Università di Firenze, Università di Perugia, INdAM consorziate nel CIAFM

DOTTORATO DI RICERCA
IN MATEMATICA, INFORMATICA, STATISTICA

CURRICULUM IN MATEMATICA
CICLO XXXI

Sede amministrativa Università degli Studi di Firenze
Coordinatore Prof. Graziano Gentili

A Wigner Equation with Decoherence

Settore Scientifico Disciplinare MAT/07

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Anni 2015/2019

Acknowledgements

This is the place where saying thanks to my supporters.
They know for themselves, so it is truly better to avoid the risk of forgetting someone special.
Still, it is a real pleasure to say explicitly thanks to the faculty board and staff of the Firenze-Perugia-INdAM Doctoral School, Cohort XXXI, in particular to the coordinator Graziano Gentili and to the indelible memory of Carlo Casolo.
Among the Florentine Physical Mathematicians, Giovanni Frosali and Giovanni Borgioli merit an affectionate mention, whereas the major aknowledgement is addressed to my advisor Luigi Barletti for his endless patience and dedication. He has been demonstrating day by day, month by month, year by year, generosity and long-suffering understanding of the personality and the overall health situation of the writer, without lacking of expressing appreciation for the little (?) managed to build at work.
It is also dutiful to thank Paolo Bordone (Università di Modena e Reggio Emilia) and Lucio Demeio (Università Politecnica delle Marche) for the precious work done together about Wigner functions with finite coherence length. Thanks to my mathematical physics Italian mates and collegues, above all Marco Coco.

It is worth to recognize the importance of the opportunity offered by the Italian *Ministero degli Affari Esteri* and the French *Ministère de l'Europe et des Affaires étrangères* regarding the grant MAE-2018, which has financed the three months staying at the Institut de Mathématiques of the Paul Sabatier University in Toulouse, where it was possible to accomplish part of the work collaborating with the MIP Laboratoire guided by Claudia Negulescu. An acknowledgement goes to the INDAM-GNFM (Italian National Group for Mathematical Physics) for the numerous funding supports in these years, as well.

It would be desiderable that people could always have the opportunity to work in an organized place which might give them long term economic security, structures and stability. As decoherence teaches us, *the environment makes the difference and strongly influeces the state of the system.* Cheers me up.

Un pensiero
a Maria Cristina Naldini
e a Giuseppe Parrini

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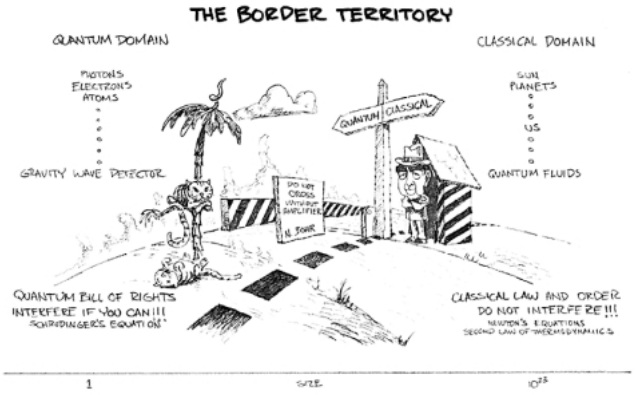
List of Abbreviations and Symbols

h	Planck constant, $\hbar \approx 6.626 \cdot 10^{-34} J/s$
$\hbar$	Reduced Planck constant, $\hbar = \frac{h}{2\pi} \approx 1.054 \cdot 10^{-34} J/s$
$\mathbb{N}$	Integers positive numbers
$\mathbb{R}$	Real Numebers
$\mathbb{R}^+$	Nonnegative real numbers
$\mathbb{C}$	Complex numbers
$\bar{z}$	Complex coniugate of $z \in \mathbb{C}$
$\Re(z)$	Real part of $z \in \mathbb{C}$
$\Im(z)$	Imaginary part of $z \in \mathbb{C}$
c_N	Constant $(2\pi)^{-N/2}$, $N \in \mathbb{N}$
$c_{N,\hbar}$	Constant $(2\pi\hbar)^{-N/2}$, $N \in \mathbb{N}$
$C^\infty(\Omega, \mathbb{C})$	Infinitely differentiable $\mathbb{C}$-valued functions on $\Omega \subseteq \mathbb{R}^N$
$C^k(\Omega, \mathbb{C})$	Continue $\mathbb{C}$-valued functions with continue derivatives till order $k \in \mathbb{N}$ over Ω
$C_0^\infty(\Omega, \mathbb{C})$	$C^\infty(\Omega, \mathbb{C})$ functions with compact support
$L^p(\Omega, \mathbb{C})$	Lebesgue Banach spaces of $\mathbb{C}$-valued functions on Ω, $1 \leq p \leq \infty$
$\|\cdot\|_p$	L^p Banach norm
$f *_p g$	Convolution product of the functions $f(x,p)$ and $g(x',p)$ w. r. t. the p variable
$\mathscr{F}$, $\mathscr{F}^{-1}$	Fourier transform on $L^2(\mathbb{R}^N)$ and its inverse transform
$\mathscr{F}_1$, ${\mathscr{F}_1}^{-1}$	Fourier transform on $L^2(\mathbb{R}^{2N})$ with respect to the first variable, and its inverse
$\mathscr{F}_2$, ${\mathscr{F}_2}^{-1}$	Fourier transform on $L^2(\mathbb{R}^{2N})$ with respect to the second variable, and its inverse
$\mathscr{W}$, $\mathscr{W}^{-1}$	Wigner transform on $L^2(\mathbb{R}^{2N})$ and it's inverse
$\mathscr{S}(\mathbb{R}^N)$	Schwartz space of rapidly decreasing functions on $\mathbb{R}^N$
$\mathscr{S}'(\mathbb{R}^N)$	Tempered distributions on $\mathbb{R}^N$
α m.i.	Multi-index α on $\mathbb{N}$
D^α	Multi-index alpha differential operator α
$(\mathscr{H}, \langle,\rangle, \|\|)$	Hilbert space on $\mathbb{C}$ with hermitian product $\langle,\rangle$ and induced norm $\|\|$
$\mathscr{L}(\mathscr{H})$	Linear space of bounded operators on $\mathscr{H}$
$\mathscr{D}(A)$	Domain of the operator A on the Hilbert space $\mathscr{H}$
$\mathscr{B}$	Borel σ-algebra in $\mathbb{R}$
Prob$\{O\}$	Probability of event O occurrance
E$\{X\}$	Expected value of random variable X

Chapter 1

Introduction



Quantum mechanics works exceedingly well in all practical applications. No example of conflict between its predictions and experiment is known. Without quantum physics, we could not explain the behaviour of the solids, the structure and function of DNA, the color of the stars, the action of lasers, or the properties of superfluids. Yet nearly a century after its inception, the debate about the relation of quantum physics to the familiar physical world continues. Why is a theory that seems to account with precision for everything we can measure still deemed lacking? [65]

One of the problems that Quantum Mechanics seems not to be able to answer is the explanation of the *quantum-to-classical* world transition.
Roughly speaking, why are the laws of Quantum Mechanics not visible to our eyes and vice versa? In this context, the quantum decoherence turns out to be a key concept, a topic which is worth to be studied thoroughly. Indeed, the interest towards the decoherence phenomenon has increased since the Eighties and its role has been recognized by material scientists and philosophers, beyond proper physicists [63,65,32].

The word *coherence* incorporates the globality of the quantum properties of a quantum system. *Decoherence* is the process of loss of quantum coherence [32,64]. It is properly a dynamic mechanism, entirely predictable on the basis of quantum evolution laws, responsible for the appearance of the classical behaviour of the particles (or disappearance of the quantum behaviour since the state of the systems becomes a statistical mixture) as a consequence of the interaction with the environment. As such, the decoherence phenomenon governs quantum-to-classical transition and it shapes our actual perception of the world. The theoretical and experimental study of decoherence processes is not only important for our understanding of fundamental physics, but it is also crucial for technological applications, such as quantum computers and spintronics [66], where quantum coherence must be preserved as long as possible. Nevertheless, decoherence is still lacking a rigorous description, where in particular we mean not a general overview, but at least a precise mathematical framing, and many attempts have been made in this direction, e.g. [22,2,18,15].

Furthermore, we would like to point out that quantum-to-classical regime transition due to decoherence is conceptually different from the semi-classical limit one. This last approach leans on the smallness of Planck's constant, i.e. $\hbar \longrightarrow 0$. Following [1] and [42], it is possible to list four main differences:

1. Decoherence regards systems which interact with an environment, namely *open quantum systems*;

2. Decoherence acts at the length-scale of the interference pattern, whereas a typical semi-classical procedure consists in evaluating a macroscopic observable on a fast oscillating probability distribution;

3. Decoherence is a dynamical effect which grows with time, while the semi-classical limit is also valid in a stationary picture;

4. From a qualitative point of view, $\hbar$ plays no role in the mechanism of decoherence, even if it must be said that, quantitatively, in many models of physical relevance the time-scale of the decoherence owes its shortness to the smallness of the Planck's constant.

In this work, we intend to present a model of dynamical quantum decoherence within the Wigner (phase-space) formulation of quantum mechanics [10], [34], [57], [50], [62]. In fact, due to its striking analogies with classical mechanics, the formulation of quantum mechanics in terms of Wigner functions is particularly suited to illustrate the quantum-to-classical regime transition. Of course,

this approach is not new and several important papers on this subject resort to (or, at least, mention) the Wigner formalism (see e.g. Refs.[5,13,32,49,58]). The novelty the reader may encounter here is that we start from a model for decoherence which is fairly general whenever the environment is viewed as a "gas" of particles of asymptotically small mass, with respect to the "heavy" particle undergoing decoherence. This model has been rigorously derived from the laws of quantum mechanics in Refs. [2,3], and, to this extent, our description can be considered as arising "from first principles". Moreover, other models (above all the Wigner-Fokker-Planck equation) can be recovered as particular cases of the general mechanism introduced here.
The thesis is organized as follows.
After a dutiful introduction to the mathematical basics of Quantum Mechanics, the Wigner phase space formulation of Quantum Mechanics is recalled because of the needs related to the model and the reasons presented above. In Chapter 3 the decoherence phenomenon, the Joos-Zeh models and the single-collision decoherence model analysed in Refs. [2,3] are briefly resumed. Then, we consider the case of many collisions, randomly distributed in time, and obtain the corresponding "mean field" limit model, which is then translated into the Wigner framework. The Wigner equation with decoherence is obtained in this way and is shown to be strictly related to other models of decoherence, such as the Wigner-Fokker-Planck equation [5,4,21,32] and the Jacoboni-Bordone Wigner function with finite coherence length [31]. We study the influence of the decoherence mechanism on the dynamics of macroscopic quantities, namely density, current and energy. About these contents you can refer to our recent work [8]. The last part (Chapter 5) is devoted to the issue of long-time asymptotics: the numerical investigation of a simple situation (i.e. the case of gaussian solutions) suggests that the correct long-time behaviour requires the addition of a Caldeira-Legget "quantum friction term" [13] and we draft some ideas on the general case. Finally, we draw some conclusions and discuss future perspectives. In the Appendix are collected the codes which have allowed to gain some didactic pictures and control the behaviour of the model, but, most of all, the results contained in Chapter 4, where our model is evinced to be indicated in an application of physical interest as a tunneling process in a decoherent environment. This part has been exposed at the 26^{th} International Conference on Transport Theory at La Sorbonne Université Pierre et Marie Curie Campus in Paris and is contained in a larger ongoing work.

Chapter 2

Basics of Quantum Mechanics & Quantum Mechanics in Phase Space

2.1 Mathematical background

Herewith are counted important basic prerequisites concerning Hilbert spaces and spectral theory of unbounded operators, as natural setting of Quantum Mechanics mathematical foundations, since when von Neumann himself has laid the groundwork for this formalism which, though some difficulties of a physical interpretation nature and the necessary extensions to the abstract algebras in order to adapt it to the quantum field theory, is still the landmark of the quantum paradigm description ([41], [39]).

2.1.1 Linear operators on Hilbert Spaces

Let recall some notations for the hermitian product. Then

Definition 1. Let V be a linear space on the field $\mathbb{C}$ of complex numbers.
A *hermitian product* is a $\mathbb{C}$-valued application $\langle \cdot, \cdot \rangle$ defined over $V \times V$ such that, for all $x, y, z \in V$ and $\lambda \in \mathbb{C}$, these properties hold:

1. $\langle x, x \rangle \geq 0$ and $\langle x, x \rangle = 0$ if and only if $x = 0$;
2. $\langle x + y, z \rangle = \langle x, z \rangle + \langle y, z \rangle$;
3. $\langle x, \lambda y \rangle = \lambda \langle x, y \rangle$;
4. $\langle x, y \rangle = \overline{\langle y, x \rangle}$.

Example 1. $\left(L^2(\mathbb{R}^N,\mathbb{C}),\|\|2\right)$ is a Hilbert Space with respect to the hermitian product given by

$$\langle\varphi,\psi\rangle = \int_{\mathbb{R}^N} \overline{\varphi(\xi)}\psi(\xi)\, d\xi, \tag{2.1}$$

for all $\varphi,\ \psi \in L^2(\mathbb{R}^N,\mathbb{C})$.

Although it may appear redundant, according to the writer, it is also necessary to clarify some operator definitions in the Hilbert spaces, so that the reader is aligned with the notations.

Definition 2. A *Hilbert space operator* $\mathscr{H}$ is a linear map

$$A\colon \mathscr{D}(A) \longrightarrow \mathscr{H},$$

where $\mathscr{D}(A)$ indicates the domain of operator A and it is the (maximal) vectorial subspace of $\mathscr{H}$ such that A is well-defined.

Let always suppose [1] $\mathscr{D}(A)$ is dense in $\mathscr{H}$ and A has closed extension.

Definition 3. An operator A on $\mathscr{H}$ is bounded (in symbols $A \in \mathscr{L}(\mathscr{H})$) if $\mathscr{D}(A) = \mathscr{H}$ and there exists $M \in \mathbb{R}^+$ such that

$$\|A\varphi\| \leq M\|\varphi\|, \qquad \text{for all } \varphi \in \mathscr{H}.$$

$\mathscr{L}(\mathscr{H})$ is a Banach space with respect to the operator norm defined as follows:

$$\|A\| = \inf_{0\neq\varphi\in\mathscr{H}} \frac{\|A\varphi\|}{\|\varphi\|}, \qquad A \in \mathscr{L}(\mathscr{H}). \tag{2.2}$$

Definition 4. Let A be an operator on $\mathscr{H}$ and let $\mathscr{D}(A^*)$ be the set of $\varphi \in \mathscr{H}$ for which there is a $\eta \in \mathscr{H}$ with

$$\langle\psi, A\varphi\rangle = \langle\eta,\psi\rangle, \qquad \text{for all } \psi \in \mathscr{D}(A).$$

For each such $\varphi \in \mathscr{D}(A^*)$, we define $A^*\varphi = \eta$. A^* is called the *adjoint* of A.

Definition 5. An operator A on $\mathscr{H}$ is said *symmetric* (or *hermitian*) if

$$\langle\psi, A\varphi\rangle = \langle A\psi,\varphi\rangle, \qquad \text{for all } \varphi,\psi \in \mathscr{D}(A). \tag{2.3}$$

We shall say that A is *self-adjoint* if it is symmetric and $\mathscr{D}(A) = \mathscr{D}(A^*)$. In this case $A = A^*$. For $A \in \mathscr{L}(\mathscr{H})$ the two definitions are equivalent.

[1] Rigorous motivations in [46], chap. VI

2.1.2 Hilbert-Schmidt and Trace Class Operators

We present some fundamental facts which regard Hilbert-Schmidt and Trace Class Operators. [46], [60].
The first result concerns the characterization of compact and self-adjoint operators on a Hilbert space and it represents the natural infinite dimension generalization of the spectral theorem for finite dimensional vectorial spaces.

Theorem 1 (Hilbert-Schmidt)**.** *Let $\mathscr{H}$ a Hilbert space and $A \in \mathscr{L}(\mathscr{H})$ a self-adjoint compact operator. Then there is a complete orthonormal system $\{\varphi_n\}_{n\in\mathbb{N}}$ for $\mathscr{H}$ such that, for $n \in \mathbb{N}$, $A\varphi_n = \lambda_n\varphi_n$. Besides the sequence $\{\lambda_n\}_{n\in\mathbb{N}} \subseteq \mathbb{R}$ tends to zero as $n \longrightarrow \infty$.*

Hence, every compact and self-adjoint operator $A \in \mathscr{L}(\mathscr{H})$ is such that there exist an orthonormal basis $\{\varphi_n\}_{n\in\mathbb{N}}$ and an infinitesimal real-valued sequence $\{\lambda_n\}_{n\in\mathbb{N}}$, such that

$$A\varphi = \sum_{n\in\mathbb{N}} \lambda_n \langle \varphi_n, \varphi\rangle \varphi_n, \quad \text{for all } \varphi \in \mathscr{H}, \tag{2.4}$$

where the convergence is in the $\mathscr{H}$ norm.

Definition 6. An operator B su $\mathscr{H}$ is said *positive* ($B \geq 0$) if for all $\psi \in \mathscr{D}(B)$ holds

$$\langle \psi, B\psi\rangle \geq 0. \tag{2.5}$$

Remark 1. Every positive and *bounded* operator $B \in \mathscr{L}(\mathscr{H})$ is self-adjoint. Indeed, for every $\psi \in \mathscr{H}$,

$$0 \leq \langle B\psi, \psi\rangle = \overline{\langle B\psi, \psi\rangle} = \langle \psi, B\psi\rangle.$$

Then, using the following equality[2]

$$4\langle \varphi, \psi\rangle = \left(\|\varphi+\psi\|^2 - \|\varphi-\psi\|^2\right) - i\left(\|\psi+i\psi\|^2 - \|\varphi-i\psi\|^2\right), \tag{2.6}$$

turns

$$\langle A\varphi, \psi\rangle = \langle \varphi, A\psi\rangle$$

for all $\varphi, \psi \in \mathscr{H}$, namely A is self-adjoint.

[2]Equation (2.6) is said *polarization identity* and represents, for $\mathbb{C}$ Hilbert spaces, a generalization of the *parallelogram rule* in $\mathbb{R}$ Hilbert spaces, tipically given by

$$2(\|\varphi\|^2 + \|\psi\|^2) = \|\varphi+\psi\| + \|\varphi-\psi\|$$

Remark 1 is no more true for operators which are not defined on the whole space. In particular, it is not true for$\mathbb{F}$-Hilbert Spaces where $\mathbb{F}$ is not $\mathbb{C}$ isomorphic field (then it is not true for $\mathbb{F}=\mathbb{R}$ either).
Besides, for all $A, B \in \mathscr{L}(\mathscr{H})$ we say that $A \geq B$ if and only if $A - B \geq 0$.

Remark 2. A positive (and self-adjoint) operator is certainly A^*A, which is defined for all $A \in \mathscr{L}(\mathscr{H})$ and is still a bounded operator. After all, for $\psi \in \mathscr{H}$, it holds

$$\langle A^*A\psi, \psi\rangle = \langle A\psi, (A^*)^*\psi\rangle = \langle A\psi, A\psi\rangle \geq 0.$$

For a positive operator we can define another operator, said *squared root operator*, as follows

Definition 7. Let $B \in \mathscr{L}(\mathscr{H})$, then $\sqrt{B}$ is the unique positive operator $Q \in \mathscr{L}(\mathscr{H})$ such that $Q^2 = B$.

