{jn})\right]^{-\frac{3}{4}}, \tag{4.48}$$

which, by definition, is independent of Δt. However, σ_{jn} carries time dependence through the derivatives of the potential evaluated at the classical trajectory. Putting all together, we can write the limit of $\widetilde{G}^{\mathrm{SB}}_{N,0}$ as

$$\begin{aligned}\lim_{N\to\infty}\widetilde{G}^{\mathrm{SB}}_{N,0} = \prod_{j=1}^{F}&\exp\int_0^t \mathrm{d}s\left(\frac{\mathrm{i}}{3}\sigma_j(s)\left[\left[\mathsf{M}_j(s)\gamma_j'+\mathsf{V}_j(s)\right]_\beta+\frac{\breve{\tilde{\mathsf{q}}}_j(s)}{\hbar}\right]^3\right)\\ &\times\exp\int_0^t \mathrm{d}s\left(-\mathrm{i}\Theta_j(s)\left[\left[\mathsf{M}_j(s)\gamma_j'+\mathsf{V}_j(s)\right]_\beta+\frac{\breve{\tilde{\mathsf{q}}}_j(s)}{\hbar}\right]\breve{\mathsf{q}}_j(s)\right)\\ &\times\delta\left(\gamma_j''-\mathsf{M}_j(t)\gamma_j'-\mathsf{V}_j(t)\right).\end{aligned} \tag{4.49}$$

Considering now the central system part of the propagator, we have

$$\begin{aligned}G^{\mathrm{S}}_{N,0} &= \left(\prod_{n=1}^{N-1}\int\mathrm{d}\mathbf{r}_n\right)\prod_{n=1}^{N}G^{\mathrm{S}}_{n,n-1}\\ &=\left(\prod_{n=1}^{N-1}\int\mathrm{d}p_n\mathrm{d}q_n\right)\left(\prod_{n=1}^{N}\int\frac{\mathrm{d}\tilde{p}_n}{2\pi\hbar}\frac{\mathrm{d}\tilde{q}_n}{2\pi\hbar}\right)\exp\left(-\frac{\mathrm{i}}{\hbar}\sum_{n=1}^{N}\phi^{\mathrm{S}}_n\right).\end{aligned} \tag{4.50}$$

We already know that

$$\phi^{\mathrm{S}}_n = \left[\frac{\Delta p_n}{\Delta t}\tilde{q}_n-\left(\frac{\Delta q_n}{\Delta t}-\frac{\bar{p}_n}{m}\right)\tilde{p}_n+\Delta V_n'\right]\Delta t, \tag{4.51}$$

then

$$\lim_{N\to\infty}G^{\mathrm{S}}_{N,0}=\frac{1}{2\pi\hbar}\int\mathcal{D}\mathbf{r}\int\mathcal{D}\tilde{\mathbf{r}}\exp\left\{-\frac{\mathrm{i}}{\hbar}\int_0^t\mathrm{d}s\left[\dot{\mathbf{r}}\wedge\tilde{\mathbf{r}}+H_{\mathrm{S}}\left(\mathbf{r}+\frac{1}{2}\tilde{\mathbf{r}}\right)-H_{\mathrm{S}}\left(\mathbf{r}-\frac{1}{2}\tilde{\mathbf{r}}\right)\right]\right\}. \tag{4.52}$$

Finally, from Eq. (4.24), Eq. (4.49) and Eq. (4.52), we find that the whole propagator takes the form

$$\begin{aligned}\widetilde{G} =&\frac{1}{2\pi\hbar}\int\mathcal{D}\mathbf{r}\int\mathcal{D}\tilde{\mathbf{r}}\exp\left(-\frac{\mathrm{i}}{\hbar}\int_0^t\mathrm{d}s\left[\dot{\mathbf{r}}\wedge\tilde{\mathbf{r}}+H_{\mathrm{S}}\left(\mathbf{r}+\frac{1}{2}\tilde{\mathbf{r}}\right)-H_{\mathrm{S}}\left(\mathbf{r}-\frac{1}{2}\tilde{\mathbf{r}}\right)\right]\right)\\ &\times\prod_{j=1}^{F}\exp\int_0^t \mathrm{d}s\left(\frac{\mathrm{i}}{3}\sigma_j(s)\left[\left[\mathsf{M}_j(s)\gamma_j'+\mathsf{V}_j(s)\right]_\beta+\frac{\breve{\tilde{\mathsf{q}}}_j(s)}{\hbar}\right]^3\right)\\ &\times\exp\int_0^t \mathrm{d}s\left(-\mathrm{i}\Theta_j(s)\left[\left[\mathsf{M}_j(s)\gamma_j'+\mathsf{V}_j(s)\right]_\beta+\frac{\breve{\tilde{\mathsf{q}}}_j(s)}{\hbar}\right]\breve{\mathsf{q}}_j(s)\right)\\ &\times\delta\left(\gamma_j''-\mathsf{M}_j(t)\gamma_j'-\mathsf{V}_j(t)\right).\end{aligned} \tag{4.53}$$

In the first line of the this propagator we find the structure of the Wigner propagator for the central system as if there were no interaction with the reservoir. The second and third lines give the mathematical structure for the dynamics of the bath modes, how they evolve and the influence they exert on the central system by means of the couplings obtained from the integrand in the second line. It is, precisely, in this same line where we find the complete description of the non-linearity of the potential and its effect on the propagator. Specifically, through the dependence of the quantity σ_j defined by

$$\sigma_{jn}(s) = \frac{U^{(3)}(Q_{jn}^{\mathrm{cl}})}{8\hbar^2}\left[m_j U^{(2)}(Q_{jn}^{\mathrm{cl}})\right]^{-\frac{3}{4}}, \tag{4.54}$$

the fingerprints of terms beyond the harmonic case are observed. In case this term get removed from the propagator, the linearity of the propagator is recovered and we fall into the limit case studied in Appendix A for the propagator of the Ullersma-Caldeira-Leggett model.

Finally, the fourth line, by means of the Dirac delta, ensures that the bath modes evolve on trajectories defined by the stability matrix of each trajectory. Thus, once the potential is fixed, these trajectories are also fixed in phase-space by means of a symplectic inverse Fourier transform. As a limiting case, we find the classic trajectories for the bath modes once the non-linear structure of the potential disappears from the propagator.

4.3 Inverse Fourier transform

Starting from Eq. (4.53), we would like to write down the propagator once the inverse Fourier transform is applied to it. Let us consider initially the system-bath part of that propagator, which is, for obvious reasons, the part of it that we want to transform. Then

$$\begin{aligned}
\widetilde{G}_j^{\mathrm{SB}} = \exp&\left\{ \mathrm{i}\int_0^t \mathrm{d}s \left(\frac{\sigma_j(s)}{3}\left[\left[\mathsf{M}_j(s)\gamma_j' + \mathsf{V}_j(s)\right]_\beta + \frac{\breve{\breve{\mathsf{q}}}_j(s)}{\hbar} \right]^3 \right) \right\} \\
&\times \exp\left\{ \mathrm{i}\int_0^t \mathrm{d}s \left(-\Theta_j(s)\left[\left[\mathsf{M}_j(s)\gamma_j' + \mathsf{V}_j(s)\right]_\beta + \frac{\breve{\breve{\mathsf{q}}}_j(s)}{\hbar} \right] \breve{\mathsf{q}}_j(s) \right) \right\} \\
&\times \delta\left(\gamma_j'' - \mathsf{M}_j(t)\gamma_j' - \mathsf{V}_j(t)\right).
\end{aligned} \tag{4.55}$$

To apply the transformation, we have to manage explicitly the phase in Eq. (4.55). By means of a convenient set of definitions given in appendix G, we can write the above expression as

$$\begin{aligned}
\widetilde{G}_j^{\mathrm{SB}} &= \exp\left\{ \mathrm{i}\left[(\alpha_j')^3 a_{3j}(t) + (\beta_j')^3 a_{6j}(t) + (\alpha_j')^2(\beta_j') a_{4j}(t) + (\alpha_j')(\beta_j')^2 a_{5j}(t) \right] \right\} \\
&\times \exp\left\{ -\mathrm{i}\left[\alpha_j' a_{1j}(t) + \beta_j' a_{2j}(t) + I_1(t) - I_2(t) \right] \right\} \\
&\times \exp\left\{ \mathrm{i}\left[(\alpha_j')^2\left[a_{13j}(t) - a_{7j}(t)\right] + (\beta_j')^2\left[a_{14j}(t) - a_{8j}(t)\right] + \alpha_j'\beta_j'\left[a_{15j}(t) - a_{9j}(t)\right] \right] \right\} \\
&\times \exp\left\{ \mathrm{i}\left[\alpha_j'\left[a_{10j}(t) - a_{16j}(t) + a_{19j}(t)\right] + \beta_j'\left[a_{11j}(t) - a_{17j}(t) + a_{20j}(t)\right] \right] \right\} \\
&\times \exp\left\{ \mathrm{i}\left[-a_{12j}(t) + a_{18j}(t) - a_{21j}(t) + a_{22j}(t) \right] \right\} \\
&\times \delta\left(\gamma_j'' - \mathsf{M}_j(t)\gamma_j' - \mathsf{V}_j(t)\right).
\end{aligned} \tag{4.56}$$

By choosing the special case of $c_j = 0$, all but $a_{3j}(t), a_{4j}(t), a_{5j}(t), a_{6j}(t)$ becomes zero. Then,

$$\widetilde{G}_j^{\mathrm{SB}} = \exp\left\{ \mathrm{i}\left[(\alpha_j')^3 a_{3j}(t) + (\beta_j')^3 a_{6j}(t) + (\alpha_j')^2(\beta_j') a_{4j}(t) + (\alpha_j')(\beta_j')^2 a_{5j}(t) \right] \right\}, \tag{4.57}$$

which reproduces the unitary case in [38].

The propagator in Eq. (4.56) can be written in a more compact way as

$$\widetilde{G}_j^{\mathrm{SB}} = \exp\left[\mathrm{i}\Phi_j(t)\right]\exp\left[\mathrm{i}\tilde{\Gamma}_j(\alpha_j',\beta_j',t)\right]\delta\left(\gamma_j''-\mathsf{M}_j(t)\gamma_j'-\mathsf{V}_j(t)\right), \tag{4.58}$$

where

$$\Phi_j(t) = I_2(t) - I_1(t) - a_{12j}(t) + a_{18j}(t) - a_{21j}(t) + a_{22j}(t), \tag{4.59}$$

and

$$\begin{aligned}\tilde{\Gamma}_j(\alpha',\beta',t) =&(\alpha_j')^3 a_{3j}(t) + (\beta_j')^3 a_{6j}(t) + (\alpha_j')^2(\beta_j')a_{4j}(t) + (\alpha_j')(\beta_j')^2 a_{5j}(t) \\ &- \beta_j' a_{2j}(t) + (\alpha_j')^2\left[a_{13j}(t) - a_{7j}(t)\right] + (\beta_j')^2\left[a_{14j}(t) - a_{8j}(t)\right] \\ &- \alpha_j' a_{1j}(t) + \alpha_j'\beta_j'\left[a_{15j}(t) - a_{9j}(t)\right] \\ &+ \alpha_j'\left[a_{10j}(t) - a_{16j}(t) + a_{19j}(t)\right] + \beta_j'\left[a_{11j}(t) - a_{17j}(t) + a_{20j}(t)\right].\end{aligned} \tag{4.60}$$

The propagator in Eq. (4.58) represents the point where we would like to calculate the inverse Fourier transform because its structure is now suitable to proceed with the integrations. In this way,

$$\begin{aligned}G_j^{\mathrm{SB}} =& \frac{\exp\left[\mathrm{i}\Phi_j(t)\right]}{(2\pi)^2}\int \mathrm{d}\alpha_j''\mathrm{d}\alpha_j'\mathrm{d}\beta_j''\mathrm{d}\beta_j' \exp\left[-\mathrm{i}\left(\alpha_j''\check{Q}_j'' - \beta_j''\check{P}_j'' - \alpha_j'\check{Q}_j' + \beta_j'\check{P}_j'\right)\right] \\ &\times \exp\left[\mathrm{i}\tilde{\Gamma}_j(\alpha_j',\beta_j',t)\right]\delta\left(\alpha_j'' - \left[\mathsf{M}_j(t)\gamma_j' + \mathsf{V}_j(t)\right]_\alpha\right) \\ &\times \delta\left(\beta_j'' - \left[\mathsf{M}_j(t)\gamma_j' + \mathsf{V}_j(t)\right]_\beta\right).\end{aligned} \tag{4.61}$$

By integating out over the γ_j'' variables, we obtain

$$\begin{aligned}G_j^{\mathrm{SB}} =& \frac{1}{(2\pi)^2}\exp\left[\mathrm{i}\Phi_j(t)\right] \\ &\times \int \mathrm{d}\alpha_j'\mathrm{d}\beta_j' \exp\left(-\mathrm{i}\left[\check{Q}_j''\left[\mathsf{M}_j(t)\gamma_j' + \mathsf{V}_j(t)\right]_\alpha - \check{P}_j''\left[\mathsf{M}_j(t)\gamma_j' + \mathsf{V}_j(t)\right]_\beta\right]\right) \\ &\times \exp\left[\mathrm{i}\left(\alpha_j'\check{Q}_j' - \beta_j'\check{P}_j'\right)\right]\exp\left[\mathrm{i}\tilde{\Gamma}_j(\alpha_j',\beta_j',t)\right].\end{aligned} \tag{4.62}$$

After some manipulations, we can write this propagator as

$$\begin{aligned}G_j^{\mathrm{SB}} =& \frac{1}{(2\pi)^2}\exp\left(\mathrm{i}\Phi_j(t)\right)\int \mathrm{d}\alpha_j'\mathrm{d}\beta_j' \exp\left(\mathrm{i}\left[\mathsf{M}_j^{-1}(t)\check{\mathsf{R}}_j'' - \check{\mathsf{R}}_j'\right) \wedge \gamma_j'\right] \\ &\times \exp\left[\mathrm{i}\tilde{\Gamma}_j(\alpha_j',\beta_j',t)\right],\end{aligned} \tag{4.63}$$

with

$$\tilde{\Phi}_j(t) = I_2(t) - I_1(t) - a_{12j}(t) + a_{18j}(t) - a_{21j}(t) + a_{22j}(t) + \check{\mathsf{R}}_j'' \wedge \mathsf{V}_j(t). \tag{4.64}$$

The phase of the above double integral is

$$\begin{aligned}\Lambda_j(\alpha_j',\beta_j',t) =&\beta_j'\left(\left[\mathsf{M}_j^{-1}(t)\check{\mathsf{R}}_j''\right]_{\check{P}_j''} - \check{P}_j'\right) - \alpha_j'\left(\left[\mathsf{M}_j^{-1}(t)\check{\mathsf{R}}_j''\right]_{\check{Q}_j''} - \check{Q}_j'\right) + \tilde{\Gamma}_j(\alpha_j',\beta_j',t) \\ =&\beta_j'\mathbb{P}_j - \alpha_j'\mathbb{Q}_j + \tilde{\Gamma}_j(\alpha_j',\beta_j',t).\end{aligned} \tag{4.65}$$

Therefore,

$$\begin{aligned}\Lambda_j(\alpha'_j,\beta'_j,t) =& (\alpha'_j)^3 a_{3j}(t) + (\beta'_j)^3 a_{6j}(t) + (\alpha'_j)^2(\beta'_j) a_{4j}(t) + (\alpha'_j)(\beta'_j)^2 a_{5j}(t) \\ &+ (\alpha'_j)^2\left[a_{13j}(t) - a_{7j}(t)\right] + (\beta'_j)^2\left[a_{14j}(t) - a_{8j}(t)\right] \\ &+ \alpha'_j\beta'_j\left[a_{15j}(t) - a_{9j}(t)\right] + \alpha'_j\left[-\mathbb{Q}_j - a_{1j}(t) + a_{10j}(t) - a_{16j}(t) + a_{19j}(t)\right] \\ &+ \beta'_j\left[\mathbb{P}_j - a_{2j}(t) + a_{11j}(t) - a_{17j}(t) + a_{20j}(t)\right].\end{aligned} \tag{4.66}$$

We can simplify even more the notation by means of the second set of auxiliary equations found in appendix G. Thus,

$$\begin{aligned}\Lambda_j(\alpha'_j,\beta'_j,t) =& (\alpha'_j)^3 A_j(t) + (\beta'_j)^3 B_j(t) + (\alpha'_j)^2(\beta'_j) C_j(t) + (\alpha'_j)(\beta'_j)^2 D_j(t) \\ &+ (\alpha'_j)^2 E_j(t) + (\beta'_j)^2 F_j(t) + \alpha'_j\beta'_j G_j(t) + \alpha'_j H_j(t) + \beta'_j J_j(t).\end{aligned} \tag{4.67}$$

and the SB part of the propagator becomes

$$G_j^{\mathrm{SB}} = \frac{1}{(2\pi)^2}\exp\left[\mathrm{i}\tilde{\Phi}_j(t)\right]\int \mathrm{d}\alpha'_j \mathrm{d}\beta'_j \exp\left[\mathrm{i}\Lambda_j(\alpha'_j,\beta'_j,t)\right]. \tag{4.68}$$

Finally, putting this into Eq. (4.53) leave us with the final expression of Wigner propagator

$$\begin{aligned}G =& \frac{1}{2\pi\hbar}\int \mathcal{D}\mathbf{r}\int \mathcal{D}\tilde{\mathbf{r}} \exp\left(-\frac{\mathrm{i}}{\hbar}\int_0^t ds\left[\dot{\mathbf{r}}\wedge\tilde{\mathbf{r}} + H_{\mathrm{S}}\left(\mathbf{r}+\frac{1}{2}\tilde{\mathbf{r}}\right) - H_{\mathrm{S}}\left(\mathbf{r}-\frac{1}{2}\tilde{\mathbf{r}}\right)\right]\right) \\ &\times\prod_{j=1}^{F}\frac{1}{(2\pi)^2}\exp\left[\mathrm{i}\tilde{\Phi}_j(t)\right]\int d\alpha'_j d\beta'_j \exp\left[\mathrm{i}\Lambda_j(\alpha'_j,\beta'_j,t)\right].\end{aligned} \tag{4.69}$$

At this point, there is no clue that serve as a guide to know if there is an specific way to transform the multivariate polynomial $\Lambda_j(\alpha'_j,\beta'_j,t)$ into a suitable expression that can generate, after integration, the Airy functions in phase-space. This situation is in clear contrast with the unitary case studied in Sec. 2.4, where by means of suitable linear transformations, it was possible to recover the Airy structure for the propagator in phase-space. Nonetheless, this issue can be clearly understood if we consider the non-linear structure of the calculation we have been working on. As is already known, the only kind of path integrals suitable to be calculated analytically are those with a quadratic dependence on its variables, i.e., gaussian integrals. Beyond that, approximative schemes has to be devised in order to calculate the path integral. Among them, we can find the centroid theory [56] and the functional expansion of the action up to quadratic order [45]. Nonetheless, despite this situation, all the physics and the calculations based on them can be developed, as far as we know, from the mixed representation of the open system propagator.