Thanks to this concept it is possible to give a sense to the operator *module*

Definition 8. Let $A \in \mathscr{L}(\mathscr{H})$. The operator *module of* A is $|A| = \sqrt{A^*A}$.

Although the notation $|\cdot|$ looks familiar, it must not deceive: on one side, $|\lambda A| = |\lambda||A|$ is still valid for all $\lambda \in \mathbb{C}$, whereas on the other side properties like $|AB| = |A||B|$ nor $|A+B| \leq |A| + |B|$ are no more valid.

The following results concern compact operator and are fundamental to continue.

Theorem 2 (Canonical form for Compact Operators)**.** *Let $A \in \mathscr{L}(\mathscr{H})$ a compact operator on the Hilbert space $\mathscr{H}$. Then there exist two orthonormal system $\{\psi_n\}_{n\in\mathbb{N}}$, $\{\varphi_n\}_{n\in\mathbb{N}}$ (which are not necessarily different, not necessarily complete) and a real valued sequence $\{\lambda_n\}_{n\in\mathbb{N}} \subseteq \mathbb{R}^+$ such that, for all $\varphi \in \mathscr{H}$,*

$$A\varphi = \sum_{n\in\mathbb{N}} \lambda_n \langle \varphi, \psi_n\rangle \varphi_n.$$

The elements belonging to sequence $\{\lambda_n\}_{n\in\mathbb{N}}$ are said singular values of the compact operator A and they coincide with the eigenvalues of $|A|$.

Compact operators own good properties. Hilbert-Schmidt and Trace-class operators, which we are going to introduce, are compact operators.

Definition 9. Let $\mathscr{H}$ a separable Hilbert space and $\{\varphi_n\}_{n\in\mathbb{N}}$ orthonormal basis of $\mathscr{H}$. Let $A \in \mathscr{L}(\mathscr{H})$ positive.
The *trace* of A is[3]

$$\operatorname{tr} A = \sum_{n\in\mathbb{N}} \langle \varphi_n, A\varphi_n\rangle \in [0,\infty].$$

[3]independently from the choice of the $\mathscr{H}$ basis, provided orthonormal.

An operator $A \in \mathscr{L}(\mathscr{H})$ is said *trace class* (or *nuclear*) if and only if $\operatorname{tr}|A| < \infty$. We indicate the set of trace class operators on the Hilbert separable space $\mathscr{H}$ as $\mathscr{J}_1(\mathscr{H})$.

Trace class operators form a (bilateral) ideal of $\mathscr{L}(\mathscr{H})$ with respect to the adjoint. Besides, if equip with the norm

$$\|A\|_{\mathscr{J}_1} := \operatorname{tr}|A|, \tag{2.7}$$

$\mathscr{J}_1(\mathscr{H})$ it results to be a Banach space.

Theorem 3. *If $A \in \mathscr{J}_1$, then A is compact. if A is compact, then $A \in \mathscr{J}_1$ if and only if its singular values series converges.*

Definition 10. Let $\mathscr{H}$ a separable Hilbert space and $A \in \mathscr{L}(\mathscr{H})$.
A is said a *Hilbert-Schmidt* operator or, briefly, HS if

$$tr(A^*A) < \infty.$$

The set HS operators on $\mathscr{H}$ is denoted by $\mathscr{J}_2(\mathscr{H})$.

Similarly to $\mathscr{J}_1$, HS operators form *-ideal of $\mathscr{L}(\mathscr{H})$.
Moreover, for all $A, B \in \mathscr{J}_2$, the following relation between the norms is deduced

$$\langle A, B\rangle_2 := \sum_{n\in\mathbb{N}} \langle \varphi_n, A^*B\varphi_n\rangle. \tag{2.8}$$

This last definition is well posed, since (2.8) absolutely conserges and it is independent on the chosen orthonormal basis of $\mathscr{H}$, $\{\varphi_n\}_{n\in\mathbb{N}}$.
Equation 2.8 defines a hermitian product, thanks to which $\mathscr{J}_2$ is a Hilbert space in turn, with induced norm

$$\|A\|_{\mathrm{HS}} = \sqrt{\langle A, A\rangle_2} = \sqrt{\operatorname{tr}(A^*A)}. \tag{2.9}$$

Hence one has

$$\|A\| \le \|A\|_{\mathrm{HS}} \le \|A\|_{\mathscr{J}_1}. \tag{2.10}$$

and, consequently,

$$\mathscr{J}_1 \subseteq \mathscr{J}_2. \tag{2.11}$$

The space of $\mathscr{J}_2$ operators admits a functional space representation, in some specific cases.

Definition 11. Let $(M, d\mu)$ a measure space and $\varphi, \psi \in L^2(M, d\mu)$.

The function $\varphi \otimes \psi$ such that

$$(\varphi \otimes \psi)(x,y) = \varphi(x)\overline{\psi}(y), \qquad \forall\, x,y \in M, \tag{2.12}$$

is said *tensor product* of φ and ψ.

Hölder's theorem leads straithforwardly to the

Proposition 1. *If $(M,d\mu)$ is a measure space and $\varphi,\psi \in L^2(M,d\mu)$, then*

$$\varphi \otimes \psi \in L^2(M\times M, d\mu\otimes d\mu) \tag{2.13}$$

and

$$\|\varphi\otimes\psi\|_{L^2(M\times M)} = \|\varphi\|_2\|\psi\|_2. \tag{2.14}$$

Proposition 2. *Se $\{\varphi_n\}_{n\in\mathbb{N}}$ e $\{\psi_n\}_{n\in\mathbb{N}}$ are orthonormal basis $L^2(M,d\mu)$, then $\{\varphi_n\otimes\psi_m\}_{n,m\in\mathbb{N}}$ is an orthonormal basis $L^2(M\times M, d\mu\otimes d\mu)$.*

When $\mathscr{H} = L^2(\mathbb{R}^N)$, then a fundamental characterization subsists for $\mathscr{J}_2(\mathscr{H})$and provide a sufficient condition for compactness of integral operators.

Theorem 4 (Characterization of HS operators)**.** *Let $(M,d\mu)$ a measure space and $\mathscr{H} = L^2(M,d\mu)$. A bounded operator $A\in\mathscr{L}(\mathscr{H})$ is HS if and only if there is a function $\rho\in L^2(M\times M, d\mu\otimes d\mu)$ such that*

$$A\psi(x) = A_\rho\psi(x) := \int_M \rho(x,y)\psi(y)\,d\mu_y, \quad \text{for all } \psi\in\mathscr{H}.$$

The map which associates $\rho\in L^2(M\times M,d\mu\otimes d\mu)$ to $A_\rho\in\mathscr{J}_2(\mathscr{H})$ is an isometry between the two spaces.

This result authorizes to work effectively and directly with operator kernels. Since the last are functions it is possible to formulate evolution problems in the form of partial differential equations. Theorem 4 leads directly to the following statement

Corollario 5. *HS norm coincides with L^2 norm over $\mathbb{R}^{2N}$, that is if $A = A_\rho \in \mathscr{J}_2$ then*

$$\|A_\rho\|_{HS} = \|\rho\|_{L^2(\mathbb{R}^{2N})}. \tag{2.15}$$

Other proprerties regarding the fact that $\mathscr{J}_2(\mathscr{H})$ is an ideal of $\mathscr{L}(\mathscr{H})$ are easily translatable in terms of integral kernels.

Definition 12. Let $\rho,\eta\in L^2(\mathbb{R}^{2N})$. We define:

- $\rho \circ \eta \in L^2(\mathbb{R}^{2N})$ given by

$$(\rho \circ \eta)(x,y) = \int_{\mathbb{R}^N} \rho(x,z)\,\eta(z,y)\,dz, \quad \forall (x,y) \in \mathbb{R}^{2N}; \tag{2.16}$$

- $\rho^* \in L^2(\mathbb{R}^{2N})$ given by

$$\rho^*(x,y) = \overline{\rho(y,x)}, \quad \forall (x,y) \in \mathbb{R}^{2N}. \tag{2.17}$$

Proposition 3. *Let A_ρ, $A_\eta \in \mathscr{J}_2(\mathscr{H})$ be HS operators with kernels $\rho, \eta \in L^2(\mathbb{R}^{2N})$, respectively. Then*

- $A_\rho A_\eta = A_{\rho\circ\eta}$;
- $A_\rho^* = A_{\rho^*}$.

2.1.3 Density matrices

From HS operators, trace class operators inherit the characterization established by Theorem 4. Farther, they have the finite trace property.

In order to carry on quantum system analysis it is worth presenting a more exclusive class of operators included in $\mathscr{J}_1$ in turn. It is about the class of *density operators*, which play the role of the wave functions in the context of mixed states. For semplicity, let denote the separable Hilbert space $L^2(\mathbb{R}^N)$ with $\mathscr{H}$.

Definition 13. $A = A_\rho \in \mathscr{J}_1(\mathscr{H}) \subseteq \mathscr{J}_2(\mathscr{H})$ is said to be a *density operator* if it owns the following properties:

1. A is positive;
2. A has unitary trace[4].

The integral kernel ρ associated to the density operator is usually named *density matrix*.

Remark 3. Since a bounded positive operator is self-adjoint, then density operators are self-adjoint.

As consequence of Hilbert Schmidt Theorem 1 and Theorem 4, the following characterization holds for density operators.

[4] ore finite trace, taking for granted that it can be normalized playing with constants

Theorem 6. *An operator $A \in \mathscr{L}(\mathscr{H})$ is a density operator if and only if there exists a complete orthonormal system $\{\varphi_n\}_{n\in\mathbb{N}} \subseteq \mathscr{H}$ and a sequence $\{\lambda_n\}_{n\in\mathbb{N}} \subseteq \mathbb{R}^+$, with $\sum_{n\in\mathbb{N}} \lambda_n = 1$, such that*

$$A = \sum_{n\in\mathbb{N}} \lambda_n \varphi_n \otimes \varphi_n \tag{2.18}$$

and any φ_n is an eigenvector forA with eigenvalue $\lambda_n > 0$. Furthermore,

$$\|A\|_{HS} = \sum_{n\in\mathbb{N}} \lambda_n^2. \tag{2.19}$$

An immediate effect is the possibility to write $A = A_\rho \in \mathscr{J}_2(\mathscr{H})$ in this form

$$\rho(x,y) = \sum_{n\in\mathbb{N}} \lambda_n \overline{\varphi_n(x)} \varphi_n(y), \qquad (x,y) \in \mathbb{R}^{2N}, \tag{2.20}$$

and clearly

$$\|\rho\|_{L^2(\mathbb{R}^{2N})} = \sum_{n\in\mathbb{N}} \lambda_n^2. \tag{2.21}$$

2.1.4 The spectral theorem

Roughly speaking, the Spectral Theorem is the result known as the possibility to diagonalize a linear operator and is often stated by saying that a self-adjoint operator has an orthonormal basis of eigenvectors. The concept of diagonalization is relatively straightforward for operators on finite-dimensional vector spaces but, as seen so far, it requires some modification for operators on infinite-dimensional spaces. In general, the Spectral Theorem identifies a class of linear operators that can be modeled by multiplication operators. The most important application of this theorem is the possibility of defining a functional calculus. That is, given a function f defined on the spectrum of a proper operator A, we might define an operator $f(A)$. Here two fundamental results of operators analysis on separable Hilbert spaces are reported (for the demonstration we suggest referring to [46], sez. VIII.3). The first theorem provides sufficient conditions for an operator being seen as a multiplicative operator on an appropriate measure space. The second one allows to extend the functional calculus to operators. Indeed, thanks to this result, the one-parameter group e^{itA} is well-posed for all $t \in \mathbb{R}$ with an appropriate A.

Theorem 7 (Spectral Theorem, *Multiplicative operators form*)**.** *Let A be a self-adjoint operator on a separable Hilbert space $\mathscr{H}$ and domain $\mathscr{D}(A) \subseteq \mathscr{H}$. There is a finite measure space $(M, d\mu)$, a unitary operator $U\colon \mathscr{H} \longrightarrow L^2(M, d\mu)$ and*

a measurable function f on M with values in $\mathbb{R} \cup \{\pm\infty\}$, but finite almost everywhere, such that

- $\psi \in \mathscr{D}(A)$ *if and only if* $f(U)\psi \in L^2(M, d\mu)$;
- *if* $\varphi \in U(\mathscr{D}(A))$, *then* $UAU^{-1}\varphi = f\varphi$.

Theorem 8 (Spectral Theorem, *Functional calculus form*)**.** *Let A be a self-adjoint operator on a separable Hilbert space $\mathscr{H}$ and domain $\mathscr{D}(A) \subseteq \mathscr{H}$. There exists one and only one map $\Psi : \mathscr{B} \longrightarrow \mathscr{L}(\mathscr{H})$ such that*

1. Ψ *is a* **-algebraic homomorphism;*
2. $\|\Psi(f)\| \leq \infty, \quad$ *for all* $f \in \mathscr{B}$;
3. *if* $A\psi = \lambda\psi$, *then* $\Psi(f)\psi = f(\lambda)\psi \quad$, *for all* $\psi \in \mathscr{D}(A)$;
4. *if* $f \geq 0$, *then* $\Psi(f) \geq 0, \quad$ *for all* $f \in \mathscr{B}$.

This last version of the Spectral Theorem is very useful in the context of Quantum Mechanics axiomatization. In particular, it is exploited concurrently with the basic measurable functions, namely the characteristic (or indicator) functions, whose we recall the following

Definition 14. $\chi_B(\cdot)$ indicates the *indicator function* of the set B belonging to the σ-algebra $\mathscr{B}$ of the borelian sets of $\mathbb{R}$. In other words, for all $\xi \in \mathbb{R}$ it is defined as

$$\chi_B(\xi) = \begin{cases} 1 & \text{if } \xi \in B, \\ 0 & \text{if } \xi \in B, \end{cases} \tag{2.22}$$

2.2 Quantum Mechanics Axioms

The mathematical structure of Quantum Mechanics can be fairly resumed in a procedure (essentially due to Von Neumann and then revisited considering Gleason's Theorem) which moves from five fundamental axioms.

Let consider a quantum mechanics system $\mathscr{S}$ with $N \in \mathbb{N}$ degrees of freedom. Its quantum mathematical description is based on five postulates.

1. The (pure) physical states of S are represented by *wave functions*, namely functions ψ in the Hilbert space $\mathscr{H} = L^2(\mathbb{R}^N, \mathbb{C})$ such that $\|\psi\|_2 = 1$.
   In a wave function ψ we cannot find a direct physical meaning[5], but it contains the whole physical information which can be gathered for the system. The way to obtain this information is provided by the following two axioms

[5] $\mathscr{H}$ can be seen as the quantum equivalent of the classic phase space

2. Physical observable quanties (in short *the observables*) are represented by linear self-adjoint operators on $\mathscr{H}$. By means of a process called *quantization*, every observable G is associated to a linear symmetric operator
$$A = A_G \colon \mathscr{D}(A) \longrightarrow \mathscr{H}. \tag{2.23}$$
The eigenfunctions of A are called *eigenstates*. The corresponding eigenvalues form the *spectrum* of A.

3. Let $\mathscr{B}$ be the borel σ-algebra in $\mathbb{R}$ and let G be an observable. The experimental measurement of the observable G (to which operator A is associated) performed with the system in the state $\psi \in \mathscr{H}$, gives a random variable $X_{A,\psi}$ such that for any $B \in \mathscr{B}$
$$\mathrm{Prob}\{X_{A,\psi} \in B\} = \langle \chi_B(A)\psi\,, \psi\rangle. \tag{2.24}$$
Hence the expected value of the measurement is
$$\mathrm{E}\{X_{A,\psi}\} = \langle A\psi, \psi\rangle. \tag{2.25}$$
The possible measurable values of G are real values because $\overline{\langle \psi, A\psi\rangle} = \langle A\psi, \psi\rangle$, but thanks to symmetry $\langle A\psi, \psi\rangle = \langle \psi, A\psi\rangle$.
The wave function information has a probabilistic nature and this fact is intrinsic and never avoidable. It means that the result of a measurement is always affected by an error, even when the appliance has got an infinite precision.

4. Any measurement perturbs the state of the system. If the system S lies in the state ψ when a measurement of observable G is performed, the result is given by the eigenvalue $\lambda \in \mathbb{R}$, then the state of after the measurement is the corresponding eigenstate of A.

5. The evolution of S is subjected to the Schrödinger equation
$$i\hbar \frac{d}{dt}\psi(t) = H\psi(t), \qquad t \in \mathbb{R}, \tag{2.26}$$
in which H is the *Hamiltonian* operator, associated to the observable total Energy of S.
The evolution law is a deterministic law, even if the objects have a random nature:
$$\psi(t) = \mathrm{e}^{-\frac{i}{\hbar}(t-t_0)H}\psi_0. \tag{2.27}$$

We underline that thanks to the spectral theory (i.e. Theorem 8) it is possible to provide the import consistency rule

$$f(X_{A,\psi}) = X_{f(A),\psi}, \qquad f\colon \mathbb{R} \longrightarrow \mathbb{R}\mathscr{B}-\text{measurable},\ A \tag{2.28}$$

valid for a $\mathscr{B}$-measurable functions $f\colon \mathbb{R} \longrightarrow \mathbb{R}$ and a self-adjoint operator A on $\mathscr{H}$.

Before concluding this axiomatic part, it is necessary to spend some other words about *simultaneous* measurements of two or more observables[6] in order to make the second and the forth axioms more complete.
If $A_1, \dots, A_k$ are self-adjoint operators which commute pairwise, then it is possible to perform simultaneous measures with the system in a state ψ.
The result of the measure is a random vector

$$(X_{A_1,\psi}, \dots, X_{A_k,\psi})$$

such that

$$\text{Prob}\{(X_{A_1,\psi}, \dots, X_{A_k,\psi}) \in B_1 \times \cdots \times B_k\} = \langle \chi_{B_1}(A_1) \cdots \chi_{B_k}(A_k)\,\psi, \psi\rangle, \tag{2.29}$$

for all the plurirectangles $B = B_1 \times \cdots \times B_k \in \mathbb{R}^k$ where $B_1, \dots, B_k \in \mathscr{B}$ are borelian sets.

We reveal in advance that these postulates are undergoing to modifications to better suit the requirements of Statistical Quantum Mechanics.

2.3 Quantization and $\mathscr{W}^{-1}$ transform

How it is possible to assign a physical observable a self-adjoint operator so as to satisfy the second axiom? There is a specific process, known as *quantization*, which has been refining over years.

In Classic Mechanics an observable has a corresponding real-valued function[7] on the phase space $\gamma(q,p) = \gamma_G(q,p)$, said *classical symbol* of G (or briefly, *simbol* of G).

Definition 15. The quantization is a procedural rule which gives every symbol γ_G a self-adjoint operator $A_G = A_\gamma$ on $\mathscr{H} = L^2(\mathbb{R}^N)$.

[6] The simultaneity of the measurements of several observables is a very delicate issue. The fundamental [43] is recommended for details in the case of observables that do not switch two by two, i.e. of non-independent measures.

[7] More precisely: a field for vectorial quantities, a scalar function otherwise.

There are two fundamental quantization, related to two fundamental observables: *position* and *momentum*. These quantizations are postulated since suggested by the experience. The classical symbol of the observable *position* is

$$\gamma_1(q,p) = q \quad \text{corresponding to quantum operator} A_q,$$

whereas the classical symbol of the observable *momentum* is

$$\gamma_2(q,p) = p \quad \text{corresponding to quantum operator} A_p. \tag{2.30}$$

A_q and A_p are defined by

$$A_q\psi(x) = \psi(x)x, \qquad \psi(x) \in \mathscr{D}(A_q) \subseteq \mathscr{H}; \tag{2.31}$$

$$A_p\psi(x) = -i\hbar\nabla\psi(x), \qquad \psi(x) \in \mathscr{D}(A_p) \subseteq \mathscr{H}. \tag{2.32}$$

We may resume in the following scheme (2.33)

position	$\xrightarrow{\text{CM}}$	q	$\xrightarrow{\text{QM}}$	A_q:	$\mathscr{D}(A_q)$	$\longrightarrow$	$\mathscr{H}$
					$\psi(x)$	$\longrightarrow$	$x\psi(x)$
momentum	$\xrightarrow{\text{CM}}$	p	$\xrightarrow{\text{QM}}$	A_p:	$\mathscr{D}(A_p)$	$\longrightarrow$	$\mathscr{H}$
					$\psi(x)$	$\longrightarrow$	$-i\hbar\nabla_x\psi(x)$

(2.33)

where to each observable is associated a classical symbol as in the Classical Mechanics (CM) context and, then, a quantum operator by an appropriate quantization rule in the Quantum Mechanics (QM) framework.
The fundamental quantization (2.33) are consistent with the second postulate because operators A_q and A_p are self-adjoint. The domains $\mathscr{D}(A_q)$, $\mathscr{D}(A_p)$ coincide with the Sobolev space $W^{1,2}(L^2(\mathbb{R}^N))$ and the operator associated to momentum is the Fourier transform of the operator associated to position, meaning that

$$A_p\psi(x) = \mathscr{F}A_q\psi(x), \tag{2.34}$$

for any $\psi \in W^{1,2}(\mathbb{R}^N)$.
Since A_q (and A_p) components are pairwise commuting operators [8], the result

[8] Indeed, for $j = 1,\ldots,N$, the components A_{q_j} of A_q fulfils $A_{q_j}\psi(x) = x_j\psi(x)$, whereas the

of a measurement of the observable position is the random vector

$$(X_{A_{q_1},\psi},\dots,X_{A_{q_N},\psi})$$

which respects equality (2.29). Then, thanks to the spectral theorem, any component A_{q_j} is such that

$$\left[\chi_{B_j}\left(A_{q_j}\right)\right]\psi(x)=\chi_{B_j}\left(x_j\right)\psi(x),\qquad x\in\mathbb{R}^N,\ \psi\in\mathscr{H},\ B_j\in\mathscr{B}. \tag{2.35}$$

From this,

$$\begin{aligned}\text{Prob}\{X_{A_q,\psi}\in B_1\times\cdots\times B_N\}&=\langle\chi_{B_1}\left(A_{q_1}\right)\cdots\chi_{B_N}\left(A_{q_N}\right)\psi,\psi\rangle=\\&=\int\limits_{\mathbb{R}^N}\prod_{j=1}^{N}\chi_{B_j}\left(x_j\right)\psi(x)\overline{\psi(x)}\,dx=\\&=\int\limits_{\mathbb{R}^N}\chi_B\left(x\right)\psi(x)\overline{\psi(x)}\,dx=\\&=\int\limits_{B_1\cdots B_N}|\psi(x)|^2\,dx.\end{aligned} \tag{2.36}$$

So we have obtained again that *the squared module of a wave function represents the density of the random variable "position measurement"*. Notice that $X_{A_q,\psi}$ is absolutely continue with respect to the Lebesgue measure.
The following computation which determin the density of the random vector "measurement of momentum" are similar to the former ones at all, but they are possible only thanks to the invertibility of the Furier transform on $\mathscr{H}=L^2(\mathbb{R}^N)$. Since, for $x\in\mathbb{R}^N,\ j=1,\dots,N,\ \psi\in\mathscr{H}$

$$\mathscr{F}\left[\chi_{B_j}\left(A_{p_j}\right)\right]\mathscr{F}^{-1}\psi(x)=\left[\chi_{B_j}\left(A_{p_j}\right)\right]\psi(x)=\chi_{B_j}\left(p_j\right)\psi(x), \tag{2.37}$$

components A_{p_j} of A_p fulfils $A_{p_j}\psi(x)=-i\hbar\frac{\partial}{\partial x_j}\psi(x)$.

then

$$\begin{aligned}\text{Prob}\{X_{A_p,\psi} \in B_1 \times \cdots \times B_N\} &= \langle \chi_{B_1}(A_{p_1}) \cdots \chi_{B_k}(A_{p_N})\psi, \psi\rangle = \\ &= \langle \mathscr{F}\chi_{B_1}(A_{p_1})\mathscr{F}^{-1} \cdots \mathscr{F}\chi_{B_N}(A_{p_N})\mathscr{F}^{-1}\mathscr{F}\psi, \mathscr{F}\psi\rangle = \\ &= \int_{\mathbb{R}^N} \prod_{j=1}^{N} \chi_{B_j}(p_j)\,|(\mathscr{F}\psi)(p)|^2\,dp = \\ &= \int_{B_1 \cdots B_N} |\mathscr{F}\psi(p)|^2\,dp.\end{aligned} \tag{2.38}$$

Once again $X_{A_p,\psi}$ is absolutely continue with density $|\mathscr{F}\psi(p)|^2$.

2.3.1 Weyl quantization

Fundamental quantization represents the starting point for other observables quantizations. For instance, the symbol associated to the observable *kinetic energy* of a free particle with mass m is

$$\gamma(q,p) \equiv \gamma(p) = \frac{|p|^2}{2m}. \tag{2.39}$$

Thanks to the rule supplied by the Spectral Theorem, the operator associated to the symbol (2.39) is

$$A_{\gamma(p)} = \gamma(A_p), \tag{2.40}$$

namely

$$A_{\gamma(p)}\psi(x) = \gamma(A_p)\psi(x) = \gamma(-i\hbar\nabla)\psi(x) = \frac{1}{2m}|-i\hbar\nabla|^2\psi(x) = \frac{\hbar^2}{2m}\Delta\psi(x). \tag{2.41}$$

An analogous behaviour is the one one of q-depending symbols. hence the following quantization rule holds:

$$A_{\gamma_1(q)} = \gamma_1(A_r); \qquad A_{\gamma_2(p)} = \gamma_2(A_p). \tag{2.42}$$

Nevertheless, when the symbol γ depends on both the two variables some ambiguities may arise, since the rule is not 1-to-1. Let consider the symbol $\gamma(q,p) = q^2 p$ on $\mathbb{R}^2$, for instance. Its quantization might be

$$A_\gamma = {A_q}^2 A_p, \tag{2.43}$$

but also $\gamma(q,p) = qpq$, then

$$A_\gamma = A_q A_p A_q. \tag{2.44}$$

The problem is that A_q and A_p do not commute, thus (2.43) and (2.44) do not define the same operator.

Hermann Weyl formulated [55][9] a quantization rule which unties this ambiguity, still respectng the fundamental quantization sanctioned by (2.31), (2.32) and the spectral theorem with (2.42).
Weyl quantization is based on Weyl transform which we are going to outline very briefly to deepen it later then.

Definition 16. The Weyl quantization of the symbol $\gamma(q,p)$ is the operator

$$A_\gamma \colon \ \mathscr{H} \supseteq \mathscr{D}(A_\gamma) \ \longrightarrow \ \mathscr{H}$$

such that

$$A_\gamma \varphi(x) = c_{N,\hbar} \int\limits_{\mathbb{R}^N} \mathscr{W}^{-1}\varphi(y)\, \gamma(y,p)\, dy.$$

Of course this has a meaning only if the integral of the symbol does exist. It is shown (e.g. in [60]) that Weyl quantization is consistent with Quantum Mechanics postulates when classic symbols γ are in the Schwartz functions class $\mathscr{S}(\mathbb{R}^N_q \times \mathbb{R}^N_p)$ and consequently when $\gamma \in L^2(\mathbb{R}^N_q \times \mathbb{R}^N_p)$ (in these cases $A_\gamma \in \mathscr{L}(\mathscr{H})$, that is $\mathscr{H} = \mathscr{D}(A_\gamma)$), whilst the issue becomes more delicate when the symbols are in $L^p(\mathbb{R}^N_q \times \mathbb{R}^N_p)$ for other values of p. In [29] you can find a complete discussion about this issue of consistency between quantization rules and Quantum Mechanics axioms.

Remark 4. Let $\gamma \in L^2(\mathbb{R}^N_q \times \mathbb{R}^N_p)$. Then the operator A_γ is an integral operator with kernel $\mathscr{W}^{-1}\gamma$, where

Definition 17. The *Weyl transform* is the map

$$\begin{aligned} \mathscr{W}^{-1} \colon \ L^2(\mathbb{R}^N_q \times \mathbb{R}^N_p) \ &\longrightarrow \ L^2(\mathbb{R}^N_x \times \mathbb{R}^N_y) \\ \gamma(q,p) \ &\longrightarrow \ \int\limits_{\mathbb{R}^N} \gamma\left(\tfrac{x+y}{2}, p\right) e^{ip\frac{x-y}{\hbar}}\, dp \end{aligned} \tag{2.45}$$

The notation $\mathscr{W}^{-1}$ ensues from the fact that the Weyl transform is actually the inverse of another transform which we are more used to handling and which we are going to introduce soon: the Wigner transform $\mathscr{W}$.

[9] [55], original article in German language; [56], posthumous translation in English language.

Weyl quantization permits to "convert" a classic observable into a quantum one effectively. At the same time this rule raised many issues concerning interesting mathematical problems within pseudodifferential operators, for which a good reference is again a [60].
Is not true that every self-adjoint operator on $\mathscr{H}$ (i.e. quantum observable) owns a corresponding classical physical quantity. The typical example is given by the following operator.

Definition 18. Let $\psi \in \mathscr{H}$ be a quantum state. The *orthogonal projection* on the (closed) vectorial subspace Span$\{\psi\}$ is the operator $P_\psi \in \mathscr{L}(\mathscr{H})$ such that

$$P_\psi \varphi = \langle \varphi, \psi \rangle \psi ,$$

for all $\varphi \in \mathscr{H}$.

P_ψ is obviously positive and then self-adjoint, as bounded. Furthermore, $P_\psi^2 = P_\psi$, that is idempotent, and unitary ($\|P_\psi\| = 1$) and the possible eigenvalues are only two: 1 and 0. This means that the projection is a quantum observable which "measures", nay try out if the system lies in a state (1) or not (0). States and Projection are hence very strictly connected. This is the base for the Quantum Mechanics to develop.
To conclude, an important property which connects expectation of a measure and operator trace holds. Its proof is a simple application of Theorem 1.

Proposition 4. *Let A a bounded self-adjoint on $\mathscr{H}$ and let $\psi \in \mathscr{D}(A)$. Then*

$$\mathrm{E}\{X_A, \psi\} = \mathrm{tr}\,(P_\psi A). \tag{2.46}$$

Proof. A is a self-adjoint operator, so it can be represented as in (2.4), with the orthonormal basis $\{\varphi_n\}_{n\in\mathbb{N}}$ of $\mathscr{H}$. Then

$$\psi = \sum_{n\in\mathbb{N}} \langle \psi, \varphi_n \rangle \varphi_n .$$

Hence

$$\begin{aligned}
\mathrm{E}\{X_A, \psi\} &= \langle A\psi, \psi \rangle = \\
&= \sum_{n\in\mathbb{N}} \langle \psi, \varphi_n \rangle \langle A\varphi_n, \psi \rangle = \\
&= \sum_{n\in\mathbb{N}} \langle \psi, \varphi_n \rangle \lambda_n \langle \varphi_n, \psi \rangle = \\
&= \sum_{n\in\mathbb{N}} \langle P_\psi A\varphi_n, \varphi_n \rangle = \\
&= \mathrm{tr}\,(P_\psi A).
\end{aligned}$$

□

Let focus on one of the consequences of the Quantum Mechanics axiomatization, which will be example of the effects of decoherence on open quantum systems.

2.3.2 The Superposition Principle

Let consider a d-dimensional quantum system $\mathscr{S}$.
The pure states of the system are unitary elements of a Hilbert space

$$\mathscr{H} = L^2(\mathbb{R}^d, \mathbb{C})$$

with respect to the L^2 norm $||\cdot||_2$.

By linearity, if ψ_1, ψ_2 are possible states of $\mathscr{S}$ (i.e. elements of $\mathscr{H}$), then any other vector

$$\psi = \alpha\psi_1 + \beta\psi_2 \qquad \text{with } \alpha, \beta \in \mathbb{C} \text{ such that } ||\psi||_2 = 1 \tag{2.47}$$

is still a state of the system $\mathscr{S}$.
This fact is known as *superposition principle* and ψ as *superposition state*.
The probability density of the "new" state ψ is

$$|\psi|^2 = |\alpha|^2|\psi_1|^2 + |\beta|^2|\psi_2|^2 + 2\Re(\alpha\beta\psi_1\psi_2), \tag{2.48}$$

namely

$$|\psi|^2 = |\alpha|^2|\psi_1|^2 + |\beta|^2|\psi_2| + 2|\alpha\beta||\psi_1|^2|\psi_2|\cos(\vartheta_1 - \vartheta_2) \tag{2.49}$$

where $\psi_j = |\psi_j|e^{\imath\vartheta_j}$ $(j = 1, 2)$ as $\mathbb{C}$-valued functions. Thus, the probability density of the superposition of two wave functions is not simply given by the sum of the two wave functions densities, as it might be natural in Classical Mechanics, but it rather owns a *mixed term* (or *interference term*), which leads to the typical interference fringes of waves packets.

In the following example the probability density of two gaussian states is explicitly computed, as it will suit us later in the discussion.

Example 2. Let consider the superposition of two well-localised orthogonal wave packets ψ_1 and ψ_2 of a one-dimensional system.
According to an appropriate reference system, the first is centred in x_0 and it runs with p_H momentum:

$$\psi_1(x) = \frac{c}{\sqrt{\sigma\sqrt{\pi}}} e^{-\frac{(x+x_0)^2}{2\sigma^2} + \imath\frac{p_H}{\hbar}x}.$$

The second is symmetric with respect to the x axis and runs with opposite momentum:

$$\psi_2(x) = \frac{c}{\sqrt{\sigma\sqrt{\pi}}} e^{-\frac{(x-x_0)^2}{2\sigma^2} - \imath\frac{p_H}{\hbar}x}.$$

If Ψ is the balanced superposition of the two states

$$\Psi = \frac{1}{\sqrt{2}}\psi_1(x) + \frac{1}{\sqrt{2}}\psi_2(x)$$

then its associated probability density is given by

$$|\Psi(x)|^2 = \frac{c^2}{2}\left[|\psi_1(x)|^2 + |\psi_2(x)|^2 + 2\Re\,\psi_1(x)\bar{\psi}_2(x)\right]$$

where $c = 1 + exp\left\{-\left(\frac{x_0^2}{\sigma^2} + \frac{p_H^2\sigma^2}{\hbar^2}\right)\right\}$, so it is not simply the sum of the probability densities associated to the former states, as expected.

It leads to the presence of interference patterns among the two bumps, typical of wave phenomena. But why do not we notice this phenomenon at a macroscopic level of observation? Why classic distribution are superposed as a sum of distributions without a mixed term presence?

In order to answer this question by the means of Quantum Mechanics itself it is important to broaden the frame towards the purview of Statistical Quantum Mechanics. A quantum system is now seen as a part of a larger system. The last is then "traced out" (in a sense we will immediately clarify), pouring its properties as environment to the one we want to concentrate on.

2.4 Statistical Quantum Mechanics Axioms

Let consider a quantum system $\mathscr{S}'$ with N degrees of freedom.
If $\mathscr{S}$ is a subsystem of $\mathscr{S}'$ with d degrees of freedom and $d << N$ (i.e. a single particle in a gas of many others particles of the same type), it is possible to focus on system $\mathscr{S}$ behaviour, regretting system $\mathscr{S}'$ behaviour unless its influence over $\mathscr{S}$ itself.
First, a wave function $\Psi(x,\eta)$ for $\mathscr{S}'$ belongs to Hilbert space

$$\mathscr{H}' = L^2(R^d \times \mathbb{R}^{N-d}).$$

Thanks to Fubini's theorem, fixed $\eta \in \mathbb{R}^{N-d}$, then the function $\psi_\eta(x) = \Psi(x,\eta)$ is a wave function for system $\mathscr{S}$: $\psi_\eta \in \mathscr{H} = L^2(\mathbb{R}^d)$. Let A be (the operator associated to) an observable physical quantity which acts on Ψ only with

respect to variable $x \in \mathbb{R}^d$. Hence, it is an operator on space $\mathscr{H}'$, and also on space $\mathscr{H}$. Therefore, A is associated to a physical quantity proper of system $\mathscr{S}$. According to "classical" Quantum Mechanics Axioms, it turns out that the expected value of A, performed when $\mathscr{S}'$ lies in the state Ψ, is given by

$$\int_{\mathbb{R}^{N-d}} \mathrm{tr}\,(P_{\psi_\eta} A)\, d\eta = \mathrm{tr}\left(\int_{\mathbb{R}^{N-d}} P_{\psi_\eta}\, d\eta A \right). \tag{2.50}$$

We can define an operator $\hat{\rho}$ as

$$\hat{\rho}\psi = \int_{\mathbb{R}^{N-d}} P_{\psi_\eta}\psi\, d\eta, \quad \text{for all } \psi \in \mathscr{H}, \tag{2.51}$$

from which we deduc that $\mathrm{E}\{A\}$ is equal to $\mathrm{tr}\,(\hat{\rho} A)$.
the following result holds

Theorem 9. *The operator defined by* (2.51) *is a density operator on* $\mathscr{H}$ *with Hilbert-Schmidt integral kernel*

$$\rho(x,y) = \int_{\mathbb{R}^{M-N}} \Psi(x,\eta)\overline{\Psi(y,\eta)}\, d\eta.$$

In the light of these considerations, we are ready to formulate the axiomatics of Statistical Quantum Mechanics.

1. The *mixed states* of a quantum system $\mathscr{S}$ with wave functions in $\mathscr{H}$ are density operators on $\mathscr{H}$. A mixed state A_ρ is a *pure state* if there exixts a wave function $\psi \in \mathscr{H}$ such that $A_\rho = P_\psi$, namely such that $\rho(x,y) = \psi(x)\overline{\psi(y)}$. Thanks to 6 every mixed state can be seen as a convex (possibly infinite) combination of pure states.

2. The second axiom does not change and can be formulated as before.

3. The measurement of an observable A, performed with system in the state A_ρ is a random variable $X_{A,\rho}$ such that for all $B \in \mathscr{B}$

$$\mathrm{Prob}\{X_{A,\rho} \in B\} = \mathrm{tr}\left(A_\rho \chi_B(A)\right). \tag{2.52}$$

   This is a well posed definition for $X_{A,\rho}$ since $\imath B A$ inherits good properties from χ by means of the Spectral Theorem. Asking the finitude of the expected value of A is a more delicate issue, but not relevant for now

4. The evolution of the system according to the hamiltonian operator H obeys to the Quantum Liouville equation or, more in general to the *von Neumann equation*

$$i\hbar\frac{d}{dt}A_\rho = \left[H, A_\rho\right], \qquad t \in \mathbb{R}, \tag{2.53}$$

where the squared parenthesis indicate the commutator between the two operators[10], once an opportune domine is defined.

Equation (2.53) is the extended version of the Schrödinger equation for mixed states. Sometimes we will confuse the two names deliberately.