Conclusions

In the present work we have developed an study of the Wigner propagator in phase-space for an open quantum system under the semiclassical framework. This study was divided in two main stages: on one hand, the construction of the propagator for a central system evolving unitarily, and on the other hand, the study of the central system undergoing a non-linear interaction with a bath reservoir at equilibrium temperature T. The former case, although simpler and non-realistic, allowed us to get a physical insight into the structure of a propagator formulated by means of path integrals while working in the semiclassical realm. The later case allowed us to model a more realistic physical system by including dissipation of energy and decoherence phenomena.

The propagator obtained within the open system framework generalizes naturally the propagator obtained under Ullersma-Caldeira-Leggett model. Specifically, our calculation implies a non-trivial quantum dynamics for the bath modes in phase-space, in clear contrast with the bilinear coupling model where the dynamics of the bath modes is indistinguishable from its classical evolution. Thus, our theory represents an approach to the true quantum behavior of the reservoir while retaining the non-local character of the dynamics due to the structure of the interaction potential. In this regard, we have also constructed a general semiclassical theory for the dynamics of dissipative systems far from equilibrium with factorizing-initial conditions, which opens the possibility for a formal and consistent study of the semiclassical spectral statistics of dissipative systems [57, 58], the study of reaction-rate theory far from equilibrium and the description of decoherent effects in terms of classical manifolds. Moreover, it could give some insights about the evolution of entanglement in semiclassical terms [59].

Regarding the open questions and problems, we should mention that there is no clue that serve as a guide to know if there is an specific way to transform the multivariate polynomial $\Lambda_j(\alpha'_j, \beta'_j, t)$ in Ec. (4.67) into a suitable expression that can generate, after integration, the Airy functions in phase-space. This situation is in clear contrast with the unitary case studied in Sec. 2.4, where by means of suitable linear transformations, it was possible to recover the Airy structure for the propagator in such a way that the interference pattern was originated from the product of Airy functions as in in Ec. (2.56). Nonetheless, it worthy to mention that in spite of this aspect of the propagator, all the physics, and the calculations based on them can start from the mixed representation of the open system propagator given in Ec. (4.69). Finally, although our description of open quantum systems is general enough, the inclusion of non-factorizing-initial conditions and more general couplings to the bath [44, 60] could be tasks to do.

Appendices

Appendix A

Wigner propagator for the Ullersma-Caldeira-Leggett model

Starting from the Wigner propagator found in Eq. (4.53)

$$\widetilde{G} = \frac{1}{2\pi\hbar}\int_{\mathbf{r}'}^{\mathbf{r}''}\mathcal{D}\mathbf{r}\int\mathcal{D}\tilde{\mathbf{r}}\exp\left(-\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}s\left[\dot{\mathbf{r}}\wedge\tilde{\mathbf{r}} + H_{\mathrm{S}}\left(\mathbf{r}+\frac{1}{2}\tilde{\mathbf{r}}\right) - H_{\mathrm{S}}\left(\mathbf{r}-\frac{1}{2}\tilde{\mathbf{r}}\right)\right]\right) \tag{A.1}$$
$$\times\prod_{j=1}^{F}\exp\int_0^t \mathrm{d}s\left(\frac{\mathrm{i}}{3}\sigma_j(s)\left[\left[\mathsf{M}_j(s)\gamma_j' + \mathsf{V}_j(s)\right]_\beta + \frac{\breve{\tilde{\mathsf{q}}}_j(s)}{\hbar}\right]^3\right)$$
$$\times\exp\int_0^t \mathrm{d}s\left(-\mathrm{i}\Theta_j(s)\left[\left[\mathsf{M}_j(s)\gamma_j' + \mathsf{V}_j(s)\right]_\beta + \frac{\breve{\tilde{\mathsf{q}}}_j(s)}{\hbar}\right]\breve{\mathsf{q}}_j(s)\right)$$
$$\times\,\delta\left(\gamma_j'' - \mathsf{M}_j(t)\gamma_j' - \mathsf{V}_j(t)\right),$$

we can study a couple of interesting limits. Specifically, we would like to test it in two well known scenarios. The first one corresponds to simple case of decoupling among the central system and the set of bath modes. The second one is much more interesting than the former. Here, we will consider the open system subject to bilinear interactions with the bath modes. As is widely known, in these two special cases, the bath dynamics in phase-space is completely determined by Dirac deltas along the classical trajectory [9]. This, in turn, means that there is no sign for true quantum phenomena as far as the linearity gives a dynamical behavior indistinguishable from the classic case.

A.1 Decoupling case with harmonic bath potential

To see if this propagator corresponds to the case of one isolated degree of freedom of the bath times the propagator of the central DOF, we consider the decoupling case $c_j = 0$. Then,

$$\widetilde{G} = \frac{1}{2\pi\hbar}\int_{\mathbf{r}'}^{\mathbf{r}''}\mathcal{D}\mathbf{r}\int\mathcal{D}\tilde{\mathbf{r}}\exp\left(-\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}s\left[\dot{\mathbf{r}}\wedge\tilde{\mathbf{r}} + H_{\mathrm{S}}\left(\mathbf{r}+\frac{1}{2}\tilde{\mathbf{r}}\right) - H_{\mathrm{S}}\left(\mathbf{r}-\frac{1}{2}\tilde{\mathbf{r}}\right)\right]\right) \tag{A.2}$$
$$\times\prod_{j=1}^{F}\exp\left\{\frac{\mathrm{i}}{3}\int_0^t \mathrm{d}s\sigma_j(s)\left(\left[\mathsf{M}_j(s)\gamma_j'\right]_\beta\right)^3\right\}\delta\left(\gamma_j'' - \mathsf{M}_j(t)\gamma_j'\right).$$

As expected, as long as there is no coupling constant, the central system and the bath becomes independent. The dynamics of the central system evolve unitarily and is described completely by the first line in the above propagator. Once c_j has beee set to zero, the bath modes do not carry any dependence of the fluctuation in the coordinate $\breve{q}(s)$. Therefore, the bath dynamics is just the product of F non-interacting bath modes whose dynamics is governed by the second and third line of the propagator above. Thus, the dynamics of the j-th bath mode is described by

$$\widetilde{G}_j(\gamma_j'', \gamma_j', t) = \exp\left\{ \frac{\mathrm{i}}{3} \int_0^t \mathrm{d}s \sigma_j(s) \left(\left[\mathsf{M}_j(s)\gamma_j' \right]_\beta \right)^3 \right\} \delta\left(\gamma_j'' - \mathsf{M}_j(t)\gamma_j' \right). \tag{A.3}$$

Going one step forward, we can see from this expression that if the bath potential, which now is decoupled from the system degree of freedom, becomes linear, i.e., quadratic at most, $\sigma_j(s) = 0$ and its dynamics will be given by

$$\widetilde{G}_j(\gamma_j'', \gamma_j', t) = \delta\left(\alpha_j'' - \alpha_j' \cos(\omega_j t) + \beta_j' \sin(\omega_j t) \right) \delta\left(\beta_j'' - \alpha_j' \sin(\omega_j t) - \beta_j' \cos(\omega_j t) \right). \tag{A.4}$$

Under the inverse symplectic Fourier transform we obtain

$$G_j(\breve{\mathbf{R}}_j'', \breve{\mathbf{R}}_j', t) = \delta\left(\breve{Q}_j'' - \breve{Q}_j' \cos(\omega_j t) - \breve{P}_j' \sin(\omega_j t) \right) \delta\left(\breve{P}_j'' - \breve{P}_j' \cos(\omega_j t) + \breve{Q}_j' \sin(\omega_j t) \right). \tag{A.5}$$

Finally, by means of the Eq. (4.22), the bath propagator takes the form

$$\begin{aligned} G_{\mathrm{B}}(\mathbf{R}_j'', \mathbf{R}_j', t) = \prod_{j=1}^{F} & \delta\left(Q_j'' - Q_j' \cos(\omega_j t) - \frac{P_j'}{m_j \omega_j} \sin(\omega_j t) \right) \\ & \times \delta\left(P_j'' - P_j' \cos(\omega_j t) + m_j \omega_j Q_j' \sin(\omega_j t) \right). \end{aligned} \tag{A.6}$$

A.2 Linear bath potential

In this case, $c_j \neq 0$ and $B_j = 0$; therefore, $\sigma_j(s) = 0$. Then, the propagator in Eq. (4.53) takes the form

$$\begin{aligned} \widetilde{G} = & \frac{1}{2\pi\hbar} \int_{\mathbf{r}'}^{\mathbf{r}''} \mathcal{D}\mathbf{r} \int \mathcal{D}\tilde{\mathbf{r}} \exp\left(-\frac{\mathrm{i}}{\hbar} \int_0^t \mathrm{d}s \left[\dot{\mathbf{r}} \wedge \tilde{\mathbf{r}} + H_{\mathrm{S}}\left(\mathbf{r} + \frac{1}{2}\tilde{\mathbf{r}} \right) - H_{\mathrm{S}}\left(\mathbf{r} - \frac{1}{2}\tilde{\mathbf{r}} \right) \right] \right) \\ & \times \prod_{j=1}^{F} \exp\left\{ -\mathrm{i} \int_0^t \mathrm{d}s \Theta_j(s) \left[\left[\mathsf{M}_j(s)\gamma_j' + \mathsf{V}_j(s) \right]_\beta + \frac{\breve{\mathsf{q}}_j(s)}{\hbar} \right] \breve{\mathsf{q}}_j(s) \right\} \\ & \times \delta\left(\gamma_j'' - \mathsf{M}_j(t)\gamma_j' - \mathsf{V}_j(t) \right). \end{aligned} \tag{A.7}$$

As we did before, let us focus our attention on the j-th term of the SB part of the propagator

$$\begin{aligned} \widetilde{G}_j = & \exp\left\{ -\mathrm{i} \int_0^t \mathrm{d}s \Theta_j(s) \left[\left[\mathsf{M}_j(s)\gamma_j' + \mathsf{V}_j(s) \right]_\beta + \frac{\breve{\mathsf{q}}_j(s)}{\hbar} \right] \breve{\mathsf{q}}_j(s) \right\} \\ & \times \delta\left(\gamma_j'' - \mathsf{M}_j(t)\gamma_j' - \mathsf{V}_j(s) \right). \end{aligned} \tag{A.8}$$

The linearization of the interaction potential implies that

$$U = \sum_{j=1}^{F} \left(\frac{1}{2} m_j \omega_j^2 Q_j^2 - c_j q Q_j + q^2 \frac{c_j^2}{2 m_j \omega_j^2} \right), \tag{A.9}$$

whereas

$$\theta_j(t) = \omega_j t. \tag{A.10}$$

Hence, by applying the the inverse symplectic Fourier transform to Eq. (A.8) we find that

$$\begin{aligned} G_j = &\exp\left\{ \frac{\mathrm{i}}{\hbar} \left(\omega_j^2 \int_0^t \mathrm{d}s \int_0^s \mathrm{d}u \sin\left[\omega_j (s-u)\right] \check{\mathfrak{q}}_j(u) \check{\mathfrak{q}}_j(s) - \omega_j \int_0^t \mathrm{d}s \check{\mathfrak{q}}_j(s) \check{\mathfrak{q}}_j(s) \right) \right\} \\ &\times \exp\left\{ \frac{\mathrm{i}}{\hbar} \left(\omega_j \check{Q}_j' \int_0^t \mathrm{d}s \cos(\omega_j s) \check{\mathfrak{q}}_j(s) + \omega_j \check{P}_j' \int_0^t \mathrm{d}s \sin(\omega_j s) \check{\mathfrak{q}}_j(s) \right) \right\} \\ &\times \delta\left(\check{Q}_j'' - \check{Q}_j' \cos(\omega_j t) - \check{P}_j' \sin(\omega_j t) - \omega_j \int_0^t \mathrm{d}s \sin[\omega_j (t-s)] \check{\mathfrak{q}}_j(s) \right) \\ &\times \delta\left(\check{P}_j'' - \check{P}_j' \cos(\omega_j t) + \check{Q}_j' \sin(\omega_j t) - \omega_j \int_0^t \mathrm{d}s \cos[\omega_j (t-s)] \check{\mathfrak{q}}_j(s) \right). \end{aligned} \tag{A.11}$$

Thus, putting together this result with the system part of the propagator, and by means of Eq. (4.22), we obtain the final form of the Wigner propagator as

$$\begin{aligned} G(\mathbf{r}'', \{\mathbf{R}_j''\}, t; \mathbf{r}', \{\mathbf{R}_j'\}, 0) = &\frac{1}{2\pi\hbar} \int_{\mathbf{r}'}^{\mathbf{r}''} \mathcal{D}\mathbf{r} \int \mathcal{D}\tilde{\mathbf{r}} \exp\left(-\frac{\mathrm{i}}{\hbar} S_{\mathrm{S}}[\mathbf{r}, \tilde{\mathbf{r}}, t] \right) \\ &\times \prod_{j=1}^{F} \delta\left(Q_j'' - Q_j^{\mathrm{cl}}(P_j', Q_j', t) \right) \delta\left(P_j'' - P_j^{\mathrm{cl}}(P_j', Q_j', t) \right) \\ &\times \exp\left\{ \frac{\mathrm{i}}{\hbar} \left(c_j \int_0^t \mathrm{d}s Q_j^{\mathrm{cl}}(P_j', Q_j', s) \tilde{q}(s) - \frac{c_j^2}{m_j \omega_j^2} \int_0^t \mathrm{d}s \tilde{q}(s) q(s) \right) \right\}. \end{aligned} \tag{A.12}$$

This result reproduces the propagator written in Ec. (3.13). It has the special feature of being written in terms of the classical trajectory of the bath modes in phase-space.

Appendix B

Properties of the $\hat{T}(\mathbf{u},\mathbf{v})$ and $\hat{d}(\mathbf{p},\mathbf{q})$ operators

B.1 Definitions

Let $\mathbf{u} = (u_1, u_2, \ldots, u_f)$ be a collection of real coordinates and $\mathbf{v} = (v_1, v_2, \ldots, v_f)$ a set of real momentum variables. Let $\hat{\mathbf{q}} = (\hat{q}_1, \hat{q}_2, \ldots, \hat{q}_f)$ and $\hat{\mathbf{p}} = (\hat{p}_1, \hat{p}_2, \ldots, \hat{p}_f)$ be the position and momentum operators. The displacement operator (DO) is defined by

$$\hat{T}(\mathbf{u},\mathbf{v}) = \exp\left[\frac{\mathrm{i}}{\hbar}(\mathbf{u}\cdot\hat{\mathbf{p}} + \mathbf{v}\cdot\hat{\mathbf{q}})\right]. \tag{B.1}$$

By taking the double Fourier transform of $\hat{T}(-\mathbf{u},-\mathbf{v})$, we can define

$$\hat{d}(\hat{\mathbf{p}},\hat{\mathbf{q}}) = \frac{1}{(2\pi\hbar)^f}\int \mathrm{d}\mathbf{u}\mathrm{d}\mathbf{v}\exp\left[\frac{\mathrm{i}}{\hbar}(\mathbf{u}\cdot\mathbf{p} + \mathbf{v}\cdot\mathbf{q})\right]\hat{T}(-\mathbf{u},-\mathbf{v}) \tag{B.2}$$

with $\mathbf{r},\mathbf{s}$ symbolizing momenta and coordinate variables respectively. To see a more complete discussion about the construction and interpretation given to these operators, see Ref. [11,61].

B.2 Properties

1. **The composition rule for two DO is given by**

$$\hat{T}(\mathbf{u},\mathbf{v})\hat{T}(\mathbf{u}',\mathbf{v}') = \exp\left[\frac{\mathrm{i}}{2\hbar}(\mathbf{u}\cdot\mathbf{v}' - \mathbf{u}'\cdot\mathbf{v})\right]\hat{T}(\mathbf{u}+\mathbf{u}',\mathbf{v}+\mathbf{v}'). \tag{B.3}$$

Proof. Let's consider the composition of two DO operators

$$\hat{T}(\mathbf{u},\mathbf{v})\hat{T}(\mathbf{u}',\mathbf{v}') = \exp\left[\frac{\mathrm{i}}{\hbar}(\mathbf{u}\cdot\hat{\mathbf{p}} + \mathbf{v}\cdot\hat{\mathbf{q}})\right]\exp\left[\frac{\mathrm{i}}{\hbar}(\mathbf{u}'\cdot\hat{\mathbf{p}} + \mathbf{v}'\cdot\hat{\mathbf{q}}]\right]$$

Seting $\hat{A} = \frac{\mathrm{i}}{\hbar}(\mathbf{u}\cdot\hat{\mathbf{p}} + \mathbf{v}\cdot\hat{\mathbf{q}})$, and $\hat{B} = \frac{\mathrm{i}}{\hbar}(\mathbf{u}'\cdot\hat{\mathbf{p}} + \mathbf{v}'\cdot\hat{\mathbf{q}})$, we obtain

$$[\hat{A},\hat{B}] = \frac{\mathrm{i}}{\hbar}(\mathbf{u}\cdot\mathbf{v}' - \mathbf{u}'\cdot\mathbf{v})\hat{1}, \qquad [\hat{A},[\hat{A},\hat{B}]] = [\hat{B},[\hat{A},\hat{B}]] = \hat{0}.$$

By means of the Glauber's formula

$$\exp(\hat{A})\exp(\hat{B}) = \exp(\hat{A}+\hat{B})\exp\left(\frac{1}{2}[\hat{A},\hat{B}]\right),$$

we obtain

$$\hat{T}(\mathbf{u},\mathbf{v})\hat{T}(\mathbf{u}',\mathbf{v}') = \exp\left(\frac{\mathrm{i}}{2\hbar}(\mathbf{u}\cdot\mathbf{v}' - \mathbf{u}'\cdot\mathbf{v})\right)\hat{T}(\mathbf{u}+\mathbf{u}',\mathbf{v}+\mathbf{v}').$$

2. **The inverse DO is given by**

$$\hat{T}^{-1}(\mathbf{u},\mathbf{v}) = \hat{T}(-\mathbf{u},-\mathbf{v}). \tag{B.4}$$

Proof. From property 1, we have

$$\begin{aligned}\hat{T}(\mathbf{u},\mathbf{v})\hat{T}(-\mathbf{u},-\mathbf{v}) =& \exp\left(\frac{\mathrm{i}}{2\hbar}(\mathbf{u}\cdot\mathbf{v} - \mathbf{u}\cdot\mathbf{v})\right)\hat{T}(\mathbf{u}-\mathbf{u},\mathbf{v}-\mathbf{v})\\ =&\hat{T}(\mathbf{0},\mathbf{0}) = \hat{1}.\end{aligned}$$

3. **The DO is unitary:**

$$\hat{T}^{\dagger}(\mathbf{u},\mathbf{v}) = \hat{T}^{-1}(\mathbf{u},\mathbf{v}). \tag{B.5}$$

Proof. Taking the Hermitian conjugate of the D.O.

$$\begin{aligned}\hat{T}^{\dagger}(\mathbf{u},\mathbf{v}) &= \exp\left(-\frac{\mathrm{i}}{\hbar}(\mathbf{u}\cdot\hat{\mathbf{p}} + \mathbf{v}\cdot\hat{\mathbf{q}})\right)\\ &= \hat{T}(-\mathbf{u},-\mathbf{v})\\ &= \hat{T}^{-1}(\mathbf{u},\mathbf{v}).\end{aligned}$$

4. **Trace of the DO**

$$\mathrm{Tr}\left[\hat{T}(\mathbf{u},\mathbf{v})\right] = (2\pi\hbar)^f\delta(\mathbf{u})\delta(\mathbf{v}) \tag{B.6}$$

Proof. By using Glauber's formula,

$$\mathrm{Tr}\left[\hat{T}(\mathbf{u},\mathbf{v})\right] = \int \mathrm{d}\mathbf{p}\mathrm{d}\mathbf{q}\mathrm{d}\mathbf{q}' e^{\frac{\mathrm{i}}{\hbar}\left(\mathbf{u}\cdot\mathbf{p}+\mathbf{v}\cdot\mathbf{q}+\frac{1}{2}\mathbf{u}\cdot\mathbf{v}\right)}\langle\mathbf{q}'|\mathbf{p}\rangle\langle\mathbf{p}|\mathbf{q}\rangle\langle\mathbf{q}|\mathbf{q}'\rangle.$$

Knowing that

$$\langle\mathbf{q}'|\mathbf{p}\rangle = (2\pi\hbar)^{-\frac{f}{2}}\exp\left(\frac{\mathrm{i}}{\hbar}\mathbf{q}'\cdot\mathbf{p}\right), \quad \langle\mathbf{q}|\mathbf{q}'\rangle = \delta(\mathbf{q}'-\mathbf{q}),$$

we obtain

$$\begin{aligned}\mathrm{Tr}\left[\hat{T}(\mathbf{u},\mathbf{v})\right] =& \frac{1}{(2\pi\hbar)^f}\int \mathrm{d}\mathbf{p}\mathrm{d}\mathbf{q} e^{\frac{\mathrm{i}}{\hbar}\left(\mathbf{u}\cdot\mathbf{p}+\mathbf{v}\cdot\mathbf{q}+\frac{1}{2}\mathbf{u}\cdot\mathbf{v}\right)},\\ =&(2\pi\hbar)^f\ \delta(\mathbf{u})\delta(\mathbf{v}).\end{aligned}$$

5. $\hat{d}(\hat{\mathbf{p}},\hat{\mathbf{q}})$ **is Hermitian**

$$\hat{d}^{\dagger}(\hat{\mathbf{p}},\hat{\mathbf{q}}) = \hat{d}(\hat{\mathbf{p}},\hat{\mathbf{q}}). \tag{B.7}$$

Proof. Since $\hat{T}^{\dagger}(-\mathbf{u},-\mathbf{v}) = \hat{T}^{-1}(-\mathbf{u},-\mathbf{v}) = \hat{T}(\mathbf{u},\mathbf{v})$, we have

$$\begin{aligned}
\hat{d}^{\dagger}(\hat{\mathbf{p}},\hat{\mathbf{q}}) =& \frac{1}{(2\pi\hbar)^f}\int \mathrm{d}\mathbf{u}\mathrm{d}\mathbf{v} \exp\left[-\frac{\mathrm{i}}{\hbar}(\mathbf{u}\cdot\mathbf{p}+\mathbf{v}\cdot\mathbf{q})\right]\hat{T}(\mathbf{u},\mathbf{v}) \\
=& \frac{1}{(2\pi\hbar)^f}\int \mathrm{d}\mathbf{u}'\mathrm{d}\mathbf{v}' \exp\left[\frac{\mathrm{i}}{\hbar}(\mathbf{u}'\cdot\mathbf{p}+\mathbf{v}'\cdot\mathbf{q})\right]\hat{T}(-\mathbf{u}',-\mathbf{v}') \\
=& \hat{d}(\hat{\mathbf{p}},\hat{\mathbf{q}}).
\end{aligned}$$

6. **Normalization in phase space:**

$$\frac{1}{(2\pi\hbar)^f}\int \mathrm{d}\mathbf{p}\mathrm{d}\mathbf{q}\hat{d}(\hat{\mathbf{p}},\hat{\mathbf{q}}) = \hat{1} \tag{B.8}$$

Proof. By calculating the integral over the whole phase space, we obtain

$$\begin{aligned}
\frac{1}{(2\pi\hbar)^f}\int \mathrm{d}\mathbf{p}\mathrm{d}\mathbf{q}\hat{d}(\hat{\mathbf{p}},\hat{\mathbf{q}}) =& \frac{1}{(2\pi\hbar)^{2f}}\int \mathrm{d}\mathbf{u}\mathrm{d}\mathbf{v} e^{-\frac{\mathrm{i}}{\hbar}(\mathbf{u}\cdot\hat{\mathbf{p}}+\mathbf{v}\cdot\hat{\mathbf{q}})}\left[\int \mathrm{d}\mathbf{p} e^{\frac{\mathrm{i}}{\hbar}\mathbf{u}\cdot\mathbf{p}}\right]\left[\int \mathrm{d}\mathbf{q} e^{\frac{\mathrm{i}}{\hbar}\mathbf{v}\cdot\mathbf{q}}\right] \\
=& \int \mathrm{d}\mathbf{u}\mathrm{d}\mathbf{v} \exp\left(-\frac{\mathrm{i}}{\hbar}(\mathbf{u}\cdot\hat{\mathbf{p}}+\mathbf{v}\cdot\hat{\mathbf{q}})\right)\delta(\mathbf{u})\delta(\mathbf{v}) \\
=& \hat{1}.
\end{aligned}$$

7. **Trace of** $\hat{d}(\hat{\mathbf{p}},\hat{\mathbf{q}})$

$$\mathrm{Tr}[\hat{d}(\hat{\mathbf{p}},\hat{\mathbf{q}})] = 1. \tag{B.9}$$

Proof. By using property 4,

$$\begin{aligned}
\mathrm{Tr}[\hat{d}(\hat{\mathbf{p}},\hat{\mathbf{q}})] =& \frac{1}{(2\pi\hbar)^f}\int \mathrm{d}\mathbf{u}\mathrm{d}\mathbf{v} \exp\left[\frac{\mathrm{i}}{\hbar}(\mathbf{u}\cdot\mathbf{p}+\mathbf{v}\cdot\mathbf{q})\right]\mathrm{Tr}[\hat{T}(-\mathbf{u},-\mathbf{v})] \\
=& \int \exp\left[\frac{\mathrm{i}}{\hbar}(\mathbf{u}\cdot\mathbf{p}+\mathbf{v}\cdot\mathbf{q})\right]\delta(\mathbf{u})\delta(\mathbf{v}) \\
=& 1.
\end{aligned}$$

8. **Composition of** $\hat{d}(\hat{\mathbf{r}})\hat{d}(\hat{\mathbf{r}}')$.

$$\hat{d}(\hat{\mathbf{r}})\hat{d}(\hat{\mathbf{r}}') = \frac{2}{\pi\hbar}\int \mathrm{d}\mathbf{r}''\hat{d}(\hat{\mathbf{r}}')\exp\left[\frac{\mathrm{i}}{\hbar}\Delta_3(\mathbf{r}'',\mathbf{r}',\mathbf{r})\right]. \tag{B.10}$$

Proof. From definition (B.2),

$$\begin{aligned}
\hat{d}(\hat{\mathbf{r}})\hat{d}(\hat{\mathbf{r}}') =& \frac{1}{(2\pi\hbar)^{2f}}\int e^{\frac{\mathrm{i}}{\hbar}[\mathbf{u}\cdot\mathbf{p}+\mathbf{u}'\cdot\mathbf{p}'+\mathbf{v}\cdot\mathbf{q}+\mathbf{v}'\cdot\mathbf{q}']} e^{\frac{\mathrm{i}}{2\hbar}(\mathbf{u}\cdot\mathbf{v}'-\mathbf{u}'\cdot\mathbf{v})\hat{1}} \\
&\times \hat{T}(-\mathbf{u}-\mathbf{u}',-\mathbf{v}-\mathbf{v}')\, d\mathbf{u}d\mathbf{u}'d\mathbf{v}d\mathbf{v}'
\end{aligned}$$

The scalar phase above can be written as

$$\mathbf{u}\cdot\mathbf{p}+\mathbf{v}\cdot\mathbf{q}+\mathbf{u}'\cdot\mathbf{p}''+\mathbf{v}'\cdot\mathbf{q}'',$$

where we have introduced the change of variables $\mathbf{p}'' = (\mathbf{p}' - \mathbf{v}/2)$, $\mathbf{q}'' = (\mathbf{q}' + \mathbf{u}/2)$ with measures related by $d\mathbf{u}d\mathbf{v} = d\mathbf{p}''d\mathbf{q}''$. By means of this expressions, the phase can be written as

$$2(\mathbf{q}'' - \mathbf{q}') \cdot \mathbf{p} - 2(\mathbf{p}'' - \mathbf{p}') \cdot \mathbf{q} + \mathbf{u}' \cdot \mathbf{p}'' + \mathbf{v}' \cdot \mathbf{q}''.$$

By introducing the second change of variables $\mathbf{u}'' - \mathbf{u}' = 2(\mathbf{q}'' - \mathbf{q}')$, and $(\mathbf{v}'' - \mathbf{v}') = 2(\mathbf{p}' - \mathbf{p}'')$, we obtain the new form of the phase as

$$\mathbf{u}'' \cdot \mathbf{p}'' + \mathbf{v}'' \cdot \mathbf{q}'' + 2[(\mathbf{p}'' \cdot \mathbf{q}' - \mathbf{q}'' \cdot \mathbf{p}') + (\mathbf{p}' \cdot \mathbf{q} - \mathbf{q}' \cdot \mathbf{p}) + (\mathbf{p} \cdot \mathbf{q}'' - \mathbf{q} \cdot \mathbf{p}'')],$$

which, by means of the symplectic product, can be written as

$$\mathbf{u}'' \cdot \mathbf{p}'' + \mathbf{v}'' \cdot \mathbf{q}'' + 2[\mathbf{r}'' \wedge \mathbf{r}' + \mathbf{r}' \wedge \mathbf{r} + \mathbf{r} \wedge \mathbf{r}''] = \mathbf{u}'' \cdot \mathbf{p}'' + \mathbf{v}'' \cdot \mathbf{q}'' + \Delta_3(\mathbf{r}'', \mathbf{r}', \mathbf{r}) \tag{B.11}$$

where we have defined the quantity $\Delta_3(\mathbf{r}'', \mathbf{r}', \mathbf{r})$ as a sum of the cyclic symplectic product of its arguments. Thus,

$$\begin{aligned}\hat{d}(\hat{\mathbf{r}})\hat{d}(\hat{\mathbf{r}}') =& \frac{2}{\pi\hbar} \int \exp\left[\frac{\mathrm{i}}{\hbar}\Delta_3(\mathbf{r}'', \mathbf{r}', \mathbf{r})\right] \\ &\times \frac{1}{(2\pi\hbar)^f} \exp\left[\frac{\mathrm{i}}{\hbar}(\mathbf{u}'' \cdot \mathbf{p}'' + \mathbf{v}'' \cdot \mathbf{q}'')\right] \hat{T}(-\mathbf{u}'', -\mathbf{v}'')\ d\mathbf{u}''d\mathbf{v}''d\mathbf{p}''d\mathbf{q}''\end{aligned}$$

and using the definition of the $\hat{d}$ operator, we can write the final form for the composition

$$\hat{d}(\hat{\mathbf{r}})\hat{d}(\hat{\mathbf{r}}') = \frac{2}{\pi\hbar} \int \hat{d}(\hat{\mathbf{r}}'') \exp\left[\frac{\mathrm{i}}{\hbar}\Delta_3(\mathbf{r}'', \mathbf{r}', \mathbf{r})\right] d\mathbf{r}''.$$

9. **Weyl symbol for the product of two operators**

$$A(\mathbf{r}) = \frac{1}{(\pi\hbar)^2} \int \mathrm{d}\mathbf{r}'\mathrm{d}\mathbf{r}'' A_1(\mathbf{r}')A_2(\mathbf{r}'') \exp\left[\frac{\mathrm{i}}{\hbar}\Delta_3(\mathbf{r}, \mathbf{r}'', \mathbf{r}')\right]. \tag{B.12}$$

Proof. The Weyl symbol is defined by $A(\mathbf{r}) = T_W[\hat{A}] = \mathrm{Tr}[\hat{A}(\hat{\mathbf{r}})\hat{d}(\hat{\mathbf{r}})]$. Moreover, by formally inverting this equation we obtain

$$\hat{A}(\hat{\mathbf{r}}) = \frac{1}{2\pi\hbar} \int \mathrm{d}\mathbf{r} A(\mathbf{r})\hat{d}(\hat{\mathbf{r}}).$$

Let $\hat{A} = \hat{A}_1\hat{A}_2$ be a product of two operators which are functions of $\hat{\mathbf{r}}$. Then,

$$A(\mathbf{r}) = \frac{1}{(2\pi\hbar)^2} \int \mathrm{d}\mathbf{r}'\mathrm{d}\mathbf{r}'' A_1(\mathbf{r}')A_2(\mathbf{r}'')\mathrm{Tr}[\hat{d}(\hat{\mathbf{r}}')\hat{d}(\hat{\mathbf{r}}'')\hat{d}(\hat{\mathbf{r}})].$$

By using properties 7 and 8,

$$\begin{aligned}\mathrm{Tr}[\hat{d}(\mathbf{r}')\hat{d}(\mathbf{r}'')\hat{d}(\mathbf{r})] =&\frac{2}{\pi\hbar}\int \mathrm{d}\mathbf{r}_1 \exp\left[\frac{\mathrm{i}}{\hbar}\Delta_3(\mathbf{r}_1,\mathbf{r}'',\mathbf{r}')\right]\mathrm{Tr}[\hat{d}(\mathbf{r}_1)\hat{d}(\mathbf{r})]\\ =&\frac{4}{(\pi\hbar)^2}\int \mathrm{d}\mathbf{r}_1\mathrm{d}\mathbf{r}_2 \exp\left[\frac{\mathrm{i}}{\hbar}\left(\Delta_3(\mathbf{r}_1,\mathbf{r}'',\mathbf{r}')+\Delta_3(\mathbf{r}_2,\mathbf{r},\mathbf{r}_1)\right)\right].\end{aligned}$$

Considering the phase in the exponential

$$\Delta_3(\mathbf{r}_1,\mathbf{r}'',\mathbf{r}')+\Delta_3(\mathbf{r}_2,\mathbf{r},\mathbf{r}_1) = 2\left(\mathbf{r}''\wedge\mathbf{r}'+\mathbf{r}_1\wedge(\mathbf{r}''-\mathbf{r}'-\mathbf{r})+\mathbf{r}_2\wedge(\mathbf{r}-\mathbf{r}_1)\right),$$

together with

$$\int \mathrm{d}\mathbf{r}_2 \exp\left[\frac{2\mathrm{i}}{\hbar}\mathbf{r}_2\wedge(\mathbf{r}-\mathbf{r}_1)\right] = (\pi\hbar)^2\delta(\mathbf{r}-\mathbf{r}_1),$$

allows us to obtain

$$\begin{aligned}A(\mathbf{r}) =&\frac{1}{(\pi\hbar)^2}\int \mathrm{d}\mathbf{r}'\mathrm{d}\mathbf{r}'' A_1(\mathbf{r}')A_2(\mathbf{r}'')\exp\left[\frac{2\mathrm{i}}{\hbar}\left(\mathbf{r}\wedge\mathbf{r}''+\mathbf{r}''\wedge\mathbf{r}'+\mathbf{r}'\wedge\mathbf{r}\right)\right]\\ =&\frac{1}{(\pi\hbar)^2}\int \mathrm{d}\mathbf{r}'\mathrm{d}\mathbf{r}'' A_1(\mathbf{r}')A_2(\mathbf{r}'')\exp\left[\frac{\mathrm{i}}{\hbar}\Delta_3(\mathbf{r},\mathbf{r}'',\mathbf{r}')\right].\end{aligned}$$

10. Weyl symbol for the product of three operators

$$\begin{aligned}B(\mathbf{r}) =&\frac{1}{(\pi\hbar)^2}\int \mathrm{d}\mathbf{r}_1\mathrm{d}\mathbf{r}_2\mathrm{d}\mathbf{r}_3 B_1(\mathbf{r}_1)B_2(\mathbf{r}_2)B_3(\mathbf{r}_3)\\ &\times\exp\left[\frac{2\mathrm{i}}{\hbar}(\mathbf{r}\wedge\mathbf{r}_3+\mathbf{r}_2\wedge\mathbf{r}_1)\right]\delta[\mathbf{r}+\mathbf{r}_2-(\mathbf{r}_3+\mathbf{r}_1)].\end{aligned} \tag{B.13}$$

Proof. Let $\hat{B}=\hat{B}_1\hat{B}_2\hat{B}_3=\hat{B}_{12}\hat{B}_3$, with all the operators being functions of $\hat{\mathbf{p}},\hat{\mathbf{q}}$. Then, by property 9,

$$B(\mathbf{r}) = \frac{1}{(\pi\hbar)^2}\int \mathrm{d}\mathbf{r}'\mathrm{d}\mathbf{r}_3 B_{12}(\mathbf{r}')B_3(\mathbf{r}_3)\exp\left[\frac{\mathrm{i}}{\hbar}\Delta_3(\mathbf{r},\mathbf{r}_3,\mathbf{r}')\right],$$