2.5 Wigner Formulation of Quantum Mechanics

Due to its striking analogies with classical mechanics, the formulation of quantum mechanics in terms of Wigner functions is particularly suited to describe the quantum-to-classical regime transition. This approach is not new and several important papers on this subject resort to (or, at least, mention) the Wigner formalism (see e.g. Refs. [5,13,32,49,58]). Therefore, we spend few words in order to introduce the Wigner transform and the related issues.

By the means of its homonymous transform, Eugene Wigner managed to obtain something very similar to a classic distribution function in the phase space from a mixed state and, in this way, to provide a representation of Quantum Mechanics which might take advantage of the Classical (Statistical) Mechanics basics.

To follow this path, it is worth to consider operator kernels for mixed states which are nothing but functions in $L^2(\mathbb{R}^N_x \times \mathbb{R}^N_y)$, as we have seen in the previous section.

2.5.1 The Wigner transform

Let define the already mentioned Wigner transform, which associates a L_2 function in the phase-space to a HS kernel, namely $\rho \in L^2(\mathbb{R}^N_x \times \mathbb{R}^N_y)$ (the phase-space function can be seen a kernel of an integral operator over $L^2(\mathbb{R}^N_q)$).

Definition 19. Let consider the map

$$\mathscr{R}\colon\ L^2(\mathbb{R}^N_x \times \mathbb{R}^N_y) \longrightarrow L^2(\mathbb{R}^N_q \times \mathbb{R}^N_\xi), \tag{2.54}$$

[10] Let A, B two operators on $\mathscr{H}$, then $[A,B] := AB - BA$ is an operator on $\mathscr{H}$

such that

$$(\mathscr{R}\rho)(q,\xi) = \rho(q+\frac{\hbar}{2}\xi, q-\frac{\hbar}{2}\xi), \qquad \rho(x,y) \in L^2(\mathbb{R}^N_x \times \mathbb{R}^N_y). \tag{2.55}$$

This is nothing but the map corresponding to variables change

$$(x,y) \longleftrightarrow (q,p)$$

given by

$$\begin{cases} q = \dfrac{x+y}{2}, \\ \xi = \dfrac{x-y}{\hbar}. \end{cases} \tag{2.56}$$

Up to $\hbar^{-N}$, i.e. less than the jacobian of the transform, $\mathscr{R}$ is a unitary operator from $L^2(\mathbb{R}^N_x \times \mathbb{R}^N_y)$ to $L^2(\mathbb{R}^N_q \times \mathbb{R}^N_\xi)$.

Let $c_N = \dfrac{1}{\sqrt{(2\pi)^N}}$ and $c_{N,\hbar} = \dfrac{1}{(2\pi\hbar)^N}$. The map

$$\mathscr{F}_2 \colon L^2(\mathbb{R}^N_q \times \mathbb{R}^N_\xi) \longrightarrow L^2(\mathbb{R}^N_q \times \mathbb{R}^N_p)$$

such that

$$(\mathscr{F}_2 g)(q,p) = c_N^2 \int_{\mathbb{R}^N} g(q,\xi) e^{-ip\cdot\xi}\, d\xi, \tag{2.57}$$

is the Fourier transform with respect to the variable ξ for $g(q,\xi)$ (up to the normalization constant c_N). The *Plancharel's idenity*,

$$\langle \mathscr{F}_2 g_1, \mathscr{F}_2 g_2 \rangle = c_N^2 \langle g_1, g_2 \rangle, \tag{2.58}$$

is then still valid for every $g_1, g_2 \in L^2(\mathbb{R}^N_q \times \mathbb{R}^N_\xi)$.

The *Wigner transform* $\mathscr{W}$ is the composition of $\mathscr{F}_2$ and $\mathscr{R}$, namely

$$\mathscr{W} = \mathscr{F}_2\mathscr{R} \colon L^2(\mathbb{R}^N_x \times \mathbb{R}^N_y) \longrightarrow L^2(\mathbb{R}^N_q \times \mathbb{R}^N_p)$$

such that, for every $\rho \in L^2(\mathbb{R}^N_x \times \mathbb{R}^N_y)$,

$$\begin{aligned} (\mathscr{W}\rho)(q,p) &= c_N^2 \int_{\mathbb{R}^N} \rho(q+\frac{\hbar}{2}\xi, q-\frac{\hbar}{2}\xi) e^{-ip\cdot\xi}\, d\xi = \\ &= c_{N,\hbar} \int_{\mathbb{R}^N} \rho(q+\frac{y}{2}, q-\frac{y}{2}) e^{-ip\cdot\frac{y}{\hbar}}\, dy. \end{aligned} \tag{2.59}$$

Thanks to (2.58) and up to $c_{N,\hbar}$, $\mathscr{W}$ defines an isometry of $L^2(\mathbb{R}^N_x \times \mathbb{R}^N_y)$ and $L^2(\mathbb{R}^N_q \times \mathbb{R}^N_p)$. Indeed it is invertible and its inverse transform is the one we have

met talking about quantization. We refer to Weyl transform $\mathscr{W}^{-1}$. Hence

$$\mathscr{W}^{-1} = \mathscr{R}^{-1}\mathscr{F}_2^{-1},$$

where, for $g \in L^2(\mathbb{R}^N_q \times \mathbb{R}^N_\xi)$,

$$(\mathscr{R}^{-1}g)(x,y) = g(\frac{x+y}{2}, \frac{x-y}{h}),$$

whereas for $f \in L^2(\mathbb{R}^N_q \times \mathbb{R}^N_p)$,

$$(\mathscr{F}_2^{-1}f)(q,\xi) = \int_{\mathbb{R}^N} f(q,p)e^{ip\cdot\xi}dp.$$

More explicitly,

$$\mathscr{W}^{-1}\colon\ L^2(\mathbb{R}^N_q \times \mathbb{R}^N_p) \longrightarrow L^2(\mathbb{R}^N_x \times \mathbb{R}^N_y),$$

is such that for every $f \in L^2(\mathbb{R}^N qp)$

$$\mathscr{W}^{-1}f(q,p) = \int\limits_{\mathbb{R}^N} f\left(\frac{x+y}{2}, p\right) e^{ip\frac{x-y}{\hbar}}\, dp. \tag{2.60}$$

From Definition 19 and the Fourier Transform properties a very simple but useful fact follows.

Proposition 5. [*Moyal-Weyl–Groenewold product*] *Let $\rho_1(x,y)$, $\rho_2(x,y)$ be two functions in $L^2(\mathbb{R}^N_x \times \mathbb{R}^N_y)$ and let $f_1(q,p) = \mathscr{W}(\rho_1)$, $f_2(q,p) = \mathscr{W}(\rho_2)$ be their respective Wigner transform in $L^2(\mathbb{R}^N_q \times \mathbb{R}^N_p)$. Then*

$$\mathscr{W}(\rho_1\rho_2) = f_1 *_p f_2 \tag{2.61}$$

where $*_p$ indicates the convolution with respect to the only variable p, i.e.

$$(f_1 *_p f_2)(q,p) = \int_{\mathbb{R}^N} f_1(q,p-p')f_2(q,p')\,dp'. \tag{2.62}$$

The Wigner transform becomes particularly of interest when it is not simply applied to a function in $L^2(\mathbb{R}^N_x \times \mathbb{R}^N_y)$.

Definition 20. A *physical Wigner function* is the Wigner transform of a density matrix.

Note that as well as a density matrix $\rho(x,y)$ has the dimensions of a density in the positions space, its Wigner transform has the dimensions of a density in the phase space.

Remark 5. In this definitional part (see 2.54) we set $\mathscr{R}$ as a map of $L^2(\mathbb{R}^N_x \times \mathbb{R}^N_y)$ in $L^2(\mathbb{R}^N_q \times \mathbb{R}^N_\xi)$. In other terms we distinguished the "quantum" position variable x from the "phase space" position variable q. This is an excess of zeal which will not occur in the following chapters: we will not differentiate the two variables, naming both x.

2.5.2 Characterization of physical Wigner functions

What is the relation between a density matrix and its Wigner function?

Let $\psi \in L^2(\mathbb{R}^N_x)$ and let $\Psi(x,y) = \psi \otimes \psi$ be the corresponding pure state. We can indicate with $w_\psi = \mathscr{W}\Psi(x,y)$ its Wigner transform and immediately observe that w_ψ is a physical Wigner function, because pure states are density matrices. This can be seen as the fundamental "wignerization", since mixed states are (infinite) convex combination of pure states.

Referring to [37] and [10] it is convenient to resume in the following theorem a characterization for physical Wigner functions. From now on, the angular parenthesis $\langle , \rangle$ will indicate the hermitian product on $L^2(\mathbb{R}^N_x \times \mathbb{R}^N_y)$ as well as on $L^2(\mathbb{R}^N_q \times \mathbb{R}^N_p)$. They will still denote the hermitian product on $\mathscr{H}$.

Theorem 10. *Let $A_\rho \in \mathscr{J}_2(\mathscr{H})$ and $w(q,p) = \mathscr{W}\rho$. Hence*

1. *The following are equivalent:*
   - *(a)* $w(q,p) \in \mathbb{R}$;
   - *(b)* A_ρ *is self-adjoint;*
   - *(c)* $\rho(x,y) = \overline{\rho(y,x)}$.
2. *The following are equivalent:*
   - *(a)* $\int_{\mathbb{R}^N_q \times \mathbb{R}^N_p} w(q,p)\, dq\, dp = 1$;
   - *(b)* $\int_{\mathbb{R}^N} \rho(x,x)\, dx = 1$;
   - *(c)* $tr\, A_\rho = 1$.
3. *The following are equivalent:*
   - *(a)* A_ρ *is positive;*
   - *(b)* $\langle \rho, \psi(x)\overline{\psi}(y)\rangle \geq 0$;
   - *(c)* $\langle w, w_\psi\rangle \geq 0$, *for every* $\psi \in L^2(\mathbb{R}^N_x)$.

The bijections established by Theorem 10 can be moderately extended. In the following proposition a connection among trace properties of the operator and integrability of the kernel Wigner transform are set.

Proposition 6. *Let $\rho \in L^2(\mathbb{R}^N_x \times \mathbb{R}^N_y)$ be the kernel of a Hilbert-Schmidt positive operator A_ρ. $f(q,p) = \mathscr{W}\rho \in L^1(\mathbb{R}^N_q \times \mathbb{R}^N_p)$ if and only if $A_\rho \in \mathscr{J}_1(\mathscr{H})$.*

Proof. A_ρ is positive (and self-adjoint), then there exists an orthonormal complete system $\{\psi_n\}_{n\in\mathbb{N}} \in \mathscr{H}$ and a sequence $\{\lambda_n\}_{n\in\mathbb{N}} \in \mathbb{R}^+$, such that

$$\rho(x,y) = \sum_{n\in\mathbb{N}} \lambda_n \psi \otimes \psi.$$

Thus,

$$\begin{aligned} \operatorname{tr}|A_\rho| = \sum_{n\in\mathbb{N}} |\lambda_n| = \sum_{n\in\mathbb{N}} \lambda_n = \sum_{n\in\mathbb{N}} \lambda_n \int_{\mathbb{R}^N} \psi_n(x)\bar{\psi}_n(x)\,dx = \\ = \int_{\mathbb{R}^N} \rho(x,x)\,dx = (\mathscr{W}^{-1}f)(x,x) = \int_{\mathbb{R}^{2N}} f(x,p)\,dp\,dx. \end{aligned} \tag{2.63}$$

□

Remark 6. The step (2.63) make possible to point out the following remarkable identy

$$\rho(x,x) = \int_{\mathbb{R}^N} f(x,p)\,dp, \qquad \text{per quasi ogni } x \in \mathbb{R}^N. \tag{2.64}$$

Another important fact concerning Wigner function is the link with symbols

Proposition 7. *Let $\rho(x,y) \in L^2(\mathbb{R}^N_x \times \mathbb{R}^N_y)$ be a density matrix and let $w(q,p)$ be its Wigner function. If A_γ is the Weyl quantization of $\gamma(q,p)$ s.t. $A_\rho A_\gamma \in \mathscr{J}_1(\mathscr{H})$, then*

$$\operatorname{tr}(A_\rho A_\gamma) = \int_{\mathbb{R}^{2N}} \gamma(q,p)\,w(q,p)\,dq\,dp. \tag{2.65}$$

From this and (2.50), equation (2.65) expresses the expectation of the measure of the quantum observable associated to the classical symbol γ in the Wigner frame. Note the strong analogy with Classical Mechanics: looking at w as phase space distribution function then the expected value of γ is given exactly by the integral over$\mathbb{R}^N_q \times \mathbb{R}^N_p$ of the product $w\gamma$. But w stands out from a classical distribution: even if w is physical, Theorem 10 assures its realty, not its positiveness.

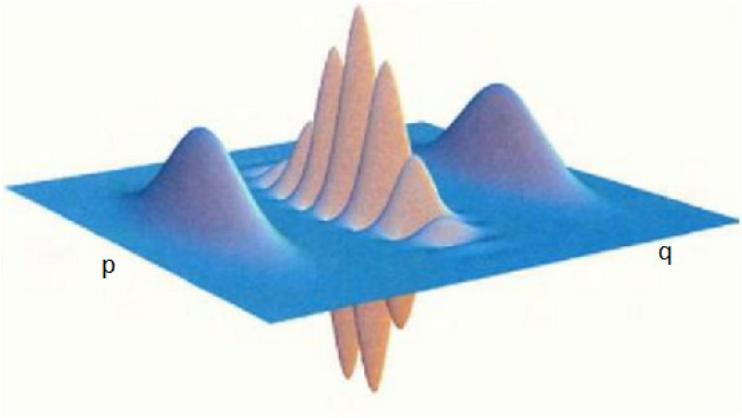


Figure 2.1: From [62]. It represents the Wigner transform $w(q,p)$ of the state $\rho(x,y) = \psi(x)\bar{\psi(y)}$ with $\psi(x) = \frac{1}{c}\{e^{-\frac{(x+a)^2}{2}} + e^{-\frac{(x-a)^2}{2}}\}$ and $c = \sqrt{2\sqrt{\pi}(1-e^{-a^2})}$. The parameter in the picture is $a = 6$. Note the superposition of two gaussian states and the presence of strong fluctuations above and below the pq plane, i.e. the zero level. This fluctuations are indeed the expression of quantum interference of the two states. For this reason, the image is normally referred as *Schrödinger's cat Wigner function.*

With this in mind, look at at Figure 2.1 "Schrödinger's cat".

Anyway, the "marginal distributions" of w result to be very similar to the classical picture ones. Thanks to the spectral theorem, if we choose

$$\gamma(q,p) = \chi_B(q) \qquad \text{with } B \text{ borelian set in } \mathbb{R}^N_q,$$

we obtain that the observable "position" measurement is given by distribution law

$$\text{Prob}\{X_{A_q} \in B\} = \text{tr}\,(A_\rho \chi_B(A_\gamma)) = \text{tr}\,(A_\rho A_\gamma) = \int\limits_{B\times\mathbb{R}^N_p} w(q,p)\,dq\,dp. \tag{2.66}$$

In other terms, the map $q \longmapsto \int\limits_{\mathbb{R}^N} w(q,p)\,dp$ is the "position" density function. This was already deducible by

$$\int\limits_{\mathbb{R}^N} w(q,p)\,dp = \rho(q,q). \tag{2.67}$$

Analogously, $p \longmapsto \int\limits_{\mathbb{R}^N} w(q,p)\,dq$ is the momentum density function.

We point out, besides, the following

Remark 7. When w is a physical Wigner function on the phase space, then the operator $A_{c_{N,\hbar}w}$ is the quantization of the symbol w, but the vice versa is not true: in general $A_{c_{N,\hbar}w}$ is *not a priori* the quantization of a *classic symbol*.

2.5.3 The Wigner Equation

As well as a mixed state fulfils the Von Neumann evolution equation, a Wigner function fulfils a *Wigner equation*, which is very similar to a classic evolution equation in the phase space.

Let A be an operator on $\mathscr{H}$ and $\rho(x,y)$ be a density matrix. There exists an orthonormal basis $\{\varphi_n\}_{n\in\mathbb{N}}$ and a sequence $\{\lambda_n\}_{n\in\mathbb{N}} \subseteq \mathbb{R}^+$, such that, as usual,

$$\rho(x,y) = \lambda_n \varphi_n(x)\overline{\varphi_n}(y),$$

thus

$$[A, A_\rho] = \sum_{n\in\mathbb{N}} \lambda_n((A\varphi_n)\otimes\varphi_n) - \varphi_n \otimes (A^*\varphi_n).$$

This fact suggests to re-define the product as

$$[A,\cdot] = A\otimes I - I\otimes A^*, \tag{2.68}$$

which, for operators of kind $\psi \otimes \varphi$, becomes

$$(A\varphi) \otimes \psi - \psi \otimes (A^* \varphi).$$

Definition 21. Let A be an operator on $\mathscr{H}$. The *wignerization* of A is given by the operator

$$A^{\text{wig}} = \mathscr{W}\,[A, \cdot]\,\mathscr{W}^{-1} \tag{2.69}$$

on the space $L^2(\mathbb{R}^N_q \times \mathbb{R}^N_p)$, with domain $\mathscr{D}(A^{\text{wig}}) = \mathscr{W}(\mathscr{D}(A))$.

Hence, in the case of a Hamiltonian $H = A_{|p|^2/2m} + A_V$, according to equation (2.53), the Wigner equation, i.e. the wignerization (2.69) of Von Neumann equation, holds

$$i\hbar \frac{dw}{dt}(t) = H^{\text{wig}} w(t), \quad t \in \mathbb{R}, \tag{2.70}$$

namely

$$i\hbar \frac{\partial}{\partial t} w = -\frac{i\hbar}{m} p \cdot \nabla_q w(t) + \delta V(q, -i\nabla_p) w, \qquad t \in \mathbb{R}, \tag{2.71}$$

or

$$\frac{\partial}{\partial t} w + \frac{p}{m} \cdot \nabla_q w(t) + \frac{i}{\hbar} \Theta[\delta V]\, w = 0 \tag{2.72}$$

where $\delta V(q, \xi) = V(q + \frac{\xi}{2}\hbar) - V(q - \frac{\xi}{2}\hbar)$ and

$$(\Theta[V]\, w)(q, p, t) = i c_{N,\hbar} \int_{\mathbb{R}^{\mathbb{N}}} \int_{\mathbb{R}^{\mathbb{N}}} \left[V\left(q + \frac{\xi}{2}\right) - V\left(q - \frac{\xi}{2}\right) \right] \mathrm{e}^{\frac{i}{\hbar}\xi \cdot (p' - p)}\, w(q, p', t)\, d\xi\, dp' \tag{2.73}$$

$$= i c_{N,\hbar} \int_{\mathbb{R}^{\mathbb{N}}} \int_{\mathbb{R}^{\mathbb{N}}} \delta V(q, \xi) \mathrm{e}^{\frac{i}{\hbar}\xi\ cdot(p' - p)}\, w(q, p', t)\, d\xi\, dp'. \tag{2.74}$$

is the wignerization of the potential V multiplicative operator, which becomes a pseudo-differential operator and can be seen as

$$(\Theta[V]\, w)(x, p, t) = \frac{i}{2\pi\hbar^2} \int_{\mathbb{R}} \int_{\mathbb{R}} \left[V\left(x + \frac{\xi}{2}\right) - V\left(x - \frac{\xi}{2}\right) \right] \mathrm{e}^{\frac{i}{\hbar}\xi(p' - p)}\, w(x, p', t)\, d\xi\, dp'$$

$$= -\sum_{k=0}^{\infty} (-1)^k \left(\frac{\hbar}{2}\right)^{2k} \left(\frac{d}{dx}\right)^{2k+1} V(x) \left(\frac{\partial}{\partial p}\right)^{2k+1} w(x, p, t). \tag{2.75}$$

It is shown in [37] that (2.72) reduces to Liouville equation for a classic distribution $f(q, p, t)$

$$\frac{\partial}{\partial t} f(t) + \frac{p}{m} \cdot \nabla_q f - \nabla_q V \cdot \nabla_p f = 0 \tag{2.76}$$

when the classic limit $\hbar \longrightarrow 0$ is taken in consideration. Formally it is already perceivable from

$$\frac{i}{c_{N,\hbar}} \int_{\mathbb{R}^{2N}} \delta V(q,\xi)\, w(q,p') e^{-i(p-p')\cdot\xi}\, d\xi\, dp' \overset{\hbar\to 0}{\longrightarrow} -\nabla_q V \cdot \nabla_p w.$$

Here, it is important to point out that Eq. 2.72 holds under the assumption that V is symmetric as $|q| \longrightarrow \infty$.

Not that if V is a quadratic potential energy, or if one takes the semiclassical limit $\hbar \to 0$, as already observed in Chapter 1, then $\Theta[V]$ reduces to the classical force term of the Liouville equation, namely in 1D case

$$\Theta[V]\, w = -V' \frac{\partial w}{\partial p}, \tag{2.77}$$

where, of course, $-V'(q)$ is the force.

Chapter 3

A mathematical model for decoherence in the Wigner picture

An important problem which has highlighted somehow the peculiarities of decoherence concerns the Wilson cloud chamber experiment: a very energetic α-particle is emitted in a radially symmetric way by a radioactive source and, inside the chamber, ionizes atoms of a super-saturated vapour. The ionized atoms become in turn condensation nuclei, triggering the formation of liquid drops. The observed tracks in real experiments look like classical particle trajectories (see Figure 3.1). Why does it happen? Darwin, Heisenberg and Mott separately suggested that the problem could be solved taking into account that the wave function in the configuration space of the entire quantum system, not in the real space. This answer is also a far-reaching intuition and was exploited by Mott in [40]. Recently it has been re-examined [19], [52] and [16], in order to give a mathematical explanation to the physics of the issue. The models involve many degrees of freedom, so writing a closed evolution equation on the density matrix of the α wave was not easy. Then the matter has been faced numerically in the case of a small environment. The cost of the simulation was exponentially increasing with the size of the environment. That is why it has been decided [27] to afford the problem by means of a toy model reducing the environment to the minimum. This has the advantage of being able to frame the problem in a "strict mathematical look". Thus, the environment has been represented by one single particle which scatters with a central particle, considered as the principal system subjected to decoherence.

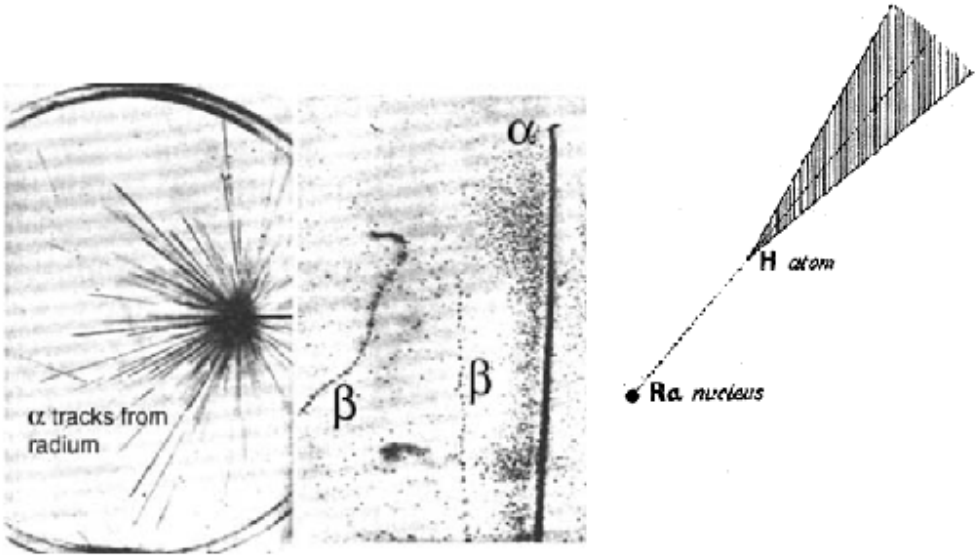


Figure 3.1: The images are typical of those obtained by Wilson during his experiences of the cloud chamber, thanks to the development of which he was awarded the Nobel Prize in Physics in 1927 [61].

3.1 Adami-Hauray-Negulescu model for decoherence

Moving from considerations of these kinds, in Refs.[1,2,3], the quantum dynamical decoherence of a heavy particle interacting with a single light particle is analysed has been analised in detail. The main result of this analysis is the following. Let $\rho(X,Y,t)$ be the reduced density matrix of the heavy particle (the degrees of freedom of the light particle are traced out). Then, in the limit of large heavy-to-light mass ratio, the interaction is concentrated in a single instant of time (say, $t=0$) and has the form of the "instantaneous" transformation

$$\rho(X,Y,0) \longmapsto \mathscr{I}(X,Y)\rho(X,Y,0),$$

where $\mathscr{I}(X,Y)$ is a "collision factor", depending on the details of the interaction. Elsewhere, $\rho(X,Y,t)$ evolves freely (up to possible external potentials V). In the one-dimensional case, this single-interaction decoherence mechanism model is therefore given by the von Neumann equation with a modified initial datum:

$$\begin{cases} i\hbar\dfrac{\partial\rho}{\partial t} = -\dfrac{\hbar^2}{2m}\left(\dfrac{\partial^2\rho}{\partial X} - \dfrac{\partial^2\rho}{\partial Y}\right) + [V(X)-V(Y)]\,\rho, \\ \\ \rho(X,Y,0) = \mathscr{I}(X,Y)\rho_0(X,Y), \end{cases} \tag{3.1}$$

where $\rho_0(X,Y)$ is the pre-interaction density matrix. The form of the collision factor $\mathscr{I}$ is completely characterized in the one-dimensional case [3] and is given by

$$\mathscr{I}(X,Y) = 1 - \Lambda(X-Y) + i\Gamma(X) - i\Gamma(Y), \tag{3.2}$$

with

$$\Lambda(X) = \int_{\mathbb{R}} (1 - \mathrm{e}^{2ikX}) |r(k)|^2 |\hat{\chi}(k)|^2 dk, \tag{3.3}$$

$$\Gamma(X) = \int_{\mathbb{R}} \mathrm{e}^{2ikX} \overline{r(-k)}\, t(k)\, \overline{\hat{\chi}(-k)}\, \hat{\chi}(k)\, dk \tag{3.4}$$

where r and t are the scattering coefficients of the interaction, and $\hat{\chi}$ is the Fourier transform of the light-particle wave function χ. A particularly simple form can be obtained by assuming that

1. χ is a gaussian wave-packet with average momentum $p_0 = \hbar k_0$ and position variance σ^2;
2. p_0 is large with respect to the momentum spread $\hbar\sigma^{-1}$;
3. σ^{-1} is small compared to the scale at which $|r(k)|^2$ varies.

In this case, as shown in Ref. [3], one can make the following approximations:

$$\Lambda(X) \approx |r(k_0)|^2 \left(1 - \mathrm{e}^{2ik_0X - \frac{X^2}{2\sigma^2}}\right), \qquad \Gamma(X) \approx 0. \tag{3.5}$$

Such approximation, providing simple and explicit expressions, will be helpful in the following.

3.2 A Wigner equation with decoherence

We now consider a quantum particle undergoing random collisions with a gas of much lighter particles, each collision being described by the single-interaction model introduced above. Let e^{tA} denote the unitary evolution group associated to the von Neumann equation

$$i\hbar \frac{\partial \rho}{\partial t} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2 \rho}{\partial X} - \frac{\partial^2 \rho}{\partial Y}\right) + [V(X) - V(Y)]\,\rho,$$

so that the solution to this equation with a generic initial datum ρ_0 is expressed (omitting the variables X and Y) as

$$\rho(t) = \mathrm{e}^{tA}\rho_0.$$

Let ν be the collision probability per unit time, and let Δt be a time-interval small enough to neglect the probability of having more than one collision inside it. The random dynamics of the heavy particle can be described by a density-matrix valued stochastic process $R(t)$ such that

$$R(t+\Delta t) = \begin{cases} \mathrm{e}^{\Delta t A} R(t), & \text{with probability } 1-\nu\Delta t, \\ \mathrm{e}^{(\Delta t - s)A} \mathscr{J} \mathrm{e}^{sA} R(t), & \text{with probability } \nu\Delta t, \end{cases}$$

for some collisional time $s \in [0, \Delta t]$. If now $\rho(t) = \langle R(t) \rangle$ is the expected value of $R(t)$, we clearly have

$$\rho(t+\Delta t) = (1-\nu\Delta t)\mathrm{e}^{\Delta t A}\rho(t) + \nu\Delta t\, \mathrm{e}^{(\Delta t - s)A} \mathscr{J} \mathrm{e}^{sA}\rho(t)$$

and then

$$\frac{\rho(t+\Delta t) - \mathrm{e}^{\Delta t A}\rho(t)}{\Delta t} = -\nu \mathrm{e}^{\Delta t A}\rho(t) + \nu \mathrm{e}^{(\Delta t - s)A} \mathscr{J} \mathrm{e}^{sA}\rho(t).$$

By using the fundamental property of the evolution group

$$\mathrm{e}^{\Delta t A} = \int_0^{\Delta t} A \mathrm{e}^{\tau A}\, d\tau + I,$$

we arrive at

$$\frac{\rho(t+\Delta t) - \rho(t)}{\Delta t} = \frac{1}{\Delta t}\int_0^{\Delta t} A \mathrm{e}^{\tau A}\rho(t)\, d\tau - \nu \mathrm{e}^{\Delta t A}\rho(t) + \nu \mathrm{e}^{(\Delta t - s)A} \mathscr{J} \mathrm{e}^{sA}\rho(t)$$

and, taking the limit $\Delta t \to 0$ and recalling that $s \in [0, \Delta t]$, we obtain

$$\frac{d\rho(t)}{dt} = A\rho(t) - \nu\rho(t) + \nu \mathscr{J}\rho(t).$$

By explicitly writing down this differential equation, and putting $\tau := \nu^{-1}$, we get

$$i\hbar \frac{\partial \rho}{\partial t} + \frac{\hbar^2}{2m}\left(\frac{\partial^2 \rho}{\partial X^2} - \frac{\partial^2 \rho}{\partial Y^2}\right) + [V(X) - V(Y)]\,\rho = \frac{i\hbar}{\tau}\left(\mathscr{J}\rho - \rho\right), \tag{3.6}$$

which is the von Neumann equation with a collisional term representing decoherence. The above formal derivation can be of course made rigorous by a suitable analysis. The rigorous derivation of Eq. (3.6), assuming the approximation (3.5), is contained in Ref. [30].

Let us adopt a phase-space description in terms of the Wigner function [10,57,62], i.e. the Wigner transform $w = \mathscr{W}\rho$ of the density matrix, where the

Wigner transform $\mathscr{W}$ is defined as in (2.59)

$$\big(\mathscr{W}\rho\big)(x,p,t) = \frac{1}{2\pi\hbar}\int_{\mathbb{R}} \rho\left(x+\frac{\xi}{2}, x-\frac{\xi}{2}, t\right) \mathrm{e}^{-i\xi p/\hbar}\, d\xi. \tag{3.7}$$

If we Wigner-transform the von Neumann equation (3.6), by using the property (2.61) $\mathscr{W}(\rho_1\rho_2) = \mathscr{W}(\rho_1) * \mathscr{W}(\rho_2)$, we arrive at the following Wigner equation

$$\frac{\partial w}{\partial t} + \frac{p}{m}\frac{\partial w}{\partial x} + \Theta[V]\, w = \frac{(\mathscr{W}\mathscr{I}) * w - w}{\tau}, \tag{3.8}$$

where $\mathscr{W}\mathscr{I}$ is the Wigner transform of the collision factor, $*$ for simplicity here denotes the p-convolution,

By using (3.2), 3.7 and (2.75), we can write

$$(\mathscr{W}\mathscr{I}) * w - w = -\gamma * w + \Theta[\hbar\Gamma]\, w \tag{3.9}$$

where

$$\gamma(p) = (\mathscr{W}\Lambda)(p) = \frac{1}{2\pi\hbar}\int_{\mathbb{R}} \Lambda(\xi)\mathrm{e}^{-i\xi p/\hbar}\, d\xi \tag{3.10}$$

is a function of p alone, because Λ is a function of the correlation variable $\xi = X - Y$.

Hence, the Wigner equation (3.8) takes the final form

$$\frac{\partial w}{\partial t} + \frac{p}{m}\frac{\partial w}{\partial x} + \Theta\Big[V - \frac{\hbar}{\tau}\Gamma\Big]\, w = -\frac{\gamma * w}{\tau}. \tag{3.11}$$

Note that the term $-\frac{\hbar}{\tau}\Gamma$ is equivalent to a potential energy and, therefore, it contributes to the unitary evolution and not to the decoherence. In the particular case of the peaked-gaussian approximation (3.5) we easily obtain

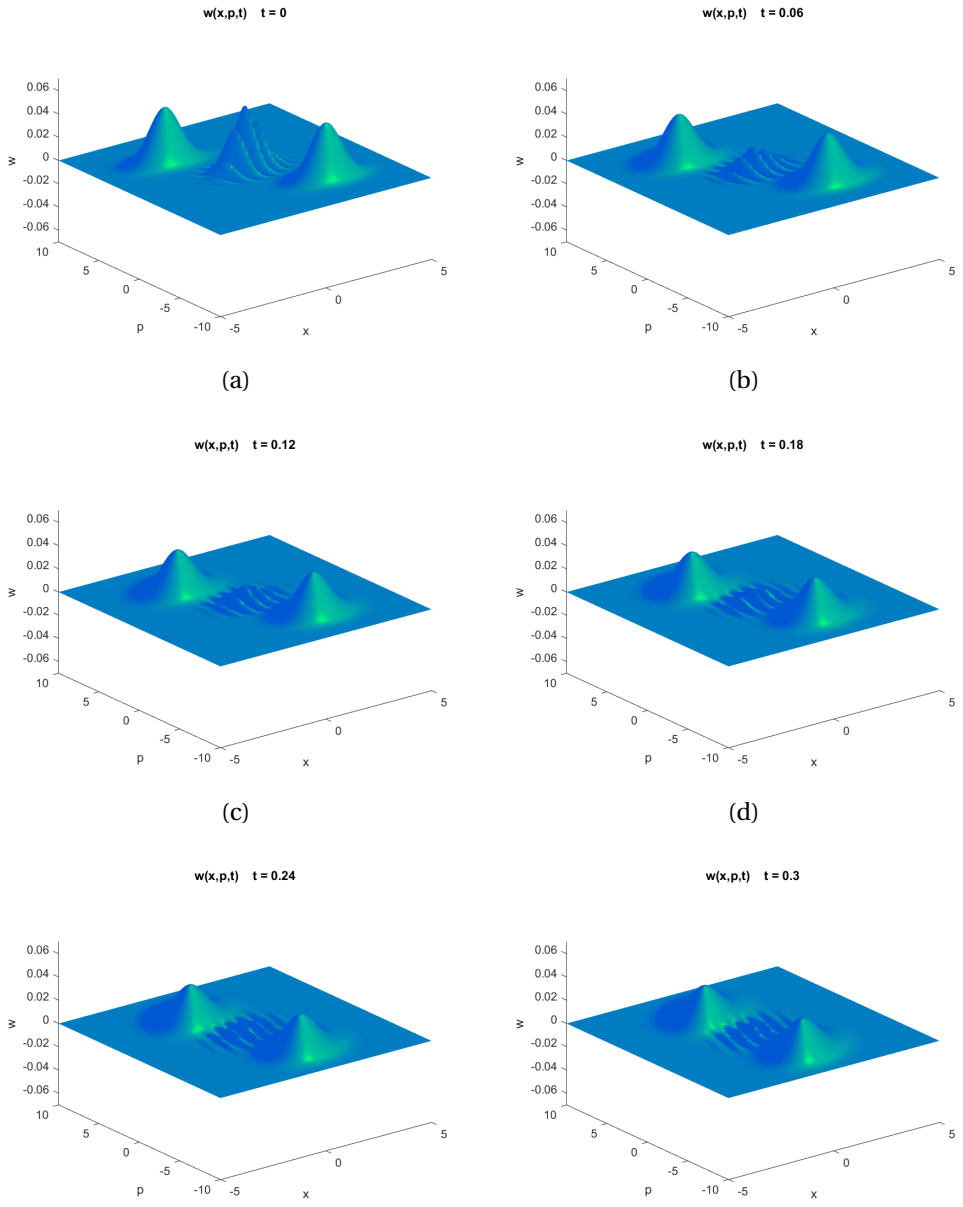
$$-\frac{\gamma * w}{\tau} \approx \frac{|r(k_0)|^2}{\tau}\left[\frac{\sigma}{\hbar\sqrt{2\pi}}\int_{\mathbb{R}} \mathrm{e}^{-\frac{\sigma^2}{2\hbar^2}(p-p'-2\hbar k_0)^2}\, w(x,p',t)\, dp' - w(x,p,t)\right]. \tag{3.12}$$

With respect to the standard Wigner equation, Eq. (3.11) contains a decoherence mechanism which is represented by the right-hand side. Such equation is our basic model of dynamical quantum decoherence.

The physical interpretation of Eq. (3.11) is given as follows. The typical $\mathscr{I}(X,Y)$ is a decaying function of the correlation distance $|X-Y|$ (see Ref. [3]). It means that the decoherence process

$$\rho(X,Y) \longmapsto \mathscr{I}(X,Y)\rho(X,Y),$$

results in a loss of spatial correlation. Switching to the Wigner picture basically



(a) (b) (c) (d) (e) (f)

Figure 3.2: Interference fringes damping

means performing a Fourier transform with respect to the correlation variable $\xi = X - Y$ and then the multiplication $\mathscr{F}(X,Y)\rho(X,Y)$ becomes a convolution with respect to the Fourier variable p. Hence, the loss of spatial correlation corresponds to a smoothing out of $w(x,p,t)$ along the p direction. In particular, from Equations (3.5) and (3.12) we can see that, in the peaked-gaussian approximation, the position spread σ of the light particle determines the reduction scale of the coherence length and, correspondingly, the momentum spread $\hbar\sigma^{-1}$ determines the smoothing scale of the Wigner function. In other terms,

this mechanism attenuates the oscillations of the Wigner function (that are typically on a scale of order $\hbar$ in phase space [50]), thus making the Wigner function progressively to lose its quantum character and to become a classical object. This is evident in Figure 3.2, obtained with a (second order) Lie-Strang numerical scheme (code in Appendix 1).