The Weyl symbol of the $\hat{B}_{12}$ operator is given by

$$B_{12}(\mathbf{r}') = \frac{1}{(\pi\hbar)^2}\int \mathrm{d}\mathbf{r}_1\mathrm{d}\mathbf{r}_2 B_1(\mathbf{r}_1)B_2(\mathbf{r}_2)\exp\left[\frac{\mathrm{i}}{\hbar}\Delta_3(\mathbf{r}',\mathbf{r}_2,\mathbf{r}_1)\right].$$

Therefore,

$$\begin{aligned}B(\mathbf{r}) =&\frac{1}{(\pi\hbar)^4}\int \mathrm{d}\mathbf{r}'\mathrm{d}\mathbf{r}_1\mathrm{d}\mathbf{r}_2\mathrm{d}\mathbf{r}_3 B_1(\mathbf{r}_1)B_2(\mathbf{r}_2)B_3(\mathbf{r}_3)\\ &\times\exp\left[\frac{\mathrm{i}}{\hbar}\left(\Delta_3(\mathbf{r},\mathbf{r}_3,\mathbf{r}')+\Delta_3(\mathbf{r}',\mathbf{r}_2,\mathbf{r}_1)\right)\right].\end{aligned}$$

Hence, by integration over the $\mathbf{r}'$ variables we arrive to

$$B(\mathbf{r}) = \frac{1}{(\pi\hbar)^2} \int \mathrm{d}\mathbf{r}_1 \mathrm{d}\mathbf{r}_2 \mathrm{d}\mathbf{r}_3 B_1(\mathbf{r}_1) B_2(\mathbf{r}_2) B_3(\mathbf{r}_3)$$
$$\times \exp\left[\frac{2\mathrm{i}}{\hbar}(\mathbf{r} \wedge \mathbf{r}_3 + \mathbf{r}_2 \wedge \mathbf{r}_1)\right] \delta[\mathbf{r} + \mathbf{r}_2 - (\mathbf{r}_3 + \mathbf{r}_1)].$$

Appendix C

Noise correlation function in the Ullersma-Calderira-Leggett model

For a bilinear coupling among the central system S and the linear bath modes B, the hamiltonian operator of the universe takes the form [37]

$$\hat{H} = \hat{H}_{\mathrm{S}} + \hat{H}_{\mathrm{B}} + \hat{H}_{\mathrm{SB}}, \tag{C.1}$$

where

$$\begin{aligned} \hat{H}_{\mathrm{S}} &= \frac{\hat{p}^2}{2m} + \hat{V}(\hat{q}), \\ \hat{H}_{\mathrm{B}} &= \sum_{j=1}^{F} \left(\frac{1}{2m_j}\hat{P}_j^2 + \frac{m_j}{2}\omega_j^2 \hat{Q}_j^2 \right), \\ \hat{H}_{\mathrm{SB}} &= -\hat{q}\sum_{j=1}^{F} c_j \hat{Q}_j + \hat{q}^2 \sum_{j=1}^{F} \frac{c_j^2}{2m_j\omega_j^2}. \end{aligned} \tag{C.2}$$

In the Heisenberg picture, the equations of motion for the environmental degrees of freedom are

$$\dot{\hat{P}}_j = \frac{\mathrm{i}}{\hbar}[\hat{H}, \hat{P}_j] = \frac{\mathrm{i}}{\hbar}([\hat{H}_{\mathrm{B}}, \hat{P}_j] + [\hat{H}_{\mathrm{SB}}, \hat{P}_j]) \ , \qquad ([\hat{H}_{\mathrm{S}}, \hat{P}_j] = 0) \tag{C.3}$$

where

$$\begin{aligned} [\hat{H}_{\mathrm{B}}, \hat{P}_j] &= \mathrm{i}\hbar m_j \omega_j^2 \hat{Q}_j, \\ [H_{\mathrm{SB}}, \hat{P}_j] &= \mathrm{i}\hbar c_j \hat{q}. \end{aligned} \tag{C.4}$$

Then

$$\dot{\hat{P}}_j = c_j\hat{q} - m_j\omega_j^2\hat{Q}_j. \tag{C.5}$$

On the other hand

$$\dot{\hat{Q}}_j = \frac{\mathrm{i}}{\hbar}[\hat{H}, \hat{Q}_j] = \frac{\mathrm{i}}{\hbar}[\hat{H}_{\mathrm{B}}, \hat{Q}_j] = \frac{\hat{P}_j}{m_j}, \tag{C.6}$$

completing the set of equations for the bath modes. In relation with the central system S, the

Heisenberg equations are

$$\dot{\hat{p}} = \frac{\mathrm{i}}{\hbar}[\hat{H}, \hat{p}] = \frac{\mathrm{i}}{\hbar}([\hat{H}_{\mathrm{S}}, \hat{p}] + [\hat{H}_{\mathrm{SB}}, \hat{p}]) = -\frac{\partial \hat{V}}{\partial \hat{q}} + \sum_{j=1}^{F}\left(c_j\hat{Q}_j - \hat{q}\frac{c_j^2}{m_j\omega_j^2}\right), \tag{C.7}$$

and

$$\dot{\hat{q}} = \frac{\mathrm{i}}{\hbar}[\hat{H}, \hat{q}] = \frac{\mathrm{i}}{\hbar}[\hat{H}_{\mathrm{S}}, \hat{q}] = \frac{\hat{p}}{m}. \tag{C.8}$$

We have obtained two sets of coupled differential equations. The standard procedure is to solve the bath modes equations and then to use this solutions into the central system equation of motion. As can be seen from Eqs. (C.5, C.6) we can write them as a single equation having the form

$$\ddot{\hat{Q}}_j + \omega_j^2\hat{Q}_j = \frac{c_j}{m_j}\hat{q}. \tag{C.9}$$

Here we have a damped equation of motion for the system coordinate. The external force being represented by $c_j\hat{q}$. The key idea here is to suppose $\hat{q}(t)$ as a stochastic function of time already given, i.e., the system coordinate couples to every oscillator in the bath in a random way such that, the differential equations listed above (for any j) are decoupled and can be solved analytically. The solution is given by

$$\hat{Q}_j(t) = \hat{Q}_j(0)\cos(\omega_j t) + \frac{\hat{P}_j(0)}{m_j\omega_j}\sin(\omega_j t) + \frac{c_j}{m_j\omega_j}\int_0^t \hat{q}(s)\sin[\omega_j(t-s)]ds. \tag{C.10}$$

This solution gives the the general form of the coordinates for the bath modes. By using this result into the central system equation

$$m\ddot{\hat{q}} + \frac{\partial \hat{V}}{\partial \hat{q}} + \hat{q}\sum_{j=1}^{F}\frac{c_j^2}{m_j\omega_j^2} = \sum_{j=1}^{F} c_j\hat{Q}_j, \tag{C.11}$$

we obtain

$$\begin{aligned} &m\ddot{\hat{q}} + \frac{\partial \hat{V}}{\partial \hat{q}} - \int_0^t ds\sum_{j=1}^{F}\frac{c_j^2}{m_j\omega_j}\sin[\omega_j(t-s)]\hat{q}(s) + \hat{q}\sum_{j=1}^{F}\frac{c_j^2}{m_j\omega_j^2} \\ &= \sum_{j=1}^{F} c_j\left(\hat{Q}_j(0)\cos(\omega_j t) + \frac{\hat{P}_j(0)}{m_j\omega_j}\sin(\omega_j t)\right). \end{aligned} \tag{C.12}$$

By means of integration by parts for the third term on the left-hand side of the above equation,

$$\begin{aligned} &\int_0^t ds\sum_{j=1}^{F}\frac{c_j^2}{m_j\omega_j}\sin[\omega_j(t-s)]\hat{q}(s) \\ &= \int_0^t ds\sum_{j=1}^{F}\frac{c_j^2}{m_j\omega_j}\left\{\frac{d}{ds}\left[\frac{\hat{q}(s)\cos[\omega_j(t-s)]}{\omega_j}\right] - \frac{1}{\omega_j}\cos[\omega_j(t-s)]\dot{\hat{q}}(s)\right\} \\ &= \sum_{j=1}^{F}\frac{c_j^2}{m_j\omega_j^2}[\hat{q}(t) - \hat{q}(0)\cos(\omega_j t)] - \int_0^t ds\sum_{j=1}^{F}\frac{c_j^2}{m_j\omega_j^2}\cos[\omega_j(t-s)]\dot{\hat{q}}(s), \end{aligned} \tag{C.13}$$

we obtain,

$$m\ddot{\hat{q}} + \frac{\partial \hat{V}}{\partial \hat{q}} + \int_0^t ds \sum_{j=1}^{F} \frac{c_j^2}{m_j \omega_j^2} \cos[\omega_j(t-s)]\dot{\hat{q}}(s) \tag{C.14}$$
$$= \sum_{j=1}^{F} c_j \left[\left(\hat{Q}_j(0) - \frac{c_j}{m_j \omega_j^2} \hat{q}(0) \right) \cos(\omega_j t) + \frac{\hat{P}_j(0)}{m_j \omega_j} \sin(\omega_j t) \right].$$

By means of the introduction of the damping kernel

$$\gamma(t) = \frac{1}{m} \sum_{j=1}^{F} \frac{c_j^2}{m_j \omega_j^2} \cos(\omega_j t), \tag{C.15}$$

the equation of motion for $\hat{q}(t)$ takes the form

$$m\ddot{\hat{q}} + \frac{\partial \hat{V}}{\partial \hat{q}} + m \int_0^t ds \gamma(t-s)\dot{\hat{q}}(s) = \hat{\xi}(t), \tag{C.16}$$

with $\hat{\xi}(t)$ the operator-valued fluctuating force defined by

$$\hat{\xi}(t) = \sum_{j=1}^{F} c_j \left[\left(\hat{Q}_j(0) - \frac{c_j}{m_j \omega_j^2} \hat{q}(0) \right) \cos(\omega_j t) + \frac{\hat{P}_j(0)}{m_j \omega_j} \sin(\omega_j t) \right]. \tag{C.17}$$

The term $m\gamma(t)\hat{q}(0)$ is known as the transient. For weak coupling one can write the fluctuating force as $\hat{\xi}(t) = \hat{\zeta}(t) - m\gamma(t)\hat{q}(0)$. Thus,

$$\hat{\zeta}(t) = \sum_{j=1}^{F} c_j \left[\hat{Q}_j(0) \cos(\omega_j t) + \frac{\hat{P}_j(0)}{m_j \omega_j} \sin(\omega_j t) \right]. \tag{C.18}$$

An important quantity to characterize the fluctuating force is the two-time correlation function $\langle \hat{\zeta}(t) \hat{\zeta}(0) \rangle_{\mathrm{B}}$. From its definition we obtain

$$\langle \hat{\zeta}(t) \hat{\zeta}(0) \rangle_{\mathrm{B}} = \sum_{j,k} c_j c_k \left\langle \left(\hat{Q}_j(0) \cos(\omega_j t) + \frac{\hat{P}_j(0)}{m_j \omega_j} \sin(\omega_j t) \right) \hat{Q}_k(0) \right\rangle_{\mathrm{B}} \tag{C.19}$$
$$= \sum_{j,k} c_j c_k \left(\langle \hat{Q}_j(0) \hat{Q}_k(0) \rangle_{\mathrm{B}} \cos(\omega_j t) + \frac{1}{m_j \omega_j} \langle \hat{P}_j(0) \hat{Q}_k(0) \rangle_{\mathrm{B}} \sin(\omega_j t) \right).$$

In thermal equilibrium the expectation values fro the operator products above can be calculated by means of the density operator

$$\hat{\rho} = \frac{1}{Z_{\mathrm{B}}} \exp\left(-\beta \hat{H}_{\mathrm{B}}\right). \tag{C.20}$$

Thus,

$$\begin{aligned}\langle\hat{Q}_j(0)\hat{Q}_k(0)\rangle_{\mathrm{B}} =& \mathrm{Tr_B}\left(\hat{Q}_j(0)\hat{Q}_k(0)\hat{\rho}_{\mathrm{B}}\right) \\ =& \frac{1}{Z_{\mathrm{B}}}\mathrm{Tr_B}\left(\hat{Q}_j(0)\hat{Q}_k(0)e^{-\beta\hat{H}_{\mathrm{B}}}\right),\end{aligned} \tag{C.21}$$

where

$$\begin{aligned}Z_{\mathrm{B}} &= \mathrm{Tr_B}\left(e^{-\beta\hat{H}_{\mathrm{B}}}\right) \\ &= \prod_{n=1}^{F}\left(\sum_{m=0}^{\infty}e^{-\beta E_{n,m}}\right) \\ &= \prod_{n=1}^{F}\frac{1}{2\sinh\left(\frac{\beta\hbar\omega_n}{2}\right)}.\end{aligned} \tag{C.22}$$

Then

$$\langle\hat{Q}_j(0)\hat{Q}_k(0)\rangle_{\mathrm{B}} = \left[\prod_{n=1}^{F}2\sinh\left(\frac{\beta\hbar\omega_n}{2}\right)\right]\mathrm{Tr_B}\left(\hat{Q}_j(0)\hat{Q}_k(0)e^{-\beta\hat{H}_{\mathrm{B}}}\right). \tag{C.23}$$

By means of

$$\hat{Q}_j(0) = \sqrt{\frac{\hbar}{2m_j\omega_j}}\left(\hat{a}_j^{\dagger}+\hat{a}_j\right), \tag{C.24}$$

we obtain

$$\begin{aligned}\mathrm{Tr_B}\left(\hat{Q}_j(0)\hat{Q}_k(0)e^{-\beta\hat{H}_{\mathrm{B}}}\right) =& \frac{\hbar}{2\sqrt{m_jm_k\omega_j\omega_k}}\left(\prod_{n\neq j,k}\frac{1}{2\sinh\left(\frac{\beta\hbar\omega_n}{2}\right)}\right) \\ &\times\sum_{m=0}^{\infty}e^{-\beta(E_{j,m}+E_{k,m})}\langle j_m,k_m|\,\hat{a}_j^{\dagger}\hat{a}_k+\hat{a}_k\hat{a}_j^{\dagger}\,|j_m,k_m\rangle.\end{aligned} \tag{C.25}$$

Therefore

$$\begin{aligned}\langle\hat{Q}_j(0)\hat{Q}_k(0)\rangle_{\mathrm{B}} =& \frac{2\hbar}{\sqrt{m_jm_k\omega_j\omega_k}}\sinh\left(\frac{\beta\hbar\omega_j}{2}\right)\sinh\left(\frac{\beta\hbar\omega_k}{2}\right) \\ &\times\sum_{m=0}^{\infty}e^{-\beta(E_{j,m}+E_{k,m})}\langle j_m,k_m|\,\hat{a}_j^{\dagger}\hat{a}_k+\hat{a}_k\hat{a}_j^{\dagger}\,|j_m,k_m\rangle.\end{aligned} \tag{C.26}$$

When $j \neq k$, $\langle j_m, k_m | \hat{a}_j^\dagger \hat{a}_k + \hat{a}_k \hat{a}_j^\dagger | j_m, k_m \rangle = 0$. When $j = k$, $\hat{a}_j^\dagger \hat{a}_j + \hat{a}_j \hat{a}_j^\dagger = 1 + 2\hat{a}_j^\dagger \hat{a}_j$. Thus,

$$\begin{aligned}\langle \hat{Q}_j^2(0) \rangle_{\mathrm{B}} =& \frac{\hbar}{m_j \omega_j} \sinh\left(\frac{\beta\hbar\omega_j}{2}\right) \sum_{m=0}^{\infty} e^{-\beta E_{j,m}} \langle j_m | 1 + 2\hat{a}_j^\dagger \hat{a}_j | j_m \rangle \\ =& \frac{2\hbar}{m_j \omega_j} \sinh\left(\frac{\beta\hbar\omega_j}{2}\right) \sum_{m=0}^{\infty} \left(m + \frac{1}{2}\right) e^{-\beta E_{j,m}} \\ =& -\frac{1}{m_j \beta \omega_j} \sinh\left(\frac{\beta\hbar\omega_j}{2}\right) \frac{d}{d\omega_j} \frac{1}{\sinh\left(\frac{\beta\hbar\omega_j}{2}\right)} \\ =& \frac{\hbar}{2 m_j \omega_j} \coth\left(\frac{\beta\hbar\omega_j}{2}\right).\end{aligned} \tag{C.27}$$

Therefore,

$$\langle \hat{Q}_j(0) \hat{Q}_k(0) \rangle_{\mathrm{B}} = \delta_{jk} \frac{\hbar}{2 m_j \omega_j} \coth\left(\frac{\beta\hbar\omega_j}{2}\right). \tag{C.28}$$

Following the same steps, it is straightforward to prove that

$$\langle \hat{P}_j(0) \hat{Q}_k(0) \rangle_{\mathrm{B}} = -\mathrm{i}\frac{\hbar}{2} \delta_{jk}. \tag{C.29}$$

Thus, by means of the these two results, Eq. (C.19) takes the form

$$\langle \hat{\zeta}(t) \hat{\zeta}(0) \rangle_{\mathrm{B}} = \sum_{j=1}^{F} \frac{\hbar c_j^2}{m_j \omega_j} \left[\coth\left(\frac{\beta\hbar\omega_j}{2}\right) \cos(\omega_j t) - \mathrm{i} \sin(\omega_j t)\right]. \tag{C.30}$$

By introducing the spectral density as

$$I(\omega) = \pi \sum_{j=1}^{F} \frac{c_j^2}{2 m_j \omega_j} \delta(\omega - \omega_j), \tag{C.31}$$

the noise correlation function takes the form

$$\langle \hat{\zeta}(t) \hat{\zeta}(0) \rangle_{\mathrm{B}} = \hbar \int_0^\infty \frac{\mathrm{d}\omega}{\pi} I(\omega) \left[\coth\left(\frac{\hbar\beta\omega}{2}\right) \cos(\omega t) - \mathrm{i} \sin(\omega t)\right]. \tag{C.32}$$

It is also possible to show, by following the above calculation, that

$$\langle \hat{\zeta}(0) \hat{\zeta}(t) \rangle_{\mathrm{B}} = \hbar \int_0^\infty \frac{\mathrm{d}\omega}{\pi} I(\omega) \left[\coth\left(\frac{\hbar\beta\omega}{2}\right) \cos(\omega t) + \mathrm{i} \sin(\omega t)\right]. \tag{C.33}$$

Thus, $\langle \hat{\zeta}(0) \hat{\zeta}(t) \rangle_{\mathrm{B}}^* = \langle \hat{\zeta}(t) \hat{\zeta}(0) \rangle_{\mathrm{B}}$. By convenience, we define $\langle \hat{\zeta}(t) \hat{\zeta}(0) \rangle_{\mathrm{B}} = \langle \hat{\zeta}_+(t) \hat{\zeta}_+(0) \rangle_{\mathrm{B}}$ and $\langle \hat{\zeta}(0) \hat{\zeta}(t) \rangle_{\mathrm{B}} = \langle \hat{\zeta}_-(t) \hat{\zeta}_-(0) \rangle_{\mathrm{B}}$, such that

$$\langle \hat{\zeta}_\pm(t) \hat{\zeta}_\pm(0) \rangle_{\mathrm{B}} = \hbar \int_0^\infty \frac{\mathrm{d}\omega}{\pi} I(\omega) \left[\coth\left(\frac{\hbar\beta\omega}{2}\right) \cos(\omega t) \mp \mathrm{i} \sin(\omega t)\right]. \tag{C.34}$$

The definition of the correlation $\langle \hat{\zeta}_-(t) \hat{\zeta}_-(0) \rangle_{\mathrm{B}}$ is just a matter of convenience for our purposes of studying the semiclassical stochastic approach. Specifically, we wanted to translate into phase-space a study that was previously done to the propagator within the configuration space in reference [51]. In that work, they formulate an study of the expected value of the influence functional in the configuration space and the connection that from that stochastic approach emerges with the dynamics of an open system. In this way, the statistical study of the influence functional is automatically transferred to the phase of influence, that is, the influence phase, and by extension, to the correlation functions of the bath.

In this regard, the use that we have made in our work of the complex conjugate of the noise correlation function $\langle\hat{\zeta}(0)\hat{\zeta}(t)\rangle_{\rm B}$ adjust the expected results for the Wigner propagator already obtained by the open system formalism.

Appendix D

Weyl transforms for products of canonical operators

D.1 Weyl transform of products having the form $\hat{p}^m\hat{q}^n$ and $\hat{q}^n\hat{p}^m$

Let us consider the operator product $\hat{A} = \hat{p}^m\hat{q}^n$. From property 9 in Appendix B, the Weyl symbol of the product of these two operators is given by

$$A(\mathbf{r}) = \frac{1}{(\pi\hbar)^2}\int \mathrm{d}\mathbf{r}'\mathrm{d}\mathbf{r}''\ A_1(\mathbf{r}')A_2(\mathbf{r}'')\exp\left[\frac{\mathrm{i}}{\hbar}\Delta_3(\mathbf{r},\mathbf{r}'',\mathbf{r}')\right].$$

Thus,

$$\begin{aligned}(\hat{p}^m\hat{q}^n)_\mathrm{W} =& \frac{1}{(\pi\hbar)^2}\int \mathrm{d}\mathbf{r}'(p')^m\exp\left(\frac{2\mathrm{i}}{\hbar}(\mathbf{r}'\wedge\mathbf{r})\right)\\ &\times\int \mathrm{d}p''\mathrm{d}q''(q'')^n\exp\left(\frac{2\mathrm{i}}{\hbar}(p''Q-q''P)\right),\end{aligned} \tag{D.1}$$

where $Q = q' - q$ and $P = p' - p$. Let us consider initially the integrals in the p'', q'' variables, such that

$$\begin{aligned}\int \mathrm{d}p''\mathrm{d}q''(q'')^n\exp\left(\frac{2\mathrm{i}}{\hbar}(p''Q-q''P)\right) =& \int \mathrm{d}p''\exp\left(\frac{2\mathrm{i}}{\hbar}p''Q\right)\\ &\times\int \mathrm{d}q''(q'')^n\exp\left(-\frac{2\mathrm{i}}{\hbar}q''P\right).\end{aligned} \tag{D.2}$$

We can write the second integral kernel as

$$(q'')^n\exp\left(-\frac{2\mathrm{i}}{\hbar}q''P\right) = \left(-\frac{\hbar}{2\mathrm{i}}\right)^n\frac{\mathrm{d}^n}{\mathrm{d}P^n}\exp\left(-\frac{2\mathrm{i}}{\hbar}q''P\right), \tag{D.3}$$

such that the result of the integral in (D.2) is

$$\int \mathrm{d}p''\mathrm{d}q''(q'')^n\exp\left(\frac{2\mathrm{i}}{\hbar}(p''Q-q''P)\right) = (\pi\hbar)^2\left(-\frac{\hbar}{2\mathrm{i}}\right)^n\delta(Q)\frac{\mathrm{d}^n}{\mathrm{d}P^n}\delta(P). \tag{D.4}$$

Then, from (D.1),

$$(\hat{p}^m\hat{q}^n)_\mathrm{W} = \left(-\frac{\hbar}{2\mathrm{i}}\right)^n \int \mathrm{d}\mathbf{r}'(p')^m \exp\left(\frac{2\mathrm{i}}{\hbar}(\mathbf{r}'\wedge\mathbf{r})\right)\delta(Q)\frac{\mathrm{d}^n}{\mathrm{d}P^n}\delta(P) \qquad (D.5)$$
$$= \left(-\frac{\hbar}{2\mathrm{i}}\right)^n \int \mathrm{d}P\ (p+P)^m \exp\left(\frac{2\mathrm{i}}{\hbar}qP\right)\frac{\mathrm{d}^n}{\mathrm{d}P^n}\delta(P).$$

By means of the Dirac delta identity [62]

$$\int_{-\infty}^{\infty} f(x)\frac{\mathrm{d}^n}{\mathrm{d}x^n}\delta(x-x_0)dx = (-1)^n\left(\frac{\mathrm{d}^n}{\mathrm{d}x^n}f(x)\right)_{x=x_0}, \qquad (D.6)$$

we can write

$$(\hat{p}^m\hat{q}^n)_\mathrm{W} = \left(\frac{\hbar}{2\mathrm{i}}\right)^n \frac{\mathrm{d}^n}{\mathrm{d}P^n}\left[(p+P)^m \exp\left(\frac{2\mathrm{i}}{\hbar}qP\right)\right]_{P=0}. \qquad (D.7)$$

On the other hand, if we want to find the Weyl symbol of the operator $\hat{B} = \hat{q}^n\hat{p}^m$, we just have to follow the same procedure as before to find

$$(\hat{q}^n\hat{p}^m)_\mathrm{W} = \left(-\frac{\hbar}{2\mathrm{i}}\right)^m \frac{\mathrm{d}^m}{\mathrm{d}Q^m}\left[(q+Q)^n \exp\left(-\frac{2\mathrm{i}}{\hbar}pQ\right)\right]_{Q=0}. \qquad (D.8)$$

The results found in (D.6) and (D.8) are quite interesting and useful, because they offer the advantage of using derivatives, instead of integrals, to calculate Weyl symbols in a easy and fast way.

Finally, by means of the binomial theorem we can write the above expressions as

$$(\hat{p}^m\hat{q}^n)_\mathrm{W} = \left(\frac{\hbar}{2\mathrm{i}}\right)^n \sum_{k=0}^{m}\binom{m}{k} p^{m-k}\frac{\mathrm{d}^n}{\mathrm{d}P^n}\left[P^k \exp\left(\frac{2\mathrm{i}}{\hbar}qP\right)\right]_{P=0}, \qquad (D.9)$$

and

$$(\hat{q}^n\hat{p}^m)_\mathrm{W} = \left(-\frac{\hbar}{2\mathrm{i}}\right)^m \sum_{k=0}^{n}\binom{n}{k} q^{n-k}\frac{\mathrm{d}^n}{\mathrm{d}Q^m}\left[Q^k \exp\left(-\frac{2\mathrm{i}}{\hbar}pQ\right)\right]_{Q=0}. \qquad (D.10)$$

D.2 Weyl transform of the Heisenberg equations for the canonical operators

Within the Heisenberg picture the evolution of an operator $\hat{A}$ is determined by the equation

$$\frac{d\hat{A}}{dt} = \frac{i}{\hbar}[\hat{H},\hat{A}]. \qquad (D.11)$$

Applied to the canonical operators, the equation allows to study its dynamical evolution in terms of differential-operator equations. Nonetheless, we are mainly interested to study the dynamics directly in phase-space rather than the Hilbert space of operators. This choice leaves us with two possibilities: On one hand we can apply the Weyl transform to the Hamiltonian operators under study and then, once in phase-space, resort to the classical equations of Hamilton to obtain the differential equations. On the other hand we can proceed by transforming directly the Heisenberg equations of motion for the canonical operators to obtain the differential equations in terms of scalar functions. Although the first choice is just a straightforward application of the Weyl transform operation, we will make use of the results of the preceding section to develop the latter procedure.

Let us consider the Weyl transform on the Heisenberg equation for the canonical operator $\hat{q}$[1]

$$\left(\frac{d\hat{q}}{dt}\right)_{\mathrm{W}} = \frac{i}{\hbar}[\hat{H}, \hat{q}]_{\mathrm{W}}. \tag{D.12}$$

On the left-hand side, the transform act on the coordinate operator in a straightforward way. Therefore, it is the right-hand side the one of interest for us. In the most simple case of a Hamiltonian for an isolated DOF having the standard form $\hat{H} = \frac{1}{2m}\hat{p}^2 + V(\hat{q})$, we have

$$[\hat{H}, \hat{q}]_{\mathrm{W}} = \frac{1}{2m}\left(\hat{p}^2\hat{q} - \hat{q}\hat{p}^2\right)_{\mathrm{W}}. \tag{D.13}$$

As long as the Weyl transform is a linear operation, we can apply it to these two terms by direct use of Eqs. (D.9), (D.10). Then, $\left(\hat{p}^2\hat{q}\right)_{\mathrm{W}} = p^2 q - i\hbar p$, and $\left(\hat{q}\hat{p}^2\right)_{\mathrm{W}} = p^2 q + i\hbar p$. Therefore, Eq. (D.12) becomes the classical Hamilton equation for the scalar coordinate q

$$\frac{dq}{dt} = \frac{p}{m}. \tag{D.14}$$

Let us now consider the Weyl transform on the Heisenberg equation for the canonical operator $\hat{p}$,

$$\begin{aligned}\left(\frac{d\hat{p}}{dt}\right)_{\mathrm{W}} =& \frac{i}{\hbar}[\hat{H}, \hat{p}]_{\mathrm{W}} \\ =& \frac{i}{\hbar}[V(\hat{q}), \hat{p}]_{\mathrm{W}}.\end{aligned} \tag{D.15}$$

Since we have not made any supposition about the mathematical for of the potential, we should make use of the Eq. (1.11) to calculate the transform of the two products above. Thus,

$$\begin{aligned}\left(\hat{V}\hat{p}\right)_{\mathrm{W}} =& \int \mathrm{d}u \exp\left\{-\frac{\mathrm{i}}{\hbar}pu\right\} \left\langle q + \frac{u}{2}\middle| V(\hat{q})\hat{p} \middle| q - \frac{u}{2}\right\rangle \\ =& \int \mathrm{d}u \exp\left\{-\frac{\mathrm{i}}{\hbar}pu\right\} V\left(q + \frac{u}{2}\right) \left\langle q + \frac{u}{2}\middle| \hat{p} \middle| q - \frac{u}{2}\right\rangle \\ =& - i\hbar \int \mathrm{d}u \exp\left\{-\frac{\mathrm{i}}{\hbar}pu\right\} V\left(q + \frac{u}{2}\right) \frac{\partial}{\partial u}\delta(u) \\ =& i\hbar\frac{\partial}{\partial u}\left[\exp\left\{-\frac{\mathrm{i}}{\hbar}pu\right\} V\left(q + \frac{u}{2}\right)\right]_{u=0} \\ =& pV(q) + \frac{i\hbar}{2}\frac{\partial V(q)}{\partial q}.\end{aligned} \tag{D.16}$$

[1]For the sake of simplicity, we will use the label W to indicate the operation of applying the Weyl transform to the quantity it is attached to.

Following the same procedure for the another transform, we obtain

$$\left(\hat{p}\hat{V}\right)_{\mathrm{W}} = pV(q) - \frac{i\hbar}{2}\frac{\partial V(q)}{\partial q}. \tag{D.17}$$

Thus, Eq. (D.15) becomes

$$\frac{dp}{dt} = -\frac{\partial V(q)}{\partial q}. \tag{D.18}$$

D.3 Equations of motion for the bath modes

The results obtained in the preceding section can be extended to include the more interesting case of an open system with hamiltonian

$$\hat{H} = \hat{H}_{\mathrm{S}} + \hat{H}_{\mathrm{B}} + \hat{H}_{\mathrm{SB}}, \tag{D.19}$$

where

$$\begin{aligned}\hat{H}_{\mathrm{S}} &= \frac{\hat{p}^2}{2m} + \hat{V}(\hat{q}),\\ \hat{H}_{\mathrm{B}} &= \sum_{j=1}^{F}\left(\frac{1}{2m_j}\hat{P}_j^2 + \frac{m_j}{2}\omega_j^2\hat{Q}_j^2\right),\\ \hat{H}_{\mathrm{SB}} &= -\hat{q}\sum_{j=1}^{F}c_j\hat{Q}_j + \hat{q}^2\sum_{j=1}^{F}\frac{c_j^2}{2m_j\omega_j^2}.\end{aligned} \tag{D.20}$$

The Heisenberg equation of motion for the operator $\hat{Q}_j$ is

$$\begin{aligned}\frac{d\hat{Q}_j}{dt} &= \frac{i}{\hbar}[\hat{H}, \hat{Q}_j]\\ \frac{d\hat{Q}_j}{dt} &= \frac{i}{\hbar}[\hat{H}_{\mathrm{B}} + \hat{H}_{\mathrm{SB}}, \hat{Q}_j].\end{aligned} \tag{D.21}$$

Then,

$$\frac{i}{\hbar}[\hat{H}_{\mathrm{B}}, \hat{Q}_j] = \frac{\hat{P}_j}{m_j}, \tag{D.22}$$

and

$$\begin{aligned}\frac{i}{\hbar}[\hat{H}_{\mathrm{SB}}, \hat{Q}_j] &= -\frac{i}{\hbar}c_j[\hat{q}\otimes\hat{Q}_j, \hat{I}_{\mathrm{S}}\otimes\hat{Q}_j]\\ &= -\frac{i}{\hbar}c_j\hat{q}\otimes\left(\hat{Q}_j\hat{Q}_j - \hat{Q}_j\hat{Q}_j\right)\\ &= \hat{0}.\end{aligned} \tag{D.23}$$

Therefore, by following the result given in Ec (D.14), the weyl transform of Ec (D.21),

$$\left(\frac{d\hat{Q}_j}{dt}\right)_{\mathrm{W}} = \frac{i}{\hbar}[\hat{H}, \hat{Q}_j]_{\mathrm{W}}, \tag{D.24}$$

becomes

$$\frac{dQ_j}{dt} = \frac{P_j}{m_j}. \tag{D.25}$$

On the other hand, for the momentum operator $\hat{P}_j$ we have

$$\begin{aligned} \frac{d\hat{P}_j}{dt} =& \frac{i}{\hbar}[\hat{H}, \hat{P}_j] \\ =& \frac{i}{\hbar}[\hat{H}_{\mathrm{B}} + \hat{H}_{\mathrm{SB}}, \hat{P}_j], \end{aligned} \tag{D.26}$$

where

$$[\hat{H}_{\mathrm{B}}, \hat{P}_j] = [\hat{V}_{\mathrm{B}}(\hat{Q}_j), \hat{P}_j]. \tag{D.27}$$

By following the same procedure of the preceding section we obtain

$$\frac{i}{\hbar}[\hat{V}_{\mathrm{B}}(\hat{Q}_j), \hat{P}_j]_{\mathrm{W}} = -\frac{\partial V_{\mathrm{B}}}{\partial Q_j}. \tag{D.28}$$

Meanwhile,

$$\begin{aligned} \frac{i}{\hbar}[\hat{H}_{\mathrm{SB}}, \hat{P}_j] &= -\frac{i}{\hbar} c_j [\hat{q} \otimes \hat{Q}_j, \hat{I}_{\mathrm{S}} \otimes \hat{P}_j] \\ &= -\frac{i}{\hbar} c_j \hat{q} \otimes \left(\hat{Q}_j \hat{P}_j - \hat{P}_j \hat{Q}_j\right) \\ &= -\frac{i}{\hbar} c_j \hat{q} \otimes [\hat{Q}_j, \hat{P}_j] \\ &= c_j \hat{q} \otimes \hat{I}_{\mathrm{B}}. \end{aligned} \tag{D.29}$$

Therefore, by knowing that the Weyl transform of the identity operator is the number one, we obtain

$$\begin{aligned} \frac{i}{\hbar}[\hat{H}_{\mathrm{SB}}, \hat{P}_j]_{\mathrm{W}} &= c_j \left(\hat{q} \otimes \hat{I}_{\mathrm{B}}\right)_{\mathrm{W}} \\ &= c_j q. \end{aligned} \tag{D.30}$$

Finally,

$$\begin{aligned} \left(\frac{d\hat{P}_j}{dt}\right)_{\mathrm{W}} = \frac{dP_j}{dt} =& \frac{i}{\hbar}[\hat{H}, \hat{P}_j]_{\mathrm{W}} \\ =& -\frac{\partial V_{\mathrm{B}}}{\partial Q_j} + c_j q \\ =& -m_j \omega_j^2 Q_j^2 + c_j q. \end{aligned} \tag{D.31}$$

Appendix E

Properties of $W(\mathbf{p},\mathbf{q})$ and $G_{\mathrm{W}}(\mathbf{r}'',t,\mathbf{r}',0)$

Starting from the definitions of the Wigner distribution function and the Wigner propagator made in the main text, we will prove some key properties that are fulfilled by these mathematical objects. Special emphasis is given to the coordinate and momentum representation of the Wigner function.