3.3 Relations with other models

By expanding $1-\mathrm{e}^{2ikX} = -2ikX + 2k^2X^2 + \cdots$, we obtain from (3.3)

$$\Lambda(X) = -iX\Lambda_1 + X^2\Lambda_2 + \cdots, \tag{3.13}$$

where, in the general case,

$$\Lambda_1 = 2\int_{\mathbb{R}} k\,|r(k)|^2\,|\hat{\chi}(k)|^2\,dk, \qquad \Lambda_2 = 2\int_{\mathbb{R}} k^2\,|r(k)|^2\,|\hat{\chi}(k)|^2\,dk, \tag{3.14}$$

and, in the approximation (3.5),

$$\Lambda_1 = 2k_0|r(k_0)|^2, \qquad \Lambda_2 = \frac{|r(k_0)|^2}{2\sigma^2}.$$

Then, we see from (3.10) and (3.13) that

$$\gamma * w \approx -\hbar\Lambda_1\frac{\partial w}{\partial p} - \hbar^2\Lambda_2\frac{\partial^2 w}{\partial p^2}, \tag{3.15}$$

and, if one also assumes $\Gamma = 0$, the following model is obtained from (3.11) and (3.9):

$$\frac{\partial w}{\partial t} + \frac{p}{m}\frac{\partial w}{\partial x} + \Theta[V]\,w = \frac{\hbar^2\Lambda_2}{\tau}\frac{\partial^2 w}{\partial p^2} + \frac{\hbar\Lambda_1}{\tau}\frac{\partial w}{\partial p}. \tag{3.16}$$

The term $\frac{\hbar\Lambda_1}{\tau}\frac{\partial w}{\partial p}$ is just a momentum drift due to our assumption that all environment particles are identical, having in particular the same momentum. This rather unphysical assumption can of course be relaxed by assuming that the light particle is chosen at random from a given population. In this case, Λ_1 survives if the light-particle distribution is asymmetric with respect to the momentum. Otherwise, if $|r(k)|^2$ and $|\hat{\chi}(k)|^2$ are even functions of k (or, simply, if $k_0 = 0$ in the approximation (3.5)), then $\Lambda_1 = 0$ and Eq. (3.16) reduces to the Wigner-Fokker-Planck equation

$$\frac{\partial w}{\partial t} + \frac{p}{m}\frac{\partial w}{\partial x} + \Theta[V]\,w = \frac{\hbar^2\Lambda_2}{\tau}\frac{\partial^2 w}{\partial p^2}, \tag{3.17}$$

which is a largely used model of decoherence [5,4,21,32].

By assuming $\Gamma = 0$ and

$$1 - \Lambda(X) = \mathrm{e}^{-|X|/\lambda}, \tag{3.18}$$

we obtain

$$\mathscr{W}(\mathscr{J}\rho) = \frac{1}{2\pi\hbar}\int_{\mathbb{R}} \mathrm{e}^{-|\xi|/\lambda}\,\rho\left(x+\frac{\xi}{2}, x-\frac{\xi}{2}, t\right)\mathrm{e}^{-i\xi p/\hbar}\,d\xi, =: w_\lambda(x,p,t).$$

In this case, our model can be written

$$\frac{\partial w}{\partial t} + \frac{p}{m}\frac{\partial w}{\partial x} + \Theta[V]\,w = \frac{w_\lambda - w}{\tau}, \tag{3.19}$$

and can be interpreted as the dynamical analogous of the approach proposed by Jacoboni and Bordone in Ref. [31], where a Wigner function with finite coherence length λ is introduced, which is exactly w_λ. In fact, the decoherence mechanism contained in Eq. (3.19) is clearly a relaxation of w to w_λ in a typical time τ. Recalling 2.61, we can also write

$$w_\lambda(x,p,t) = (\mathscr{W}\mathscr{J}) * w = \frac{1}{\pi}\int_{\mathbb{R}} \frac{\hbar/\lambda}{(\hbar/\lambda)^2 + (p-p')^2}\,w(x,p',t)\,dp',$$

from which we see that the effect of the finite coherence length is a Lorentzian broadening of the Wigner function in momentum space, as already remarked in Ref. [31].

Our approach allows a straightforward generalization of Eq. (3.19). In fact, it is enough to assume that the population of lighth particles has a non vanishing momentum p_0 to enrich Eq. (3.19) with the additional parameter p_0, namely

$$w_{\lambda,p_0}(x,p,t) = \frac{1}{\pi}\int_{\mathbb{R}} \frac{\hbar/\lambda}{(\hbar/\lambda)^2 + (p-p_0-p')^2}\,w(x,p',t)\,dp',$$

which embeds the momentum transfer from the environment to the particle undergoing decoherence.

We would like furthermore add that, like ours, Jacoboni-Bordone's model [31] foresees the possibility to adopt any kernel $\Lambda_\lambda(\xi)$ which fulfils these properties:

1. $\Lambda_\lambda(\xi)$ is smooth, differentiable, nonnegative and vanishes at infinity;
2. $\lim_{\lambda\to\infty}\Lambda_\lambda(\xi) = 1$ so that standard case is recovered;
3. $\Lambda_\lambda(0) = 1$.

3.4 Balance laws

In the following we assume $\Gamma = 0$, because, as we can see from Eq. (3.11), the general case with $\Gamma \neq 0$ can be recovered by substituting V with $V - \frac{\hbar}{\tau}\Gamma$.

Balance laws can be deduced from the Wigner equation (3.11) by taking suitable moments with respect to p. In particular, we are interested in the momenta till second order, namely following quantities:

$$\begin{aligned} N(x,t) &= \int_{\mathbb{R}} w(x,p,t)\,dp, && \text{(number density)},\\ J(x,t) &= \frac{1}{m}\int_{\mathbb{R}} p\,w(x,p,t)\,dp, && \text{(current density)},\\ E(x,t) &= \frac{1}{2m}\int_{\mathbb{R}} p^2\,w(x,p,t)\,dp, && \text{(kinetic energy density)}. \end{aligned} \tag{3.20}$$

In order to compute balance laws for N, J and E, we need to take the corresponding moments of Eq. (3.11) and, in particular, we need the momenta of $\Theta[V]\,w$ and $\gamma * w$. By using the series expansion in Eq. (2.75), it is readily seen that

$$\begin{aligned} &\int_{\mathbb{R}} \left(\Theta[V]\,w\right)(x,p,t)\,dp = 0,\\ &\frac{1}{m}\int_{\mathbb{R}} p\left(\Theta[V]\,w\right)(x,p,t)\,dp = \frac{1}{m}V'(x)N(x,t),\\ &\frac{1}{2m}\int_{\mathbb{R}} p^2\left(\Theta[V]\,w\right)(x,p,t)\,dp = V'(x)\,J(x,t). \end{aligned} \tag{3.21}$$

Moreover, from (3.10) and (3.3) we obtain

$$\int_{\mathbb{R}} \gamma(p)\,dp = \Lambda(0) = 0, \tag{3.22}$$

which means that the number of particles is conserved, and

$$\int_{\mathbb{R}} p\,\gamma(p)\,dp = -i\hbar\Lambda'(0), \qquad \int_{\mathbb{R}} p^2\,\gamma(p)\,dp = -\hbar^2\Lambda''(0). \tag{3.23}$$

With a little additional algebra we arrive at

$$\begin{aligned} &\frac{1}{m}\int_{\mathbb{R}} p\left(\gamma * w\right)(x,p,t)\,dp = -\frac{i\hbar}{m}\Lambda'(0)\,N(x,t),\\ &\frac{1}{2m}\int_{\mathbb{R}} p^2\left(\gamma * w\right)(x,p,t)\,dp = -\frac{i\hbar}{m}\Lambda'(0)\,J(x,t) + \frac{\hbar^2}{2m}\Lambda''(0)\,N(x,t). \end{aligned} \tag{3.24}$$

From (3.13) we see that $i\Lambda'(0) = \Lambda_1$ and $\Lambda''(0) = 2\Lambda_2$ (where the constants Λ_j are given by (3.14)). Then, by multiplying the Wigner equation (3.11) by 1, p/m

and $p^2/2m$, respectively, and integrating both sides with respect to p, we obtain the following system of Euler-like equations:

$$\begin{cases} \dfrac{\partial N}{\partial t} + \dfrac{\partial J}{\partial x} = 0, \\ \dfrac{\partial J}{\partial t} + \dfrac{\partial \mathscr{J}_J}{\partial x} + \dfrac{1}{m} V' N = \dfrac{\hbar \Lambda_1}{m\tau} N, \\ \dfrac{\partial E}{\partial t} + \dfrac{\partial \mathscr{J}_E}{\partial x} + V' J = \dfrac{\hbar \Lambda_1}{m\tau} J - \dfrac{\hbar^2 \Lambda_2}{m\tau} N, \end{cases} \tag{3.25}$$

where

$$\mathscr{J}_J(x,t) = \frac{1}{m^2} \int_{\mathbb{R}} p^2 w(x,p,t)\, dp = \frac{1}{m} E(x,t)$$

and

$$\mathscr{J}_E(x,t) = \frac{1}{2m^2} \int_{\mathbb{R}} p^3 w(x,p,t)\, dp$$

are the currents associated to J and E, respectively. As usual, this system contains the extra unknown $\mathscr{J}_E$ (but also $\mathscr{J}_J$ would be an unknown in higher spatial dimensions) and needs to be closed by making suitable assumptions (see e.g. Refs. [11,34,48] and references therein).

The right-hand sides of Eq. (3.25) are due to decoherence collisions. We can notice that the terms depending on Λ_1 are due to the momentum injection from the environment (see the discussion in the first part of Sec. 3.3), while the term depending on Λ_2 (which is a positive constant, as it is apparent from (3.14)) represents energy dissipation in the environment.

Chapter 4

Quantum decoherence effects on a scattering process

In this chapter we aim to test the efficacy of our Wigner equation model for decoherence on a situation of physical interest as a tunneling process through a potential barrier in a decoherent environment.

It is indicated, for example in [33], that one typical quantum property, the coherence length, is reduced by decoherence. According to the Schrödinger equation, a free wave packet would spread, thereby increasing its size and extending its coherence properties over a larger region of space. Decoherence is expected to counteract this behaviour and reduce the coherence length.
In [26] the authors analyze, from a theoretical point of view in the Wigner formalism, the problem of electron dynamics inside nanometric systems, where the coherence of the electron ensemble is maintained in a very short region. For very short devices indeed, transport properties, such as tunnelling through potential barriers, are significantly influenced by the distance between the contacts, which spoil such a coherence, so that the interference processes between the carrier wavefunction and the internal potential profile result affected by the proximity of the contacts. By means of the model presented in the previous chapter we are able to point out the following

Property 1. In a tunneling process through a potential barrier, the decoherence phenomenon (i.e. finite coherence length related to finitude of the semiconductor device, see [26,23,33,49]) favours transmission in an otherwise reflection-dominated regime.

We would like to stress that this phenomenon occurs because long wavelength components of the potential cannot interfere effectively with low energy electron states, hence reflection is someway inhibited. If the coherence length of the system is short, electrons cannot "feel" the wavelengths needed to be

reflected by the potential profile. An experimental measurement of this effect is still sought, since the hypothesis of an abrupt vanishing of coherence at the contacts and the need for a sharp control of the spatial dimensions of the nano-device make the experimental results really sensitive to the accuracy of the geometrical definition of the sample and to the effectiveness of the decoherence processes within the contacts.

Here below we numerically solve the evolution equation with decoherence resulting from the one-dimensional scattering problem. The finitude of the device is contained in the decoherence term (which reduces then essentially to parameter λ as seen in Section 3.3 in relation to [31]), so that the problem can be faced on the entire real spacial domain. The final state is observed in terms of average quantities (momentum and position) and density profiles, but the proper "measure" of the effect is given by the observation of the transmission coefficients we will be aware of later.

4.1 The physical model

Let consider a gaussian wave packet, supposed free at $t \longrightarrow -\infty$, which enters a region where a potential barrier is present. Here, we are no more interested to observe the classical behaviour effects appearance (i.e. the damping of interference fringes), but rather to verify Property 1. This is why, instead of a superposition initial state, we take a single bump centred in x_0 with average momentum p_0 as initial condition:

$$\psi_0(x) = \left(\frac{2\sigma_p}{\pi\hbar^2}\right)^{\frac{1}{4}} e^{-\frac{\sigma_p(x-x_0)^2}{\hbar^2} + i\frac{p_0(x-x_0)}{\hbar}}, \tag{4.1}$$

where σ_p is the initial momentum variance.
To the wave function in (4.1) there corresponds an initial density matrix

$$\rho_0(x,y) = \overline{\psi_0(x)}\psi_0(y), \tag{4.2}$$

and an initial Wigner function

$$w_0(x,p) = \frac{1}{\pi\hbar}\mathrm{e}^{-2\frac{\sigma_p(x-x_0)^2+\sigma_x(p-p_0)^2}{\hbar^2}}, \tag{4.3}$$

where the initial position variance σ_x fulfils

$$\sigma_x\sigma_p = \frac{\hbar^4}{4}, \tag{4.4}$$

requiring a minimal uncertainty wave packet.
We suppose that the initial Wigner function starts in free motion at large distance from the origin.

We recall Eq. (3.11) in the form (3.19)

$$\frac{\partial w}{\partial t} + \frac{p}{m}\frac{\partial w}{\partial x} + \Theta[V]\, w = \frac{w_\lambda - w}{\tau}, \tag{4.5}$$

where

$$w_\lambda = \gamma_\lambda *_p w, \tag{4.6}$$

with a correlation length parameter λ contained in the collisional kernel

$$\gamma_\lambda(p) = \frac{1}{2\pi\hbar}\int_{\mathbb{R}} \Lambda_\lambda(\xi)\, e^{-\frac{i}{\hbar}p\xi}\, d\xi$$

being responsible for the damping of the density matrix for large values of ξ.

For the numerics we have chosen a gaussian potential located in the central region

$$V(x) = V_0 e^{-\frac{x^2}{a^2}} \tag{4.7}$$

and the gaussian decoherence function

$$\Lambda_\lambda(\xi) = {r_0}^2\left(1 - e^{-\frac{\xi^2}{2\lambda^2}}\right). \tag{4.8}$$

in accordance to Equation (3.13).

4.1.1 Nondimensionalization

In order to numerically solve the problem we reduce to a dimensionless evolution equation. In this regard, we take in account characteristic quantities as the characteristic lenght a, the characteristic potential barrier height V_0, and time $T = \sqrt{\frac{V_0}{ma^2}}$, which represents the time a particle of energy V_0 takes to overpass the barrier.
Hence, we introduce a dimensionless energy

$$E_K = \frac{p_0^2}{2mV_0} \tag{4.9}$$

and an initial dimensionless momentum variance

$$\sigma_0 = \frac{\sigma_p}{mV_0}. \tag{4.10}$$

The nondimensionalized variables are

$$x' = \frac{x}{a}, \qquad t' = \frac{t}{T}, \qquad p' = \frac{p}{\sqrt{mV_0}}, \tag{4.11}$$

and the dimensionless Planck constant becomes

$$\bar{h} = \hbar \frac{a}{\sqrt{mV_0}}.$$

The initial dimensionless momentum is then

$$p'_0 = \sqrt{2E_K} \tag{4.12}$$

and the initial dimensionless position x'_0 is empirically chosen so that the initial packet bump is far from the potential. These parameters characterize, hence, the initial Wigner function in the new variables, which has been divided by $\sqrt{mV_0}$ to nondimensionalize. Moreover, the new potential has been divided by the quantity V_0, as well.
In sake of simplicity, from now on, we will get rid of the primes in the notations and consider the unprimed variables as dimensionless.

In the new variables, the evolution equation recalled in (4.5) becomes

$$\frac{\partial w}{\partial t} + p\frac{\partial w}{\partial x} + \Theta[V]\, w = \frac{1}{\tau}(w_\lambda - w) \tag{4.13}$$

with an initial condition

$$w_0(x,p) = \frac{1}{\pi\bar{h}} e^{-2\left[\frac{\sigma_0(x-x_0)^2}{\bar{h}^2} + \bar{h}^2\sigma_0(p-p_0)^2\right]} \tag{4.14}$$

4.2 The numerical method

The solution of (4.13) can be numerically found using a splitting scheme algorithm. This numerical method consists in decoupling the problem in two (or more) subproblems.
Indeed our evolution equation can be split in two parts: one of "free transport" evolution and one of "due-to-potential" evolution. The idea of using this method is borrowed from the one proposed initially in [12] for the one-dimensional classical Vlasov equation for collisionless plasmas,

$$\frac{\partial f}{\partial t} + p\frac{\partial f}{\partial x} - E\frac{\partial f}{\partial p} = 0, \tag{4.15}$$

which has been adapted to the quantum case for the Wigner equation (Reff. [6], [7], [20]). In the study of plasma waves, the electric field E is also an unknown quantity and it obeys the Poisson equation, which is included in the numerical scheme. We do not have other unknowns but w. Furthermore, we need to modify the method because of the decoherence term nature, which appears, as seen in the previous chapter, as a p-convolution of the decoherence kernel $\gamma_\lambda(p)$ and the unknown.

In its original formulation [12] for the classical nonlinear Vlasov-Poisson system, the splitting scheme performs the numerical integration along the characteristics in the phase space. A discretized mesh

$$x_l = l\Delta x \quad \text{and} \quad p_j = j\Delta p - p_M, \quad \text{for } l = 0,...,N;\ j = 0,...,M$$

is introduced in the phase space, and the solution is advanced in time from t to $t+\Delta t$ by alternating an integration along x for half time-step, an integration along p for a whole time step and a final integration again along x for half time-step. When integrating along x, the transport equation

$$\frac{\partial f}{\partial t} + p\frac{\partial f}{\partial x} = 0 \tag{4.16}$$

is solved from t to $t+\Delta t/2$ and the solution is given by

$$f(x_l, p_j, t+\Delta t/2) = f(x_l - p_j\Delta t/2).$$

This corresponds to a shift of the solution along x by the quantity $pj\Delta t/2$ for each p_j . The evaluation of f on the off-mesh points $(x_l - p_j\Delta t/2, p_j)$ is best done by Fourier transforming with respect to x, since a shift in the x variable by $pj\Delta t/2$ amounts to a multiplication of the Fourier transform by the phase factor $\exp(-ikp_j\Delta t/2)$. When integrating along p, the equation

$$\frac{\partial f}{\partial t} - E\frac{\partial f}{\partial p} = 0$$

is solved from $t+\Delta t$ and the solution is given by

$$f(x_l, p_j, t+\Delta t) = f(x_l, p_j + E\Delta t, t).$$

This corresponds to a shift of the solution along p by the quantity $pj\Delta t$ for each x_l. Again, the evaluation of f on the off-mesh points $(x_l, p_j + E\Delta t)$ is best done by Fourier transforming with respect to p, and here the Fourier transform is multiplied by the phase factor $\exp(ikp_j\Delta t)$. The splitting is equivalent to

replacing each actual characteristic curve, within a mesh cell, with a sequence of three connected segments, the first and the last being parallel to the x-axis while the second is parallel to the p-axis. For this reason, the integrations along x are referred to as horizontal shifts and the integration along p as vertical shift. It has also to be noted that, at each time step after the initial one, the first horizontal shift can be combined with the second horizontal shift of the previous time step in a unique horizontal shift, thus saving computational time.
The splitting-scheme algorithm illustrated here above can be applied to the numerical solution of the Wigner equation (1) for $w(x,p,t)$, even though there are no characteristics in the quantum case. The differential term of the Vlasov equation is replaced in equation (4.13) by a pseudo-differential term plus the decoherence term. It can be easily again approached by Fourier transforming with respect to the p variable and this is equivalent to apply the inverse Wigner transform and solve the "potential-plus-decoherent" evolution on Δt and come back to the Wigner function by Wigner transform. It would not be necessary to transform at the first shift because we could use the advantages of the Wigner formulation where a free transport term appears and, hence, interpolate on the mesh, but we prefer to use twice a multiplicative form both for the transport and the "potential-plus-decoherence" step. In the second shift it is absolutely indispensable, because of convolution operator presence.

Horizontal shift The splitting sequence retains the same structure, because the equation of the of horizontal shift is still like (4.16):

$$\frac{\partial w}{\partial t} + p\frac{\partial w}{\partial x} = 0, \tag{4.17}$$

which can be solved by Fourier transforms in position. If

$$\hat{w}(k,p,t) = \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} w(x,p,t)e^{ikx}dx$$

is the (inverse) Fourier transform of $w(x,p,t)$ (with respect to x-to-k variable), equation (4.17) becomes

$$\frac{\partial \hat{w}}{\partial t} + ip\hat{w} = 0, \tag{4.18}$$

then

$$\hat{w}(k_i,p_j,t+\frac{\Delta t}{2}) = e^{-\imath p\frac{\Delta t}{2}}\hat{w}(k_i,p_j,t). \tag{4.19}$$

The solution $w(x_l, p_j, t+\frac{\Delta t}{2})$ is then obtained by the Fourier transform with respect to k-to-x variable

$$w(x,p,t) = \frac{1}{\sqrt{2\pi}} \int \hat{w}(k,p,t) e^{-ixp} dk. \tag{4.20}$$

Vertical shift The vertical shift is intended to solve the equation

$$\frac{\partial w}{\partial t} + \left\{ \Theta[V] + \frac{1-\gamma_\lambda *_p}{\tau} \right\} w = 0. \tag{4.21}$$

We transform with respect to the p-to-k variable, obtaining

$$\frac{\partial \tilde{w}}{\partial t} + \delta(V)\tilde{w} + \frac{1-\tilde{\gamma}_\lambda}{\tau}\tilde{w} = 0, \tag{4.22}$$

being

$$\tilde{w}(x,k,t) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} w(x,p,t) e^{ikp} dp. \tag{4.23}$$

Hence,

$$\tilde{w}(x_l, k_j, t+\Delta t) = e^{-V+\frac{1-\tilde{\gamma}_\lambda}{\tau}} \tilde{w}\left(x_l, k_j, \frac{\Delta t}{2}\right). \tag{4.24}$$

We Fourier transform again to obtain $w(x_l, p_j, t+\Delta t)$.

4.3 Numerical results

In this section, the numerical solution of the Wigner equation with decoherence for the physical situation discussed in Section 4.1 with the choice[1]

$$\Lambda_\lambda(\eta) = \left(\cosh\frac{\eta}{\lambda}\right)^{-1} \tag{4.25}$$

is presented.

Three cases are discussed, corresponding to different values of the dimensionless energy E_K for which, in the quantum standard dynamics (i.e. $\lambda \longrightarrow \infty$), the regime is

1. reflection-dominated, for $E_K = 0.5$;
2. neutral, for $E_K = 1$;
3. transmission-dominated, for $E_K = 1.5$ and $E_K = 2$.

[1] due to regularity reasons in the phase-space origin

For each one, we vary the values of the decoherence parameter (or coherence length) λ and we report the quantity which gives an approximated value of the transmission coefficient, as in [53],

$$T = \frac{1}{2}\left(1 + \frac{\langle p\rangle_\infty}{p_0}\right), \tag{4.26}$$

where

$$\langle p\rangle(\infty) = \lim_{t\to\infty}\int_{\mathbb{R}}\int_{\mathbb{R}} p\, w(x,p,t)\, dx\, dp = \lim_{t\to\infty}\int_{\mathbb{R}} J(x,p)dx \tag{4.27}$$

is the average momentum at the final time step, i.e. the asymptotic value of the current (see (3.20)). Another parameter we take into account is τ, i.e. the dimensionless equivalent of the collisional characteristic time.

4.3.1 First case

To begin we focus on the case in which the initial energy is one half of the potential height and refection dominates in the standard case ($\lambda \longrightarrow \infty$). Figure 4.1 shows the density profile $N(x)$ at $\frac{1}{5}$ of the final time step ($t = 60$ in the dimensionless units) and Figure 4.2 at the final time step, both for seven different values of λ (as indicated in the legends) and $\tau = 10$. The initial gaussian packet travels freely in the early stages of the evolution, moves towards the potential region, with the average momentum staying constant before the bulk of the packet reaches the potential. The packet (see the density figures) presents the natural increasing spread, this effect becoming more pronounced at smaller correlation lengths (see Figure 4.2). As the packet reaches the potential, oscillations are set on the density profile and the average momentum drops; the oscillations appear to be smoothened as the correlation length becomes shorter, and the drop in the average momentum is also less pronounced at shorter values of λ (see Figure 4.3 where $\tau = 10$).
After the interaction with the potential, a transmitted and a reflected packet separate, travelling away from the origin in opposite directions; the transmitted packet is broader and higher as λ becomes smaller. The average momentum settles to a constant value, clearly larger for smaller values of λ; the transmission coefficient, reported in Tables 4.1 –4.3, also shows increasing values in this case as λ becomes smaller. The Wigner function keeps oscillating indefinitely near the potential region, although the contribution of these oscillations to the density becomes negligible with time; as the correlation length becomes smaller, the oscillations are seen to be damped away. This behaviour is in

agreement with the results of [7], where the increased transmission due to the decoherence was attributed to a reduced momentum exchanged between the packet and the potential caused by the correlation damping.

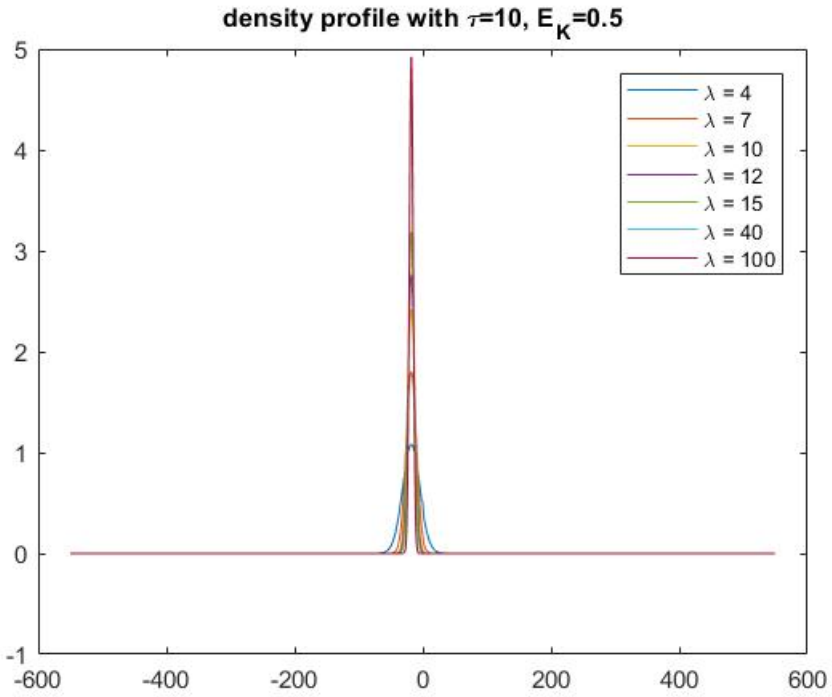


Figure 4.1: Density profile as function of x in the first case $E_K = 0.5$ (reflection-dominated regime) at time $t = 12$ with $\tau = 10$, $\sigma_0 = 0.1E_K$, $p_0 = \sqrt{2E_K}$, $\bar{h} = 0.5$ and different values of λ, as displayed in the legend, from $\lambda = 4$ to $\lambda = 100$ (i.e. $\lambda \to \infty$). All quantities are in dimensionless units.

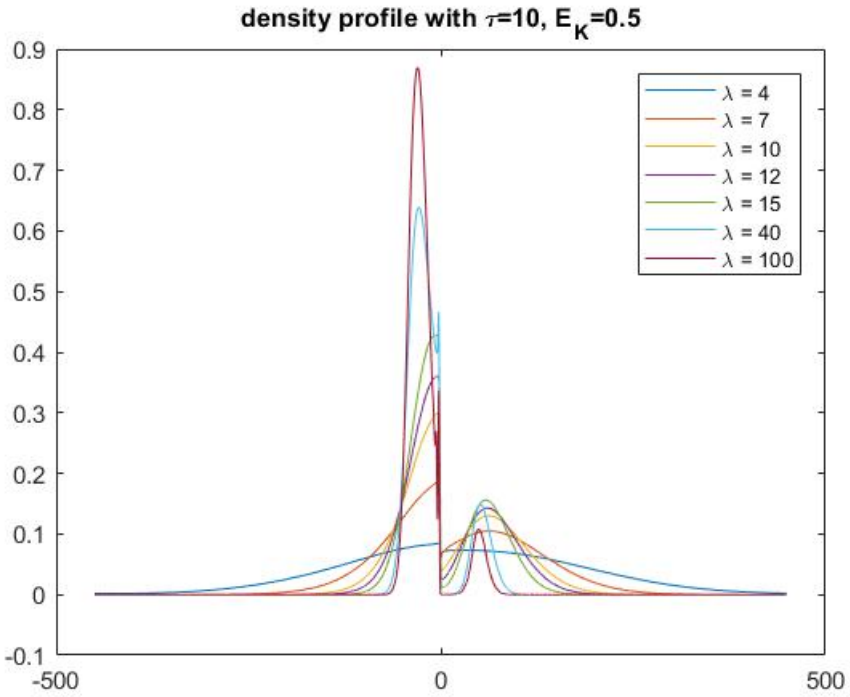


Figure 4.2: Density profile as function of x in the first case $E_K = 0.5$ (reflection-dominated regime) at time $t = 60$ with $\tau = 10$, $\sigma_0 = 0.1E_K$, $p_0 = \sqrt{2E_K}$, $\bar{h} = 0.5$ and different values of λ, as displayed in the legend, from $\lambda = 4$ to $\lambda = 100$ (i.e. $\lambda \to \infty$). All quantities are in dimensionless units.

4.3.2 Second case

The initial energy is here at the same level of the potential height. As in the case with $E_K = 0.5$, the final time of simulation is $t = 60$ in dimensionless units. We show again the density profile at the final time in Figure 4.4. The values for the correlation length λ are the same. The early evolution of the initial gaussian packet is similar to the evolution observed in the previous case, with the packet becoming lower and broader and with the effect being again more pronounced at smaller correlation lengths. The onset of oscillations on the density profile is observed again, but a portion of the packet has already travelled past the potential region before the oscillations stop. As the interaction with the potential becomes negligible, we observe again a transmitted and a reflected packet travelling away from the origin in opposite directions; both the transmitted and the reflected packets, however, become now broader and smaller as λ is decreased. The overall effect is to favour transmission and the transmission coefficients also show increasing values in this case as λ becomes smaller.

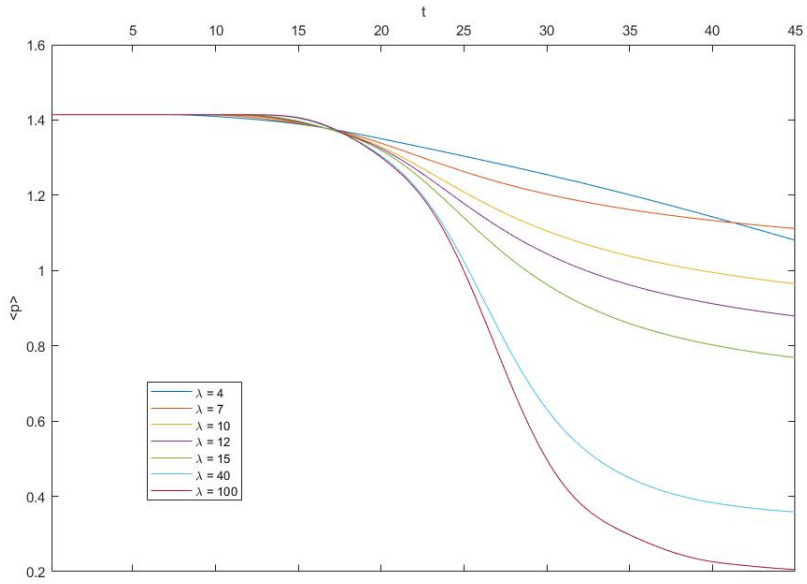


Figure 4.3: Average momentum $< p >$ as functions of time t, from $t = 0$ to $t = 45$ for the case $E_K = 0.5$ with $\tau = 10$, $\sigma_0 = 0.1E_K$, $p_0 = \sqrt{2E_K}$, $\bar{h} = 0.5$ and different values of λ, as displayed in the legend, from $\lambda = 4$ to $\lambda = 100$ (i.e. $\lambda \to \infty$). All quantities are in dimensionless units.

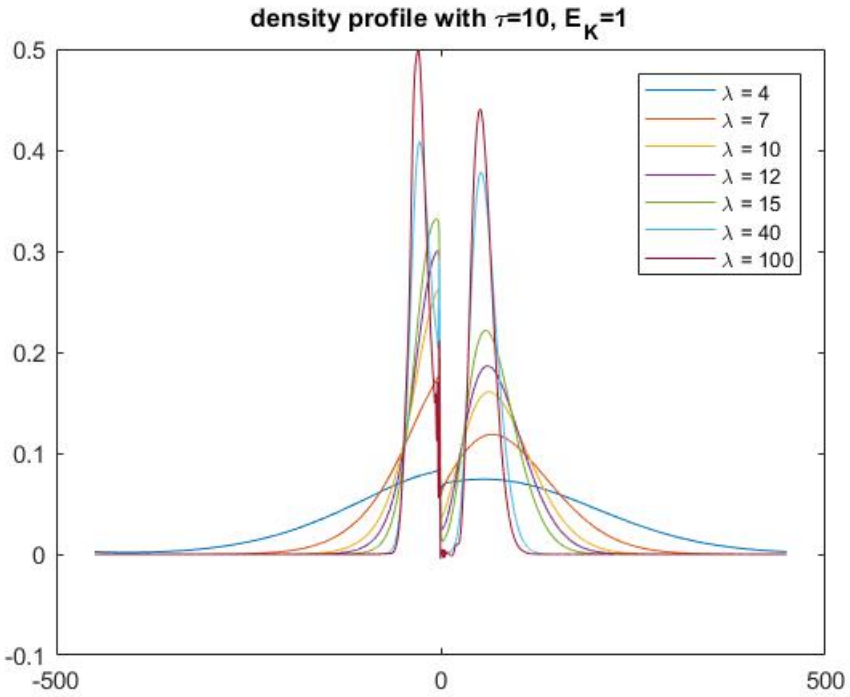


Figure 4.4: Density profile as function of x in the second case $E_K = 1$ at time $t = 60$ with $\tau = 10$, $\sigma_0 = 0.1E_K$, $p_0 = \sqrt{2E_K}$, $\bar{h} = 0.5$ and different values of λ, as displayed in the legend, from $\lambda = 4$ to $\lambda = 100$ (i.e. $\lambda \to \infty$). All quantities are in dimensionless units.

4.3.3 Third and fourth cases

The initial energy is now higher than the potential one. The final time of simulation is still $t = 60$ in dimensionless units. The values for the correlation length λ are the same as in the previous cases. By comparing Figures 4.8 and 4.9 for the average momentum with the corresponding Figures 4.3 and 4.5, we see that the effect of a decreasing λ on transmission is now much weaker; the average momentum, after the drop from the initial value during the interaction, settles to a constant which is almost independent of the coherence length λ. The Tables 4.1–4.3 show that in this case the transmission coefficient remains constant (to the second digit) as the correlation length λ is varied. The density profiles show a similar behaviour as in the previous two cases, with the onset of oscillations during the interaction of the packet with the potential, followed by a separation into reflected and transmitted portions, which become lower and broader as the value of λ is reduced. In the end we would like to point out that the parameter τ influences immediately the transmission for high values of λ, as we could imagine since it is related to the number of collision in a time unit.

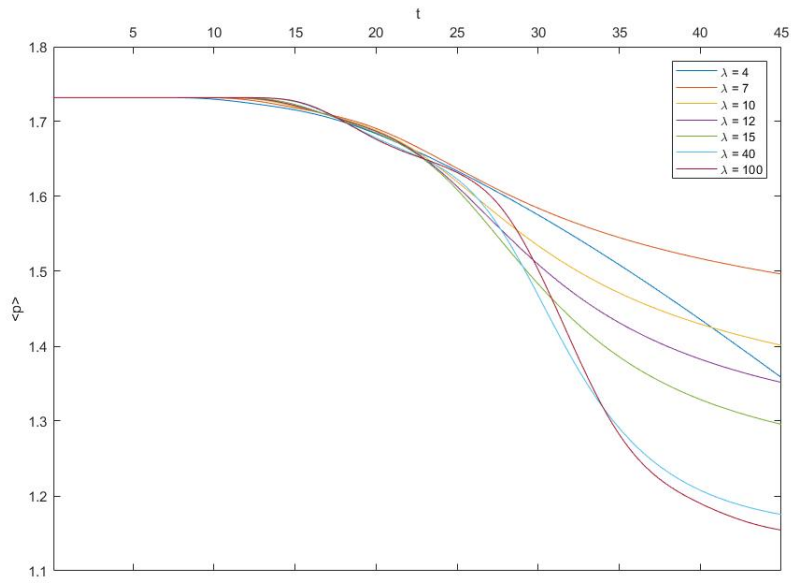
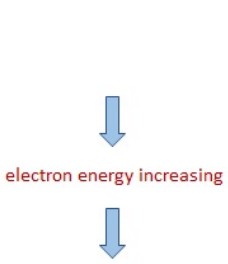


Figure 4.5: Average momentum $< p >$ as functions of time t, from $t = 0$ to $t = 45$ for the case $E_K = 1$ with $\tau = 10$, $\sigma_0 = 0.1E_K$, $p_0 = \sqrt{2E_K}\,\bar{h} = 0.5$ and different values of λ, as displayed in the legend, from $\lambda = 4$ to $\lambda = 100$ (i.e. $\lambda \to \infty$). All quantities are in dimensionless units.

The previous analysis and, in particular, the results in Tables 4.1–4.3 allow us asserting that decoherence (low values of λ) favours transmission (T values are incremented) in reflection-dominated regimes, while the effect is almost irrelevant in transmission-dominated ones.