E.1 Wigner function in the $|\mathbf{q}\rangle$ and $|\mathbf{p}\rangle$ representations

The Wigner function is defined as the Weyl transform of the density operator as

$$\begin{aligned} W(\mathbf{p},\mathbf{q}) =& \frac{1}{(2\pi\hbar)^f}\mathrm{Tr}[\hat{\rho}(\hat{\mathbf{p}},\hat{\mathbf{q}})\hat{d}(\mathbf{p},\mathbf{q})], \\ =& \frac{1}{(2\pi\hbar)^{2f}}\int \mathrm{d}\mathbf{u}\mathrm{d}\mathbf{v}\exp\left[\frac{\mathrm{i}}{\hbar}(\mathbf{u}\cdot\mathbf{p}+\mathbf{v}\cdot\mathbf{q})\right]\mathrm{Tr}\left[\hat{\rho}\,\hat{T}(-\mathbf{u},-\mathbf{v})\right]. \end{aligned} \tag{E.1}$$

where $\hat{d}$ has been defined in appendix B. In order to calculate the trace, we will use the coordinate basis $\{|\mathbf{q}'\rangle\}$ such that

$$\begin{aligned} \mathrm{Tr}\left[\hat{\rho}\,\hat{T}(-\mathbf{u},-\mathbf{v})\right] &= \int \mathrm{d}\mathbf{q}'\exp\left[-\frac{\mathrm{i}}{2\hbar}(\mathbf{u}\cdot\mathbf{v}+2\mathbf{v}\cdot\mathbf{q}')\right]\langle\mathbf{q}'|\,\hat{\rho}\exp\left[\frac{\mathrm{i}}{\hbar}\mathbf{u}\cdot\hat{\mathbf{p}}\right]|\mathbf{q}'\rangle \\ &= \int \mathrm{d}\mathbf{q}'e^{-\frac{\mathrm{i}}{2\hbar}(\mathbf{u}\cdot\mathbf{v}+2\mathbf{v}\cdot\mathbf{q}')}\langle\mathbf{q}'|\,\hat{\rho}\,|\mathbf{q}'+\mathbf{u}\rangle, \end{aligned} \tag{E.2}$$

Where, in the last line, we have made use of the translation operator acting on the $|\mathbf{q}'\rangle$ state. Hence,

$$\begin{aligned} W(\mathbf{p},\mathbf{q}) =& \frac{1}{(2\pi\hbar)^{2f}}\int \mathrm{d}\mathbf{q}'\mathrm{d}\mathbf{u}\mathrm{d}\mathbf{v}e^{\frac{i}{\hbar}(\mathbf{u}\cdot\mathbf{p}+\mathbf{v}\cdot\mathbf{q}-\frac{1}{2}\mathbf{u}\cdot\mathbf{v}-\mathbf{v}\cdot\mathbf{q}')}\langle\mathbf{q}'|\,\hat{\rho}\,|\mathbf{q}'+\mathbf{u}\rangle \\ =& \frac{1}{(2\pi\hbar)^{f}}\int \mathrm{d}\mathbf{q}'\mathrm{d}\mathbf{u}e^{\frac{\mathrm{i}}{\hbar}\mathbf{u}\cdot\mathbf{p}}\,\delta\left[\mathbf{q}'-\left(\mathbf{q}-\frac{\mathbf{u}}{2}\right)\right]\langle\mathbf{q}'|\,\hat{\rho}\,|\mathbf{q}'+\mathbf{u}\rangle \\ =& \int \mathrm{d}\mathbf{u}e^{\frac{\mathrm{i}}{\hbar}\mathbf{u}\cdot\mathbf{p}}\left\langle\mathbf{q}-\frac{\mathbf{u}}{2}\right|\frac{\hat{\rho}}{(2\pi\hbar)^f}\left|\mathbf{q}+\frac{\mathbf{u}}{2}\right\rangle. \end{aligned} \tag{E.3}$$

An equivalent version can be obtained if we consider the substitution $\mathbf{u}\to-\mathbf{u}$,

$$W(\mathbf{p},\mathbf{q}) = \int \mathrm{d}\mathbf{u}e^{-\frac{\mathrm{i}}{\hbar}\mathbf{u}\cdot\mathbf{p}}\left\langle\mathbf{q}+\frac{\mathbf{u}}{2}\right|\frac{\hat{\rho}}{(2\pi\hbar)^f}\left|\mathbf{q}-\frac{\mathbf{u}}{2}\right\rangle. \tag{E.4}$$

The wigner function can be written in the momentum representation by means of a change of basis as

$$W(\mathbf{p},\mathbf{q}) = \int \mathrm{d}\mathbf{w} e^{-\frac{\mathrm{i}}{\hbar}\mathbf{q}\cdot\mathbf{w}} \left\langle \mathbf{p}+\frac{\mathbf{w}}{2}\right| \frac{\hat{\rho}}{(2\pi\hbar)^f} \left|\mathbf{p}-\frac{\mathbf{w}}{2}\right\rangle \\ = \int \mathrm{d}\mathbf{w} e^{\frac{\mathrm{i}}{\hbar}\mathbf{q}\cdot\mathbf{w}} \left\langle \mathbf{p}-\frac{\mathbf{w}}{2}\right| \frac{\hat{\rho}}{(2\pi\hbar)^f} \left|\mathbf{p}+\frac{\mathbf{w}}{2}\right\rangle . \tag{E.5}$$

E.2 Properties of the Wigner function

1. **Wigner function is real.**

Proof.

$$\begin{aligned} W^*(\mathbf{p},\mathbf{q}) =& \frac{1}{(2\pi\hbar)^f} \left(\mathrm{Tr}[\hat{\rho}(\hat{\mathbf{p}},\hat{\mathbf{q}})\hat{d}(\mathbf{p},\mathbf{q})]\right)^* \\ =& \frac{1}{(2\pi\hbar)^f} \mathrm{Tr}[\hat{d}^\dagger(\mathbf{p},\mathbf{q})\hat{\rho}^\dagger(\hat{\mathbf{p}},\hat{\mathbf{q}})] \\ =& \frac{1}{(2\pi\hbar)^f} \mathrm{Tr}[\hat{\rho}(\hat{\mathbf{p}},\hat{\mathbf{q}})\hat{d}(\mathbf{p},\mathbf{q})] \\ =& W(\mathbf{p},\mathbf{q}). \end{aligned}$$

2. **Wigner function is normalized in phase space.**

Proof.

$$\begin{aligned} \int \mathrm{d}\mathbf{p}\mathrm{d}\mathbf{q} W(\mathbf{p},\mathbf{q}) =& \int \mathrm{d}\mathbf{u}\mathrm{d}\mathbf{p}\mathrm{d}\mathbf{q} \exp\left\{-\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{u}\right\} \left\langle \mathbf{q}+\frac{\mathbf{u}}{2}\right| \frac{\hat{\rho}}{(2\pi\hbar)^f} \left|\mathbf{q}-\frac{\mathbf{u}}{2}\right\rangle \\ =& \int \mathrm{d}\mathbf{u}\mathrm{d}\mathbf{q} \left\langle \mathbf{q}+\frac{\mathbf{u}}{2}\right| \hat{\rho} \left|\mathbf{q}-\frac{\mathbf{u}}{2}\right\rangle \left[\int \frac{\mathrm{d}\mathbf{p}}{(2\pi\hbar)^f} \exp\left\{-\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{u}\right\}\right] \\ =& \int \mathrm{d}\mathbf{u}\mathrm{d}\mathbf{q} \left\langle \mathbf{q}+\frac{\mathbf{u}}{2}\right| \hat{\rho} \left|\mathbf{q}-\frac{\mathbf{u}}{2}\right\rangle \delta(\mathbf{u}) \\ =& \int \mathrm{d}\mathbf{q} \left\langle \mathbf{q}\right| \hat{\rho} \left|\mathbf{q}\right\rangle \\ =& \mathrm{Tr}\left[\hat{\rho}\right] = 1. \end{aligned}$$

3. **The marginals densities of the Wigner function are the position and momentum probability densities.**

Proof. By considering a general mixed state described by the operator $\hat{\rho} = \sum_i P_i \left|\psi_i\right\rangle \left\langle\psi_i\right|$, we obtain

⋆ *Coordinate probability density.*

$$\begin{aligned}\int \mathrm{d}\mathbf{p}W(\mathbf{p},\mathbf{q}) &= \int \mathrm{d}\mathbf{u}\mathrm{d}\mathbf{p}\exp\left\{-\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{u}\right\}\left\langle \mathbf{q}+\frac{\mathbf{u}}{2}\right| \frac{\hat{\rho}}{(2\pi\hbar)^f}\left|\mathbf{q}-\frac{\mathbf{u}}{2}\right\rangle \\ &= \int \mathrm{d}\mathbf{u}\left\langle \mathbf{q}+\frac{\mathbf{u}}{2}\right|\hat{\rho}\left|\mathbf{q}-\frac{\mathbf{u}}{2}\right\rangle \delta(\mathbf{u}) \\ &= \langle \mathbf{q}|\,\hat{\rho}\,|\mathbf{q}\rangle \\ &= \sum_i P_i\langle \mathbf{q}|\psi_i\rangle\langle\psi_i|\mathbf{q}\rangle \\ &= \sum_i P_i|\psi_i(\mathbf{q})|^2.\end{aligned}$$

For the special case of a pure state, $\hat{\rho} = |\psi\rangle\langle\psi|$,

$$\int \mathrm{d}\mathbf{p}W(\mathbf{p},\mathbf{q}) = |\psi(\mathbf{q})|^2.$$

⋆ *Momentum probability density.*

$$\begin{aligned}\int \mathrm{d}\mathbf{q}W(\mathbf{p},\mathbf{q}) &= \int \mathrm{d}\mathbf{w}\mathrm{d}\mathbf{q}\exp\left\{-\frac{\mathrm{i}}{\hbar}\mathbf{q}\cdot\mathbf{w}\right\}\left\langle \mathbf{p}+\frac{\mathbf{w}}{2}\right| \frac{\hat{\rho}}{(2\pi\hbar)^f}\left|\mathbf{p}-\frac{\mathbf{w}}{2}\right\rangle \\ &= \int \mathrm{d}\mathbf{w}\left\langle \mathbf{p}+\frac{\mathbf{w}}{2}\right|\hat{\rho}\left|\mathbf{p}-\frac{\mathbf{w}}{2}\right\rangle \delta(\mathbf{w}) \\ &= \langle \mathbf{p}|\,\hat{\rho}\,|\mathbf{p}\rangle \\ &= \sum_i P_i\langle \mathbf{p}|\psi_i\rangle\langle\psi_i|\mathbf{p}\rangle \\ &= \sum_i P_i|\psi_i(\mathbf{p})|^2.\end{aligned}$$

For the special case of a pure state, $\hat{\rho} = |\psi\rangle\langle\psi|$,

$$\int \mathrm{d}\mathbf{q}W(\mathbf{p},\mathbf{q}) = |\psi(\mathbf{p})|^2.$$

4. **Wigner function is bounded.**

Proof. For pure states, $\hat{\rho} = |\psi\rangle\langle\psi|$ and

$$W(\mathbf{p},\mathbf{q}) = \int \frac{\mathrm{d}\mathbf{u}}{(2\pi\hbar)^f}\exp\left\{-\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{u}\right\}\psi\left(\mathbf{q}+\frac{\mathbf{u}}{2}\right)\psi^*\left(\mathbf{q}-\frac{\mathbf{u}}{2}\right)$$

The Cauchy-Schwartz inequality says

$$\left|\int_a^b \mathrm{d}z f^*(z)g(z)\right| \leq \sqrt{\int_a^b \mathrm{d}z\,|f(z)|^2\,dz\int_a^b |g(z)|^2}.$$

By setting $a=-\infty, b=\infty, f=\psi\left(\mathbf{q}-\mathbf{u}/2\right), g=(2\pi\hbar)^{-f}\psi\left(\mathbf{q}+\mathbf{u}/2\right)e^{-\mathrm{i}\mathbf{p}\cdot\mathbf{u}/\hbar}$ we obtain

$$\int_{-\infty}^{\infty}\mathrm{d}\mathbf{u}\left|\psi\left(\mathbf{q}-\frac{\mathbf{u}}{2}\right)\right|^2=2^f,\qquad \frac{1}{(2\pi\hbar)^{2f}}\int_{-\infty}^{\infty}\mathrm{d}\mathbf{u}\left|\psi\left(\mathbf{q}+\frac{\mathbf{u}}{2}\right)\right|^2=\frac{2^f}{(2\pi\hbar)^{2f}}.$$

Thus,

$$|W(\mathbf{p},\mathbf{q})|=\left|\int\frac{\mathrm{d}\mathbf{u}}{(2\pi\hbar)^f}\exp\left\{-\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{u}\right\}\psi\left(\mathbf{q}+\frac{\mathbf{u}}{2}\right)\psi^*\left(\mathbf{q}-\frac{\mathbf{u}}{2}\right)\right|\le\sqrt{\left(\frac{1}{\pi\hbar}\right)^{2f}}.$$

Therefore,

$$|W(\mathbf{p},\mathbf{q})|\le\left(\frac{2}{h}\right)^f.$$

5. **The overlap of two Wigner functions is proportional to the inner product of the corresponding wave-functions.**

Proof.

$$\begin{aligned}&\int\mathrm{d}\mathbf{p}\mathrm{d}\mathbf{q}W_\psi(\mathbf{p},\mathbf{q})W_\phi(\mathbf{p},\mathbf{q})\\ &=\int\mathrm{d}\mathbf{u}\mathrm{d}\mathbf{v}\mathrm{d}\mathbf{p}\mathrm{d}\mathbf{q}\frac{e^{-\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot(\mathbf{u}+\mathbf{v})}}{(2\pi\hbar)^{2f}}\left\langle\mathbf{q}+\frac{\mathbf{u}}{2}\right|\hat\rho_\psi\left|\mathbf{q}-\frac{\mathbf{u}}{2}\right\rangle\left\langle\mathbf{q}+\frac{\mathbf{v}}{2}\right|\hat\rho_\phi\left|\mathbf{q}-\frac{\mathbf{v}}{2}\right\rangle\\ &=\int\frac{\mathrm{d}\mathbf{u}\mathrm{d}\mathbf{q}}{(2\pi\hbar)^f}\left\langle\mathbf{q}+\frac{\mathbf{u}}{2}\right|\hat\rho_\psi\left|\mathbf{q}-\frac{\mathbf{u}}{2}\right\rangle\left\langle\mathbf{q}-\frac{\mathbf{u}}{2}\right|\hat\rho_\phi\left|\mathbf{q}+\frac{\mathbf{u}}{2}\right\rangle\\ &=\int\frac{\mathrm{d}\mathbf{u}\mathrm{d}\mathbf{q}}{(2\pi\hbar)^f}\left[\psi\left(\mathbf{q}+\frac{\mathbf{u}}{2}\right)\phi^*\left(\mathbf{q}+\frac{\mathbf{u}}{2}\right)\right]\left[\phi\left(\mathbf{q}-\frac{\mathbf{u}}{2}\right)\psi^*\left(\mathbf{q}-\frac{\mathbf{u}}{2}\right)\right].\end{aligned}$$

Setting $\mathbf{Q_1}=\mathbf{q}+\mathbf{u}/2$ and $\mathbf{Q_2}=\mathbf{q}-\mathbf{u}/2$, then $d\mathbf{q}d\mathbf{u}=|J|d\mathbf{Q_1}d\mathbf{Q_2}=d\mathbf{Q_1}d\mathbf{Q_2}$ and

$$\begin{aligned}\int\mathrm{d}\mathbf{p}\mathrm{d}\mathbf{q}W_\psi(\mathbf{p},\mathbf{q})W_\phi(\mathbf{p},\mathbf{q})=&\frac{1}{h^f}\int\mathrm{d}\mathbf{Q_1}\left[\psi\left(\mathbf{Q_1}\right)\phi^*\left(\mathbf{Q_1}\right)\right]\\ &\times\int\mathrm{d}\mathbf{Q_2}\left[\phi\left(\mathbf{Q_2}\right)\psi^*\left(\mathbf{Q_2}\right)\right]\\ =&\frac{1}{h^f}\left|\langle\psi|\phi\rangle\right|^2.\end{aligned}$$

6. **Overlap for orthogonal wave-functions**

$$\text{If }\langle\psi|\phi\rangle=0\implies\int\mathrm{d}\mathbf{p}\mathrm{d}\mathbf{q}W_\psi(\mathbf{p},\mathbf{q})W_\phi(\mathbf{p},\mathbf{q})=0.$$

Proof. It is a direct consequence of property 5.

7. **Overlap of the Wigner function with itself**

$$\text{Since }\langle\psi|\psi\rangle=1\implies\int\mathrm{d}\mathbf{p}\mathrm{d}\mathbf{q}W^2(\mathbf{p},\mathbf{q})=\frac{1}{h^f}$$

Proof. It is a direct consequence of property 5.

8. **Translational behavior of the Wigner function.**

- ⋆ If $\psi(\mathbf{q}) \to \psi(\mathbf{q}-\mathbf{b})$ then $\mathrm{W}(\mathbf{p},\mathbf{q}) \to \mathrm{W}(\mathbf{p},\mathbf{q}-\mathbf{b})$.

  Proof. Let's consider a density operator $\hat{\rho} = \sum_i P_i \left|\psi_i\right\rangle \left\langle\psi_i\right|$, such that

$$
\begin{aligned}
W(\mathbf{p},\mathbf{q}) =& \int \mathrm{d}\mathbf{u} e^{-\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{u}} \left\langle \mathbf{q}+\frac{\mathbf{u}}{2}\right| \frac{\hat{\rho}}{(2\pi\hbar)^f} \left|\mathbf{q}-\frac{\mathbf{u}}{2}\right\rangle \\
=& \sum_i P_i \int \frac{\mathrm{d}\mathbf{u}}{(2\pi\hbar)^f} e^{-\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{u}} \psi_i\left(\mathbf{q}+\frac{\mathbf{u}}{2}\right) \psi_i^*\left(\mathbf{q}-\frac{\mathbf{u}}{2}\right).
\end{aligned}
$$

  Under the shift $\psi_i(\mathbf{q}) \to \psi_i(\mathbf{q}-\mathbf{b})$, we obtain

$$
\begin{aligned}
W(\mathbf{p},\mathbf{q}) \to & \sum_i P_i \int \frac{\mathrm{d}\mathbf{u}}{(2\pi\hbar)^f} e^{-\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{u}} \psi_i\left(\mathbf{q}-\mathbf{b}+\frac{\mathbf{u}}{2}\right) \psi_i^*\left(\mathbf{q}-\mathbf{b}-\frac{\mathbf{u}}{2}\right) \\
=& \int \mathrm{d}\mathbf{u} e^{-\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{u}} \left\langle (\mathbf{q}-\mathbf{b})+\frac{\mathbf{u}}{2}\right| \frac{\hat{\rho}}{(2\pi\hbar)^f} \left|(\mathbf{q}-\mathbf{b})-\frac{\mathbf{u}}{2}\right\rangle \\
=& W(\mathbf{p},\mathbf{q}-\mathbf{b}).
\end{aligned}
$$

- ⋆ If $\psi(\mathbf{q}) \to \psi(\mathbf{q}) \exp\left(\frac{i}{\hbar}\mathbf{q}\cdot\mathbf{p}'\right) \implies W(\mathbf{p},\mathbf{q}) \to W(\mathbf{p}-\mathbf{p}',\mathbf{q})$.

  Proof. Let's consider a density operator $\hat{\rho} = \sum_i P_i \left|\psi_i\right\rangle \left\langle\psi_i\right|$, such that

$$
W(\mathbf{p},\mathbf{q}) = \sum_i P_i \int \frac{\mathrm{d}\mathbf{u}}{(2\pi\hbar)^f} e^{-\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{u}} \psi_i\left(\mathbf{q}+\frac{\mathbf{u}}{2}\right) \psi_i^*\left(\mathbf{q}-\frac{\mathbf{u}}{2}\right).
$$

  Under the shift $\psi(\mathbf{q}) \to \psi(\mathbf{q}) \exp\left(\frac{i}{\hbar}\mathbf{q}\cdot\mathbf{p}'\right)$, we obtain

$$
\begin{aligned}
W(\mathbf{p},\mathbf{q}) \to & \sum_i P_i \int \frac{\mathrm{d}\mathbf{u}}{(2\pi\hbar)^f} e^{-\frac{\mathrm{i}}{\hbar}(\mathbf{p}-\mathbf{p}')\cdot\mathbf{u}} \psi_i\left(\mathbf{q}+\frac{\mathbf{u}}{2}\right) \psi_i^*\left(\mathbf{q}-\frac{\mathbf{u}}{2}\right) \\
=& \int \mathrm{d}\mathbf{u} e^{-\frac{\mathrm{i}}{\hbar}(\mathbf{p}-\mathbf{p}')\cdot\mathbf{u}} \left\langle \mathbf{q}+\frac{\mathbf{u}}{2}\right| \frac{\hat{\rho}}{(2\pi\hbar)^f} \left|\mathbf{q}-\frac{\mathbf{u}}{2}\right\rangle \\
=& W(\mathbf{p}-\mathbf{p}',\mathbf{q}).
\end{aligned}
$$

9. **Invariance of the Wigner function under time and space reflection**

- ⋆ If $\psi(\mathbf{q}) \to \psi(-\mathbf{q})$ then $\mathrm{W}(\mathbf{p},\mathbf{q}) \to \mathrm{W}(-\mathbf{p},-\mathbf{q})$.

  Proof.

$$
\begin{aligned}
W(\mathbf{p},\mathbf{q}) \to & \sum_i P_i \int \frac{\mathrm{d}\mathbf{u}}{(2\pi\hbar)^f} e^{-\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{u}} \psi_i\left(-\mathbf{q}-\frac{\mathbf{u}}{2}\right) \psi_i^*\left(-\mathbf{q}+\frac{\mathbf{u}}{2}\right) \\
=& \sum_i P_i \int \frac{\mathrm{d}\mathbf{Q}}{(2\pi\hbar)^f} e^{\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{Q}} \psi_i\left(-\mathbf{q}+\frac{\mathbf{Q}}{2}\right) \psi_i^*\left(-\mathbf{q}-\frac{\mathbf{Q}}{2}\right) \\
=& \sum_i P_i \int \frac{\mathrm{d}\mathbf{Q}}{(2\pi\hbar)^f} e^{-\frac{\mathrm{i}}{\hbar}(-\mathbf{p})\cdot\mathbf{Q}} \psi_i\left(-\mathbf{q}+\frac{\mathbf{Q}}{2}\right) \psi_i^*\left(-\mathbf{q}-\frac{\mathbf{Q}}{2}\right) \\
=& \int \mathrm{d}\mathbf{Q} e^{-\frac{\mathrm{i}}{\hbar}(-\mathbf{p})\cdot\mathbf{Q}} \left\langle (-\mathbf{q})+\frac{\mathbf{Q}}{2}\right| \frac{\hat{\rho}}{(2\pi\hbar)^f} \left|(-\mathbf{q})-\frac{\mathbf{Q}}{2}\right\rangle \\
=& W(-\mathbf{p},-\mathbf{q}).
\end{aligned}
$$

⋆ If $\psi(\mathbf{q}) \to [\psi(\mathbf{q})]^* \implies W(\mathbf{p},\mathbf{q}) \to W(-\mathbf{p},\mathbf{q})$.

Proof.

$$\begin{aligned}
W(\mathbf{p},\mathbf{q}) \to &\sum_i P_i \int \frac{\mathrm{d}\mathbf{u}}{(2\pi\hbar)^f} e^{-\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{u}} \psi_i^*\left(\mathbf{q}+\frac{\mathbf{u}}{2}\right)\psi_i\left(\mathbf{q}-\frac{\mathbf{u}}{2}\right) \\
=&\sum_i P_i \int \frac{\mathrm{d}\mathbf{Q}}{(2\pi\hbar)^f} e^{\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{Q}} \psi_i\left(\mathbf{q}+\frac{\mathbf{Q}}{2}\right)\psi_i^*\left(\mathbf{q}-\frac{\mathbf{Q}}{2}\right) \\
=&\sum_i P_i \int \frac{\mathrm{d}\mathbf{Q}}{(2\pi\hbar)^f} e^{-\frac{\mathrm{i}}{\hbar}(-\mathbf{p})\cdot\mathbf{Q}} \psi_i\left(\mathbf{q}+\frac{\mathbf{Q}}{2}\right)\psi_i^*\left(\mathbf{q}-\frac{\mathbf{Q}}{2}\right) \\
=&\int \mathrm{d}\mathbf{Q} e^{-\frac{\mathrm{i}}{\hbar}(-\mathbf{p})\cdot\mathbf{Q}} \left\langle \mathbf{q}+\frac{\mathbf{Q}}{2}\right| \frac{\hat{\rho}}{(2\pi\hbar)^f} \left|\mathbf{q}-\frac{\mathbf{Q}}{2}\right\rangle \\
=&W(-\mathbf{p},\mathbf{q}).
\end{aligned}$$

10. Expectation values.

⋆ $\langle f(\hat{\mathbf{q}})\rangle = \int \mathrm{d}\mathbf{p}\mathrm{d}\mathbf{q} f(\mathbf{q}) W(\mathbf{p},\mathbf{q})$.

Proof. The expectation value in standard Quantum mechanics is given by $\langle f(\hat{\mathbf{q}})\rangle = \langle\psi| f(\hat{\mathbf{q}}) |\psi\rangle$. On the other hand, in phase space quantum mechanics,

$$\begin{aligned}
\int \mathrm{d}\mathbf{p}\mathrm{d}\mathbf{q} f(\mathbf{q}) W(\mathbf{p},\mathbf{q}) =& \int \mathrm{d}\mathbf{u}\mathrm{d}\mathbf{q} f(\mathbf{q}) \left\langle \mathbf{q}+\frac{\mathbf{u}}{2}\right| \hat{\rho} \left|\mathbf{q}-\frac{\mathbf{u}}{2}\right\rangle \delta(\mathbf{u}) \\
=& \int \mathrm{d}\mathbf{q} f(\mathbf{q}) \langle\mathbf{q}|\hat{\rho}|\mathbf{q}\rangle \\
=& \int \mathrm{d}\mathbf{q} \psi(\mathbf{q}) f(\mathbf{q}) \psi^*(\mathbf{q}) \\
=&\langle f(\hat{\mathbf{q}})\rangle.
\end{aligned}$$

⋆ $\langle g(\hat{\mathbf{p}})\rangle = \int \mathrm{d}\mathbf{p}\mathrm{d}\mathbf{q} g(\mathbf{p}) W(\mathbf{p},\mathbf{q})$

Proof. Following the same lines as above,

$$\begin{aligned}
\int \mathrm{d}\mathbf{p}\mathrm{d}\mathbf{q} g(\mathbf{p}) W(\mathbf{p},\mathbf{q}) =& \int \mathrm{d}\mathbf{p}\mathrm{d}\mathbf{w} g(\mathbf{p}) \left\langle \mathbf{p}+\frac{\mathbf{w}}{2}\right| \hat{\rho} \left|\mathbf{p}-\frac{\mathbf{w}}{2}\right\rangle \delta(\mathbf{w}) \\
=& \int \mathrm{d}\mathbf{p} g(\mathbf{p}) \langle\mathbf{p}|\hat{\rho}|\mathbf{p}\rangle \\
=& \int \mathrm{d}\mathbf{p} \psi(\mathbf{p}) g(\mathbf{p}) \psi^*(\mathbf{p}) \\
=&\langle g(\hat{\mathbf{p}})\rangle.
\end{aligned}$$

⋆ $\langle \hat{H}(\hat{\mathbf{p}},\hat{\mathbf{q}})\rangle = \int \mathrm{d}\mathbf{p}\mathrm{d}\mathbf{q} H(\mathbf{p},\mathbf{q}) \mathrm{W}(\mathbf{p},\mathbf{q})$

Proof. It is a direct consequence of the linearity of the integral and the expectations proved previously.

11. Linearity of mixed states in phase space.

Proof. Let us consider a mixed quantum state $\hat{\rho} = \sum_i P_i \hat{\rho}_i = \sum_i P_i |\psi_i\rangle \langle\psi_i|$, then

$$\begin{aligned} W(\mathbf{p},\mathbf{q}) &= \int \mathrm{d}\mathbf{u} \exp\left\{-\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{u}\right\} \left\langle \mathbf{q}+\frac{\mathbf{u}}{2}\right| \frac{\hat{\rho}}{(2\pi\hbar)^f} \left|\mathbf{q}-\frac{\mathbf{u}}{2}\right\rangle \\ &= \sum_i P_i \int \mathrm{d}\mathbf{u} \exp\left\{-\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{u}\right\} \left\langle \mathbf{q}+\frac{\mathbf{u}}{2}\right| \frac{\hat{\rho}_i}{(2\pi\hbar)^f} \left|\mathbf{q}-\frac{\mathbf{u}}{2}\right\rangle \\ &= \sum_i P_i W_i(\mathbf{p},\mathbf{q}). \end{aligned}$$

12. **Wave function from the Wigner distribution**

$$\psi(\mathbf{q}) = \frac{1}{\psi^*(\mathbf{0})} \int \mathrm{d}\mathbf{p} \exp\left\{\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{q}\right\} W\left(\mathbf{p},\frac{\mathbf{q}}{2}\right).$$

Proof. For a pure state, $\hat{\rho} = |\psi\rangle \langle\psi|$, then

$$W\left(\mathbf{p},\frac{\mathbf{q}}{2}\right) = \frac{1}{(2\pi\hbar)^f} \int_{-\infty}^{\infty} \mathrm{d}\mathbf{u} \exp\left\{-\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{u}\right\} \psi\left(\frac{\mathbf{q}}{2}+\frac{\mathbf{u}}{2}\right) \psi^*\left(\frac{\mathbf{q}}{2}-\frac{\mathbf{u}}{2}\right)$$

Multiplying both sides by $e^{\mathrm{i}\mathbf{p}\cdot\mathbf{q}/\hbar}$ and taking the integral over the $\mathbf{p}$ variables we obtain

$$\begin{aligned} \int \mathrm{d}\mathbf{p} \exp\left\{\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{q}\right\} W\left(\mathbf{p},\frac{\mathbf{q}}{2}\right) &= \int_{-\infty}^{\infty} \mathrm{d}\mathbf{u}\psi\left(\frac{\mathbf{q}}{2}+\frac{\mathbf{u}}{2}\right) \psi^*\left(\frac{\mathbf{q}}{2}-\frac{\mathbf{u}}{2}\right) \delta(\mathbf{u}-\mathbf{q}) \\ &= \psi(\mathbf{q})\, \psi^*(\mathbf{0}). \end{aligned}$$

E.3 Properties of the Wigner propagator

The properties of the Wigner propagator depends upon the properties of the Weyl symbol of the unitary evolution operator. This weyl symbol is usually called Weyl propagator. Let us check a couple of simple properties of this object.

1. $U_{\mathrm{W}}(\mathbf{r},0) = 1$.

Proof. At initial time $t = 0$, $\hat{U} = \hat{1}$ and

$$\begin{aligned} U_{\mathrm{W}}(\mathbf{r},0) &= \int \mathrm{d}\mathbf{u} e^{-\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{u}} \left\langle \mathbf{q}+\frac{\mathbf{u}}{2}\right| \hat{U}(0) \left|\mathbf{q}-\frac{\mathbf{u}}{2}\right\rangle \\ &= \int \mathrm{d}\mathbf{u} e^{-\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{u}} \delta(\mathbf{u}) = 1. \end{aligned}$$

2. $U^*_{\mathrm{W}}(\mathbf{r},t) = U_{\mathrm{W}}(\mathbf{r},-t) = U^{-1}_{\mathrm{W}}(\mathbf{r},t)$.

Proof. We know that $\hat{U}^\dagger = \hat{U}^{-1}$, then,

$$\begin{aligned}
U_{\mathrm{W}}^*(\mathbf{r},t) =& \int \mathrm{d}\mathbf{u} e^{\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{u}} \left\langle \mathbf{q}-\frac{\mathbf{u}}{2}\right| \hat{U}^\dagger(t) \left|\mathbf{q}+\frac{\mathbf{u}}{2}\right\rangle \\
=& \int \mathrm{d}\mathbf{u} e^{\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{u}} \left\langle \mathbf{q}-\frac{\mathbf{u}}{2}\right| \hat{U}^{-1}(t) \left|\mathbf{q}+\frac{\mathbf{u}}{2}\right\rangle \\
=& \int \mathrm{d}\mathbf{v} e^{-\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{v}} \left\langle \mathbf{q}+\frac{\mathbf{v}}{2}\right| \hat{U}^{-1}(t) \left|\mathbf{q}-\frac{\mathbf{v}}{2}\right\rangle \\
=& U_{\mathrm{W}}^{-1}(\mathbf{r},t).
\end{aligned}$$

On the other hand

$$\begin{aligned}
U_{\mathrm{W}}(\mathbf{r},-t) =& \int \mathrm{d}\mathbf{v} e^{-\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{v}} \left\langle \mathbf{q}+\frac{\mathbf{v}}{2}\right| \hat{U}(-t) \left|\mathbf{q}-\frac{\mathbf{v}}{2}\right\rangle \\
=& \int \mathrm{d}\mathbf{v} e^{-\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{v}} \left\langle \mathbf{q}+\frac{\mathbf{v}}{2}\right| \hat{U}^{-1}(t) \left|\mathbf{q}-\frac{\mathbf{v}}{2}\right\rangle .
\end{aligned}$$

Therefore,

$$U_{\mathrm{W}}^*(\mathbf{r},t) = U_{\mathrm{W}}(\mathbf{r},-t) = U_{\mathrm{W}}^{-1}(\mathbf{r},t).$$

3. **$G_{\mathbf{W}}(\mathbf{r}'',0;\mathbf{r}',0) = \delta(\mathbf{r}''-\mathbf{r}')$.**

   Proof. By considering the definition of Wigner propagator,

$$\begin{aligned}
G_{\mathrm{W}}(\mathbf{r}'',t;\mathbf{r}',0) =& \frac{1}{(2\pi\hbar)^2}\int \mathrm{d}\tilde{\mathbf{r}} e^{\frac{\mathrm{i}}{\hbar}(\mathbf{r}'-\mathbf{r}'')\wedge\tilde{\mathbf{r}}} U_{\mathrm{W}}\left(\frac{\tilde{\mathbf{r}}'+\tilde{\mathbf{r}}''}{2}+\frac{\tilde{\mathbf{r}}}{2},t\right) \\
&\times U_{\mathrm{W}}^*\left(\frac{\tilde{\mathbf{r}}'+\tilde{\mathbf{r}}''}{2}-\frac{\tilde{\mathbf{r}}}{2},t\right),
\end{aligned}$$

   and the fact that at initial time $t=0$, $U_{\mathrm{W}}(\mathbf{r},0)=1$, then

$$G_{\mathrm{W}}(\mathbf{r}'',t;\mathbf{r}',0) = \frac{1}{(2\pi\hbar)^2}\int \mathrm{d}\tilde{\mathbf{r}} \exp\left[\frac{\mathrm{i}}{\hbar}(\mathbf{r}'-\mathbf{r}'')\wedge\tilde{\mathbf{r}}\right] = \delta(\mathbf{r}'-\mathbf{r}'').$$

4. **Wigner propagator is real**

   Proof. Since Wigner function is real, then

$$\begin{aligned}
W(\mathbf{r}'',t) =& \left[\int \mathrm{d}\mathbf{r}' G_{\mathrm{W}}(\mathbf{r}'',t;\mathbf{r}',0) W(\mathbf{r}',0)\right]^* \\
=& \int \mathrm{d}\mathbf{r}' G_{\mathrm{W}}^*(\mathbf{r}'',t;\mathbf{r}',0) W(\mathbf{r}',0) \\
=& \int \mathrm{d}\mathbf{r}' G_{\mathrm{W}}(\mathbf{r}'',t;\mathbf{r}',0) W(\mathbf{r}',0),
\end{aligned}$$

   therefore,

$$G_{\mathrm{W}}^*(\mathbf{r}'',t;\mathbf{r}',0) = G_{\mathrm{W}}(\mathbf{r}'',t;\mathbf{r}',0).$$

5. $G_{\mathrm{W}}(\mathbf{r}'',t;\mathbf{r}',0) = G_{\mathrm{W}}(\mathbf{r}',0;\mathbf{r}'',t) = G_{\mathrm{W}}(\mathbf{r}',-t;\mathbf{r}'',0)$.

Proof. Straightforward by application of property 2 in the Wigner propagator representation

$$G_{\mathrm{W}}(\mathbf{r}'', t; \mathbf{r}', 0) = \frac{1}{(2\pi\hbar)^2} \int \mathrm{d}\tilde{\mathbf{r}} e^{\frac{\mathrm{i}}{\hbar}(\mathbf{r}'-\mathbf{r}'')\wedge\tilde{\mathbf{r}}} U_{\mathrm{W}} \left(\frac{\tilde{\mathbf{r}}' + \tilde{\mathbf{r}}''}{2} + \frac{\tilde{\mathbf{r}}}{2}, t \right) U_{\mathrm{W}}^{*} \left(\frac{\tilde{\mathbf{r}}' + \tilde{\mathbf{r}}''}{2} - \frac{\tilde{\mathbf{r}}}{2}, t \right).$$

Appendix F

Phase transformation of the unitary Wigner propagator

By considering Eq. (2.54), we see that the phase of the propagator in Eq. (2.53) is a multivariate polynomial in α_0, β_0. This polynomial has mixed terms that prevent the direct integration into Airy functions. Hence, it is necessary to transform this phase into a new one suitable for the integration of the propagator. At this point one may wonder about the structure of such kind of transformations. The answer comes from the mathematical structure of the Airy function: As long as we seek for linear transformations we are able to maintain the cubic + linear term as we will see in the following.

To begin with, let us consider the polynomial

$$P_0(\alpha_0, \beta_0) = a\alpha_0^3 + b\alpha_0^2\beta_0 + c\alpha_0\beta_0^2 + d\beta_0^3 - \alpha_0 Q + \beta_0 P, \tag{F.1}$$

with coefficients a, b, c, d defined in Eq. (G.1) of Appendix G. From this polynomial we would like to go to a phase without mixed terms. To accomplish this objective, we propose the first linear transformation over this polynomial

$$\alpha_0 = \mu_1, \qquad \beta_0 = \nu_1 - \lambda_1\mu_1, \tag{F.2}$$

with the Jacobian satisfying $|J_1| = 1$, whereas the dimensionless parameter λ_1 will enable us to remove terms from P. By applying this transformation to P we obtain

$$\begin{aligned} P_1(\mu_1, \nu_1) = &- (Q + \lambda_1 P)\mu_1 + P\nu_1 + (a - \lambda_1 b + c\lambda_1^2 - d\lambda_1^3)\mu_1^3 \\ &+ (b - 2\lambda_1 c + 3d\lambda_1^2)\nu_1\mu_1^2 + (c - 3d\lambda_1)\mu_1\nu_1^2 + d\nu_1^3. \end{aligned} \tag{F.3}$$

With the purpose of removing from this phase the quadratic term in ν_1, we must impose the condition

$$\lambda_1 = \frac{c}{3d}. \tag{F.4}$$

Then, leaving λ_1 implicitly to get a simpler expression, the polynomial takes the form

$$P_1(\mu_1, \nu_1) = -(Q+\lambda_1 P)\mu + (b - 2\lambda_1 c + 3\lambda_1^2 d)\nu\mu^2 + (a - \lambda_1 b + \lambda_1^2 c - \lambda_1^3 d)\mu^3 + P\nu + d\nu^3. \tag{F.5}$$

From this expression we define the following relations among the coefficients

$$a_1 = a - \lambda_1 b + \lambda_1^2 c - \lambda_1^3 d, \qquad b_1 = b - 2\lambda_1 c + 3\lambda_1^2 d, \qquad d_1 = d. \tag{F.6}$$

Therefore,

$$P_1(\mu_1, \nu_1) = -(Q + \lambda_1 P)\mu_1 + P\nu_1 + a_1\mu_1^3 + b_1\nu_1\mu_1^2 + d_1\nu_1^3. \tag{F.7}$$

Following the same steps as above, we introduce a new transformation as

$$\mu_1 = \mu_2, \qquad \nu_1 = (\nu_2 - \lambda_2\mu_2), \tag{F.8}$$

with $|J_2| = 1$. Thus, the polynomial takes the new form

$$\begin{aligned} P_2(\mu_2, \nu_2) =& -(Q + \lambda_1 P + \lambda_2 P + 3d_1\lambda_2\nu_2^2)\mu_2 + (b_1 + 3\lambda_2^2 d_1)\nu_2\mu_2^2 \\ &+ (a_1 - \lambda_2 b_1 - \lambda_2^3 d_1)\mu_2^3 + P\nu_2 + d_1\nu_2^3. \end{aligned} \tag{F.9}$$

In order to eliminate the factor of μ_2^3 we solve for its coefficient. Once we do that, we obtain three solutions for the parameter λ_2. As long as the polynomial shall be real, we keep only the real solution given by

$$\begin{aligned} \lambda_2 =& \frac{1}{6^{2/3}}\left(-9a_1d_1^2 + \sqrt{3d_1^3(4b_1^3 + 27a_1^2 d_1)}\right)^{1/3} \\ &\times\left[-\frac{2^{1/3}}{d_1} + 2(3)^{1/3} b_1\left(-9a_1d_1^2 + \sqrt{3d_1^3(4b_1^3 + 27a_1^2 d_1)}\right)^{-2/3}\right]. \end{aligned} \tag{F.10}$$

By means of the new set of coefficients

$$b_2 = b_1 + 3\lambda_2^2 d_1, \qquad c_2 = -3d_1\lambda_2, \qquad d_2 = d_1. \tag{F.11}$$

the polynomial takes the new form

$$P_2(\mu_2, \nu_2) = -(Q + \lambda_1 P + \lambda_2 P)\mu_2 + c_2\nu_2^2\mu_2 + b_2\nu_2\mu_2^2 + P\nu_2 + d_2\nu_2^3. \tag{F.12}$$

Let us introduce here the third transformation defined by

$$\nu_2 = \nu_3, \qquad \mu_2 = (\mu_3 - \lambda_3\nu_3), \tag{F.13}$$

with $|J_3| = 1$. Then

$$\begin{aligned} P_3(\mu_3, \nu_3) =& \left(-Q - P(\lambda_1 + \lambda_2 - 1)\right)\mu_3 + (c_2\mu_3 - 2\lambda_3 b_2\mu_3)\nu_3^2 \\ &+ (d_2 - \lambda_3 c_2 + \lambda_3^2 b_2)\nu_3^3 + b_2\mu_3^2\nu_3. \end{aligned} \tag{F.14}$$

If we want to remove the quadratic term ν_3^2, the parameter λ_3 must be

$$\lambda_3 = \frac{c_2}{2b_2}, \tag{F.15}$$

Therefore, by defining the new set of coefficients

$$b_3 = b_2, \qquad d_3 = d_2 - \frac{c_2^2}{4b_2}, \tag{F.16}$$

we find that

$$\begin{aligned} P_3(\mu_3, \nu_3) =& -\left(Q + P(\lambda_1 + \lambda_2)\right)\mu_3 + d_3\nu_3^3 + b_3\mu_3^2\nu_3 \\ &+ \left(P[1 + \lambda_1\lambda_3 + \lambda_2\lambda_3] + \lambda_3 Q\right)\nu_3 \end{aligned} \tag{F.17}$$

Finally, we propose the last transformation as

$$\mu_3 = \frac{\nu_4 - \mu_4}{2\lambda_4}, \qquad \nu_3 = \frac{\nu_4 + \mu_4}{2}, \tag{F.18}$$

with $J_4 = (-2\lambda_4)^{-1}$. Then,

$$\begin{aligned} P_4(\mu_4, \nu_4) =& \left(\frac{d_3}{8} + \frac{b_3}{8\lambda_4^2}\right)\mu_4^3 + \left(\frac{3d_3}{8} - \frac{b_3}{8\lambda_4^2}\right)\mu_4^2\nu_4 \\ &+ \left(\frac{P}{2}\left[1 + \lambda_1\lambda_3 + \lambda_2\lambda_3 + \frac{\lambda_1}{\lambda_4} + \frac{\lambda_2}{\lambda_4}\right] + \frac{Q}{2}\left[\lambda_3 + \frac{1}{\lambda_4}\right]\right)\mu_4 \\ &+ \left(\frac{d_3}{8} + \frac{b_3}{8\lambda_4^2}\right)\nu_4^3 + \left(\frac{3d_3}{8} - \frac{b_3}{8\lambda_4^2}\right)\nu_4^2\mu_4 \\ &+ \left(\frac{P}{2}\left[1 + \lambda_1\lambda_3 + \lambda_2\lambda_3 - \frac{\lambda_1}{\lambda_4} - \frac{\lambda_2}{\lambda_4}\right] + \frac{Q}{2}\left[\lambda_3 - \frac{1}{\lambda_4}\right]\right)\nu_4. \end{aligned} \tag{F.19}$$

In order to eliminate the quadratic contribution in both variables, we have to impose the condition

$$\lambda_4 = \sqrt{\frac{b_3}{3d_3}}. \tag{F.20}$$

Then

$$P_4(\mu_4, \nu_4) = \frac{d_3}{2}\mu_4^3 + \left(\frac{P}{2}\left[1 + \lambda_1\lambda_3 + \lambda_2\lambda_3 + \frac{\lambda_1}{\lambda_4} + \frac{\lambda_2}{\lambda_4}\right] + \frac{Q}{2}\left[\lambda_3 + \frac{1}{\lambda_4}\right]\right)\mu_4 \tag{F.21}$$

$$+ \frac{d_3}{2}\nu_4^3 + \left(\frac{P}{2}\left[1 + \lambda_1\lambda_3 + \lambda_2\lambda_3 - \frac{\lambda_1}{\lambda_4} - \frac{\lambda_2}{\lambda_4}\right] + \frac{Q}{2}\left[\lambda_3 - \frac{1}{\lambda_4}\right]\right)\nu_4. \tag{F.22}$$

From this result, it is clear that the polynomial P_4 is now a function of the linear and cubic variables only. With the purpose of writing this result in a more compact way, we introduce the last set of definitions as

$$\rho = \frac{d_3}{2}, \qquad \chi = \frac{P}{2}\left[1 + \lambda_1\lambda_3 + \lambda_2\lambda_3\right] + \frac{Q}{2}\lambda_3, \qquad \xi = \frac{P}{2}\left[\frac{\lambda_1}{\lambda_4} + \frac{\lambda_2}{\lambda_4}\right] + \frac{Q}{2\lambda_4}. \tag{F.23}$$

Hence, the final form of the polynomial is

$$P_4(\mu_4, \nu_4) = \rho\mu_4^3 + (\chi + \xi)\mu_4 + \rho\nu_4^3 + (\chi - \xi)\nu_4. \tag{F.24}$$

In the same way, under the whole set of transformations, the total Jacobian change the measures as

$$d\alpha_0 d\beta_0 = |J_1 J_2 J_3 J_4|\ d\mu_4 d\nu_4 = (2\lambda_4)^{-1} d\mu_4 d\nu_4. \tag{F.25}$$

By using this into Eq. (2.53) we obtain

$$\begin{aligned} G(\breve{\mathbf{r}}'', t; \breve{\mathbf{r}}', 0) =& \int \frac{\mathrm{d}\alpha_0 \mathrm{d}\beta_0}{(2\pi)^2} \exp\left(\mathrm{i}\left[a\alpha_0^3 + b\alpha_0^2\beta_0 + c\alpha_0\beta_0^2 + d\beta_0^3 - \alpha_0 Q + \beta_0 P\right]\right) \\ =& \frac{1}{2\lambda_4(2\pi)^2} \int \mathrm{d}\mu_4 \mathrm{d}\nu_4 \exp\left(\mathrm{i}\left[\rho\mu_4^3 + (\chi+\xi)\,\mu_4 + \rho\nu_4^3 + (\chi-\xi)\,\nu_4\right]\right) \\ =& \frac{1}{2\lambda_4} \int_{-\infty}^{\infty} \frac{\mathrm{d}\mu_4}{2\pi} \exp\left(\mathrm{i}\left[\rho\mu_4^3 + (\chi+\xi)\,\mu_4\right]\right) \int_{-\infty}^{\infty} \frac{\mathrm{d}\nu_4}{2\pi} \exp\left(i\left[\rho\nu_4^3 + (\chi-\xi)\,\nu_4\right]\right) \\ =& \frac{1}{2\lambda_4} \int_0^{\infty} \frac{\mathrm{d}\mu_4}{\pi} \cos\left(\rho\mu_4^3 + (\chi+\xi)\,\mu_4\right) \int_0^{\infty} \frac{\mathrm{d}\nu_4}{\pi} \cos\left(\rho\nu_4^3 + (\chi-\xi)\,\nu_4\right). \end{aligned} \tag{F.26}$$

Thus, by means of the following integration

$$\begin{aligned} \int_0^{\infty} \frac{\mathrm{d}z}{\pi} \cos\left(rz^3 + sz\right) =& (3r)^{-1/3} \int_0^{\infty} \frac{\mathrm{d}z'}{\pi} \cos\left(\frac{[z']^3}{3} + s(3r)^{-1/3} z'\right) \\ =& \frac{1}{\sqrt[3]{3r}} \mathrm{Ai}\left(\frac{s}{\sqrt[3]{3r}}\right), \end{aligned} \tag{F.27}$$

we obtain the final propagator in Eq. (2.56).

Appendix G

Phase coefficients for the Fourier-space version of the propagator

G.1 First set of coefficients

When writing explicitly the Wigner propagator in Eq. (2.52) we have made an overall simplification in notation by means of the following auxiliary equations. They are completely independent of the system dynamics.

$$
\begin{aligned}
a &= \frac{1}{3}\int_0^t \mathrm{d}s\sigma(t')\sin^3(\theta), \qquad \text{(G.1)}\\
b &= \int_0^t \mathrm{d}s\sigma(t')\sin^2(\theta)\cos(\theta),\\
c &= \int_0^t \mathrm{d}s\sigma(t')\sin(\theta)\cos^2(\theta),\\
d &= \frac{1}{3}\int_0^t \mathrm{d}s\sigma(t')\cos^3(\theta),
\end{aligned}
$$

G.2 Second set of coefficients

When writing explicitly the Wigner propagator in Eq. (4.55) we have made an overall simplification in notation by means of the following auxiliary equations. Most of them depends upon the system dynamics, expressed in terms of its trajectory q_n and its quantum fluctuations $\tilde{q}_n$. This, in turn, implies that it is not possible to know them explicitly unless we have solved completely the dynamics of this DOF.

$$\begin{aligned}
I_1(t) &= \frac{1}{\hbar}\int_0^t \mathrm{d}s\Theta_j(s)\breve{\tilde{\mathsf{q}}}_j(s)\breve{\mathsf{q}}_j(s), \\
I_2(t) &= \frac{1}{\hbar}\int_0^t \mathrm{d}s \int_0^s \mathrm{d}u\Theta_j(s)\Theta_j(u)\sin\left[\theta_j(s)-\theta_j(u)\right]\breve{\tilde{\mathsf{q}}}_j(u)\breve{\mathsf{q}}_j(s), \\
I_3(s) &= \int_0^s \mathrm{d}u\Theta_j(u)\sin\left[\theta_j(s)-\theta_j(u)\right]\breve{\tilde{\mathsf{q}}}_j(u), \\
a_{1j}(t) &= \int_0^t \mathrm{d}s\Theta_j(s)\sin[\theta_j(s)]\breve{\mathsf{q}}_j(s), \\
a_{2j}(t) &= \int_0^t \mathrm{d}s\Theta_j(s)\cos[\theta_j(s)]\breve{\mathsf{q}}_j(s), \\
a_{3j}(t) &= \frac{1}{3}\int_0^t \mathrm{d}s\sigma_j(s)\sin^3[\theta_j(s)]), \\
a_{4j}(t) &= \int_0^t \mathrm{d}s\sigma_j(s)\sin^2[\theta_j(s)]\cos[\theta_j(s)], \\
a_{5j}(t) &= \int_0^t \mathrm{d}s\sigma_j(s)\sin[\theta_j(s)]\cos^2[\theta_j(s)], \\
a_{6j}(t) &= \frac{1}{3}\int_0^t \mathrm{d}s\sigma_j(s)\cos^3[\theta_j(s)], \\
a_{7j}(t) &= \frac{1}{\hbar}\int_0^t \mathrm{d}s\sigma_j(s)\sin^2(\theta_j)I_3(s), \\
a_{8j}(t) &= \frac{1}{\hbar}\int_0^t \mathrm{d}s\sigma_j(s)\cos^2(\theta_j)I_3(s), \\
a_{9j}(t) &= \frac{2}{\hbar}\int_0^t \mathrm{d}s\sigma_j(s)\sin(\theta_j)\cos(\theta_j)I_3(s), \\
a_{10j}(t) &= \frac{1}{\hbar^2}\int_0^t \mathrm{d}s\sigma_j(s)\sin[\theta_j(s)]I_3^2(s), \\
a_{11j}(t) &= \frac{1}{\hbar^2}\int_0^t \mathrm{d}s\sigma_j(s)\cos[\theta_j(s)]I_3^2(s), \\
a_{12j}(t) &= \frac{1}{3\hbar^3}\int_0^t \mathrm{d}s\sigma_j(s)I_3^3(s), \\
a_{13j}(t) &= \frac{1}{\hbar}\int_0^t \mathrm{d}s\sigma_j(s)\sin^2[\theta_j(s)]\breve{\tilde{\mathsf{q}}}_j(s), \\
a_{14j}(t) &= \frac{1}{\hbar}\int_0^t \mathrm{d}s\sigma_j(s)\cos^2[\theta_j(s)]\breve{\tilde{\mathsf{q}}}_j(s), \\
a_{15j}(t) &= \frac{2}{\hbar}\int_0^t \mathrm{d}s\sigma_j(s)\sin[\theta_j(s)]\cos[\theta_j(s)]\breve{\tilde{\mathsf{q}}}_j(s), \\
a_{16j}(t) &= \frac{2}{\hbar^2}\int_0^t \mathrm{d}s\sigma_j(s)\sin[\theta_j(s)]I_3(s)\breve{\tilde{\mathsf{q}}}_j(s), \\
a_{17j}(t) &= \frac{2}{\hbar^2}\int_0^t \mathrm{d}s\sigma_j(s)\cos[\theta_j(s)]I_3(s)\breve{\tilde{\mathsf{q}}}_j(s), \\
a_{18j}(t) &= \frac{1}{3\hbar^3}\int_0^t \mathrm{d}s\sigma_j(s)I_3^2(s)\breve{\tilde{\mathsf{q}}}_j(s),
\end{aligned} \tag{G.2}$$

$$a_{19j}(t) = \frac{1}{\hbar^2}\int_0^t \mathrm{d}s\sigma_j(s)\sin[\theta_j(s)]\breve{\mathsf{q}}_j^2(s), \quad \text{(G.3)}$$

$$a_{20j}(t) = \frac{1}{\hbar^2}\int_0^t \mathrm{d}s\sigma_j(s)\cos[\theta_j(s)]\breve{\mathsf{q}}_j^2(s),$$

$$a_{21j}(t) = \frac{1}{\hbar^3}\int_0^t \mathrm{d}s\sigma_j(s)I_3(s)\breve{\mathsf{q}}_j^2(s),$$

$$a_{22j}(t) = \frac{1}{\hbar^3}\int_0^t \mathrm{d}s\sigma_j(s)\breve{\mathsf{q}}_j^3(s)$$

G.3 Third set of coefficients

$$A_j(t) = a_{3j}(t) \qquad B_j(t) = a_{6j}(t), \qquad C_j(t) = a_{4j}(t), \qquad D_j(t) = a_{5j}(t), \quad \text{(G.4)}$$

$$E_j(t) = a_{13j}(t) - a_{7j}(t) \qquad F_j(t) = a_{14j}(t) - a_{8j}(t), \qquad G_j(t) = a_{15j}(t) - a_{9j}(t), \quad \text{(G.5)}$$

$$H_j(t) = -\mathbb{Q}_j - a_{1j}(t) + a_{10j}(t) - a_{16j}(t) + a_{19j}(t), \quad \text{(G.6)}$$

$$J_j(t) = \mathbb{P}_j - a_{2j}(t) + a_{11j}(t) - a_{17j}(t) + a_{20j}(t). \quad \text{(G.7)}$$

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