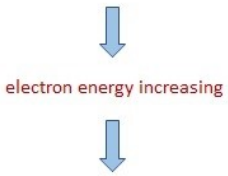
Table 4.1: Transmission Coefficients table for $\tau = 3$



decoherence increasing

λ / E_K	100	40	15	12	10	7	4
0,50	0,1560	0,3345	0,6834	0,7488	0,7924	0,8187	0.6979
1,00	0,6896	0,7442	0,8661	0,8916	0,9065	0,8861	0.7211
1,50	0,8975	0,8955	0,9272	0,9380	0,9421	0,9042	0.7262
2,00	0,9614	0,9526	0,9556	0,9595	0,9578	0,9101	0.7268

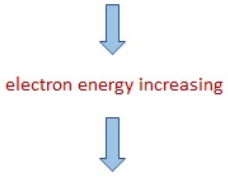
Table 4.2: Transmission Coefficients table for $\tau = 10$



decoherence increasing

λ / E_K	100	40	15	12	10	7	4
0,50	0,1241	0,1931	0,4659	0,5493	0,6153	0,7294	0,8191
1,00	0,6792	0,7012	0,7870	0,8162	0,8404	0,8842	0,8920
1,50	0,8992	0,8961	0,9017	0,9092	0,9172	0,9349	0,9119
2,00	0,9635	0,9589	0,9555	0,9502	0,9522	0,9585	0,9000

Table 4.3: Transmission Coefficients table for $\tau = 15$



decoherence increasing

λ / E_K	100	40	15	12	10	7	4
0,50	0,1194	0,1669	0,3914	0,4723	0,5403	0,6659	0,8076
1,00	0,6776	0,6931	0,7624	0,7893	0,8131	0,8597	0,9073
1,50	0,8995	0,8970	0,8975	0,9023	0,9084	0,9247	0,9371
2,00	0,9639	0,9608	0,9510	0,9498	0,9501	0,9547	0,9495

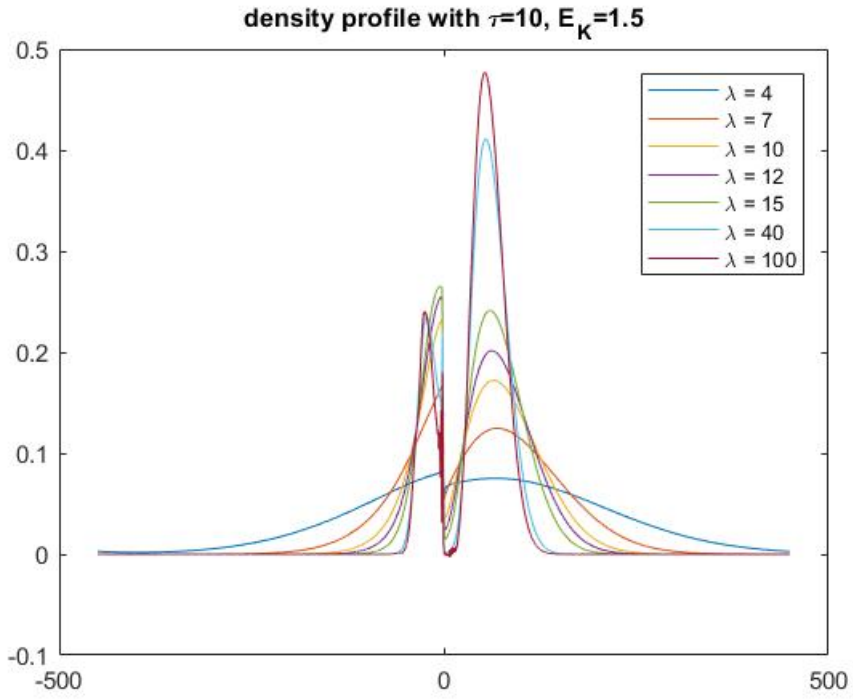


Figure 4.6: Density profile as function of x in the third case $E_K = 1.5$ (transmission-dominated regime) at time $t = 60$ with $\tau = 10$, $\sigma_0 = 0.1E_K$, $p_0 = \sqrt{2E_K}$, $\bar{h} = 0.5$ and different values of λ, as displayed in the legend, from $\lambda = 4$ to $\lambda = 100$ (i.e. $\lambda \to \infty$). All quantities are in dimensionless units.

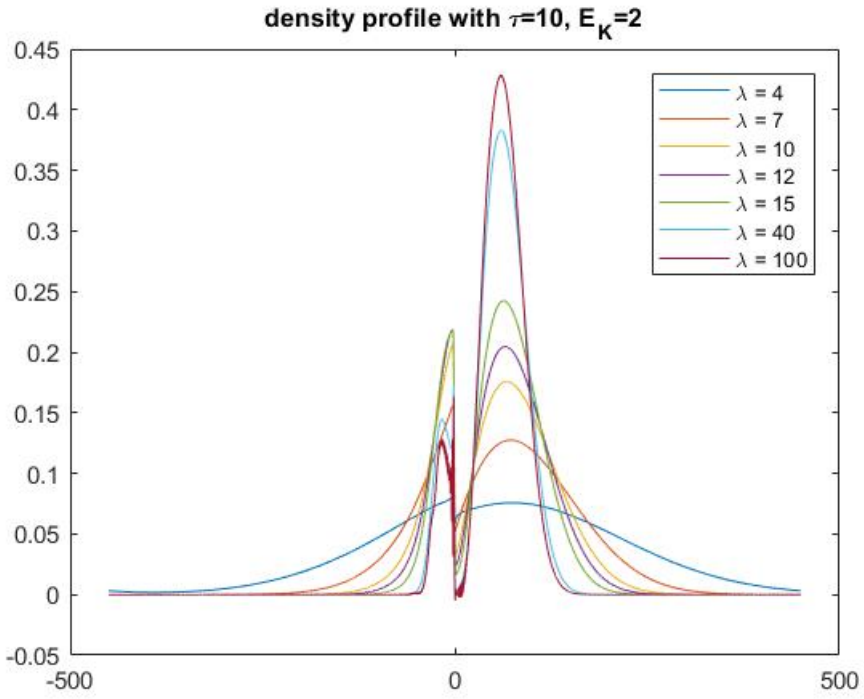


Figure 4.7: Density profile as function of x in the third case $E_K = 1.5$ (higher transmission-dominated regime) at time $t = 60$ with $\tau = 10$, $\sigma_0 = 0.1E_K$, $p_0 = \sqrt{2E_K}$, $\bar{h} = 0.5$ and different values of λ, as displayed in the legend, from $\lambda = 4$ to $\lambda = 100$ (i.e. $\lambda \to \infty$). All quantities are in dimensionless units.

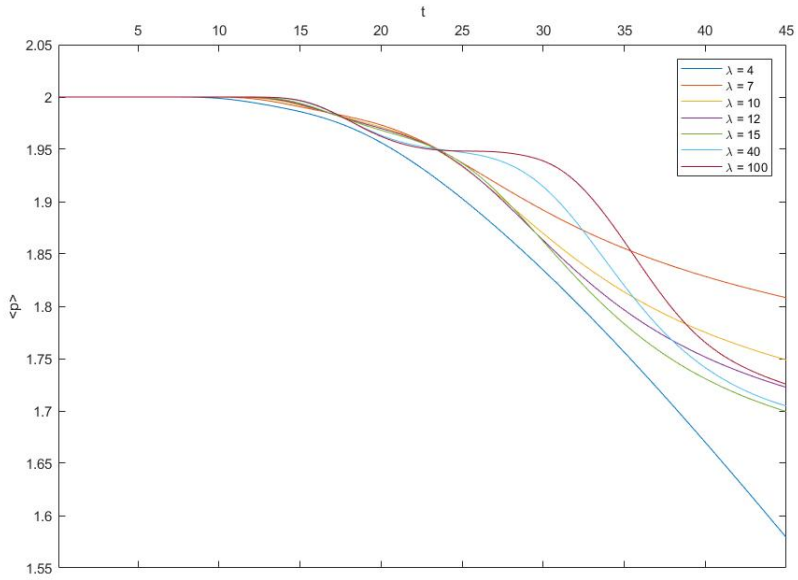


Figure 4.8: Average momentum $< p >$ as functions of time t, from $t = 0$ to $t = 45$ for the case $E_K = 1.5$ with $\tau = 10$, $\sigma_0 = 0.1E_K$, $p_0 = \sqrt{2E_K}$, $\bar{h} = 0.5$ and different values of λ, as displayed in the legend, from $\lambda = 4$ to $\lambda = 100$ (i.e. $\lambda \to \infty$). All quantities are in dimensionless units.

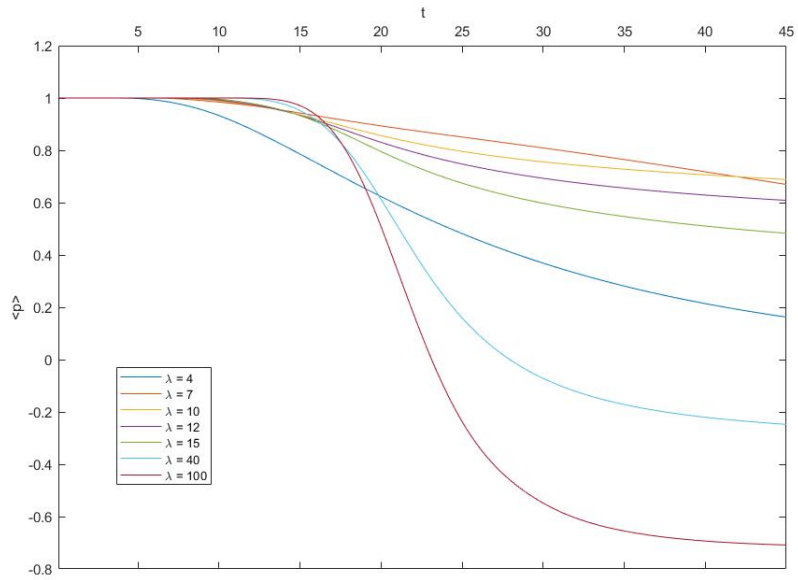


Figure 4.9: Average momentum $< p >$ as functions of time t, from $t = 0$ to $t = 45$ for the case $E_K = 2$ with $\tau = 10$, $\sigma_0 = 0.1E_K$, $p_0 = \sqrt{2E_K}$, $\bar{h} = 0.5$ and different values of λ, as displayed in the legend, from $\lambda = 4$ to $\lambda = 100$ (i.e. $\lambda \to \infty$). All quantities are in dimensionless units.

Chapter 5

Large-time asymptotics for the model

At this point, we would like to study the behaviour of our model for decoherence, as presented in Chapter 3, for large values of t (i.e. $t \to +\infty$). It can be immediately observed that the solution $w(x,p,t)$ of the Wigner equation (3.11) tends to be completely smoothed out to a constant value. Correspondingly, within the density matrix formalism, the coherence length associated to ρ, i.e. the decay of $\rho(X,Y,t)$ along the correlation coordinate $X-Y$, tends to vanish. This is an unphysical behaviour which was already pointed out by Joos and Zeh [32].

5.1 Large-time behaviour for a gaussian wave packet

Inspired by the approach adopted in Ref. [32], rather than embarking in a general analysis which will be outlined in the next section, we shall discuss the issue of large-time asymptotics by performing numerical simulation in a very simple (but physically meaningful) situation, that is the case of a gaussian distribution.

Let us work within the Wigner-Fokker-Planck approximation (3.17), and assume that the potential is harmonic, namely

$$V(x) = \frac{\kappa}{2} x^2,$$

with $\kappa \geq 0$. Recalling Eq. (2.77), the resulting equation is

$$\frac{\partial w}{\partial t} + \frac{p}{m}\frac{\partial w}{\partial x} - \kappa \frac{\partial w}{\partial p} = \frac{\Lambda_0}{\tau}\frac{\partial^2 w}{\partial p^2}, \tag{5.1}$$

where for simplicity we have set

$$\Lambda_0 = \hbar^2 \Lambda_2.$$

It is readily seen that (3.17) admits solutions of the form

$$w(x,p,t) = \mathrm{e}^{-[A(t)\,p^2 + B(t)\,px + C(t)\,x^2 + D(t)]}, \tag{5.2}$$

where $1/\sqrt{2A(t)}$ is the momentum spread (and, therefore, $\hbar\sqrt{2A(t)}$ is the coherence-length spread, according to the discussion closing Section 3.2), $B(t)$ is a covariance parameter, $1/\sqrt{2C(t)}$ is the position spread and $D(t)$ is a normalization parameter. It is to be noticed that the corresponding density matrix still has a gaussian form, which is exactly the one considered by Joos and Zeh. The substitution of (5.2) into the Wigner-Fokker-Plank equation (3.17) leads straightforwardly to the following system of ODEs for the unknown functions $A(t)$, $B(t)$, $C(t)$ and $D(t)$:

$$\begin{cases} \dot{A} = -\dfrac{1}{m}\,B - \dfrac{4\Lambda_0}{\tau}\,A^2, \\ \dot{B} = -\dfrac{2}{m}\,C - \dfrac{4\Lambda_0}{\tau}\,AB + 2\kappa\,A, \\ \dot{C} = -\dfrac{\Lambda_0}{\tau}\,B^2 + \kappa\,B, \\ \dot{D} = \dfrac{2\Lambda_0}{\tau}\,A. \end{cases} \tag{5.3}$$

This system for A, B and C (which is decoupled from the equation for D) possesses the unique, asymptotically stable, equilibrium point $(A,B,C) = (0,0,0)$. This means that, as expected, the Wigner function is completely smoothed out towards a constant value (which is of course 0). Correspondingly, the coherence length goes to zero. The model is therefore not satisfactory for large times, since, as remarked by Joos and Zeh [32], the coherence must be maintained at least at the length-scale of the thermal De Broglie wavelength

$$\lambda_{\mathrm{th}} = \frac{\hbar}{\sqrt{2mk_BT}}, \tag{5.4}$$

where T is the temperature of the environment particle bath, and k_B is the Boltzmann constant.

By looking at the equilibrium conditions for system (5.3) we can guess that the addition to the first equation of a linear term in A, with positive coefficient,

is able to shift the equilibrium from $A = 0$ to a positive value. How such a term could arise from Eq. (5.1)? If we want to preserve the gaussian form (5.2) of the solution, we see that there are not many more possibilities than adding a derivative of w with respect to p and multiply it by p. We realised that this is provided by a "quantum friction" term proposed by Caldeira and Legget [13]. In fact, for high temperatures and in the density matrix formalism, this term appears at the right-hand side of the von Neumann equation (3.6) as

$$i\hbar\frac{\eta}{2}(X-Y)\left(\frac{\partial\rho}{\partial X}-\frac{\partial\rho}{\partial Y}\right),$$

where $\eta \geq 0$ is a "friction" coefficient [13,21]. Translating this term into the Wigner formalism, and adding it to the Wigner equation (5.1), we obtain

$$\frac{\partial w}{\partial t}+\frac{p}{m}\frac{\partial w}{\partial x}-\kappa\frac{\partial w}{\partial p}=\frac{\Lambda_0}{\tau}\frac{\partial^2 w}{\partial p^2}+\eta\frac{\partial}{\partial p}(pw), \tag{5.5}$$

which has exactly the needed form. Substituting (5.2) in (5.5) yields the new system of ODEs

$$\begin{cases} \dot{A}=-\dfrac{1}{m}B-\dfrac{4\Lambda_0}{\tau}A^2+2\eta A \\ \dot{B}=-\dfrac{2}{m}C-\dfrac{4\Lambda_0}{\tau}AB+2\kappa A+\eta B, \\ \dot{C}=-\dfrac{\Lambda_0}{\tau}B^2+\kappa B, \\ \dot{D}=\dfrac{2\Lambda_0}{\tau}A-\eta, \end{cases} \tag{5.6}$$

possessing the asymptotically stable equilibrium point

$$(A_0,B_0,C_0)=\left(\frac{\tau\eta}{2\Lambda_0},0,\frac{m\tau\kappa\eta}{2\Lambda_0}\right). \tag{5.7}$$

Note that the asymptotic coherence length is

$$\hbar\sqrt{2A_0}=\hbar\sqrt{\frac{\tau\eta}{\Lambda_0}}=\frac{\hbar}{\sqrt{mk_BT}},$$

where the last equality holds if one takes the relation

$$\Lambda_0=\tau m\eta k_BT,$$

as it is done, e.g., in Ref. [21]. Hence, we obtain that the asymptotic coherence length is of the order of the thermal De Broglie wavelength (5.4), exactly as

physically expected. We also note that the simultaneous presence of the friction and of the harmonic potential stabilises the position spread towards the asymptotic value

$$\frac{1}{\sqrt{2C_0}} = \sqrt{\frac{\Lambda_0}{2\tau\kappa\eta}} = \sqrt{\frac{k_B T}{\kappa}}$$

(where the last equality holds if one takes Λ_0 as above).

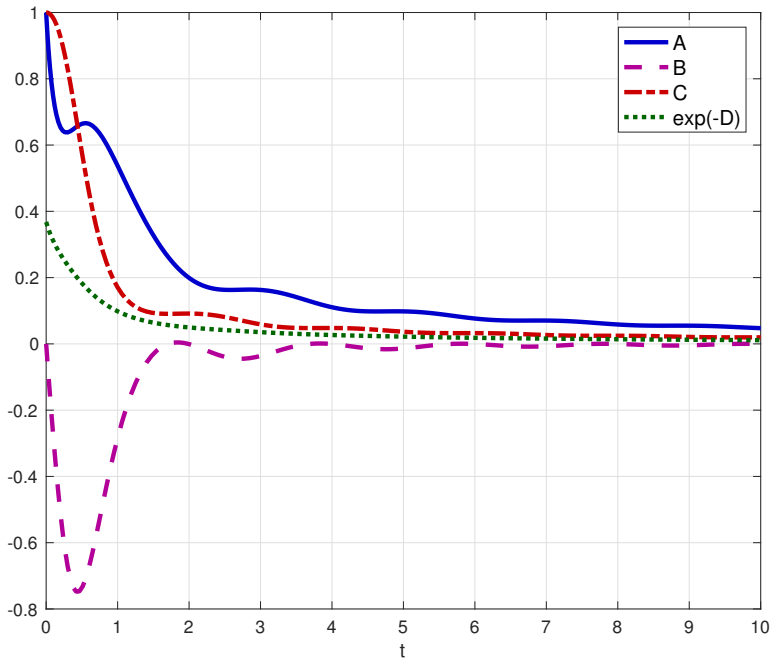


Figure 5.1: Evolution of the parameters A (continuous blue line), B (purple dashed line) and C (red dot-dashed line) of the Wigner function (5.2) in absence of friction ($\eta = 0$). The overall normalisation coefficient $\exp(-D)$ (dotted green line) is also shown. We assume to work in arbitrary units in which $m = 0.4$, $\tau = 1$, $\Lambda_0 = 1$ and $\kappa = 1$.

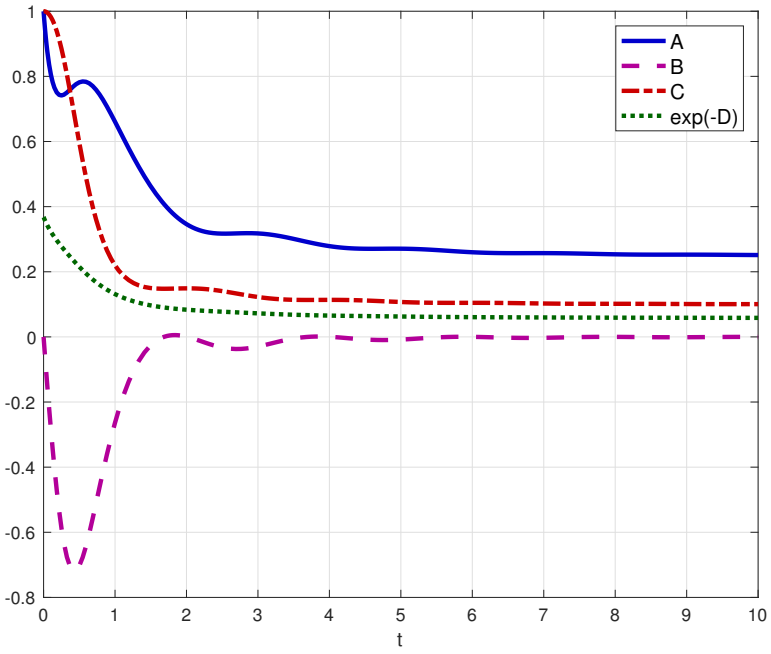


Figure 5.2: The same as in Figure 5.1 but with the addition of the friction. The values of the parameters are $m = 0.4$, $\tau = 1$, $\Lambda_0 = 1$, $\kappa = 1$ and $\eta = 0.5$.

In Figures 5.1–5.3 we show some solutions to system (5.6). In Figure 5.1 we set $\eta = 0$ and we can see that in the absence of friction both $A(t)$ and $C(t)$ approach zero as $t \to \infty$. This means that the Wigner function becomes infinitely spread out in both momentum and position, and tends to zero everywhere ($D(t) \to +\infty$). When a friction is added (Figure 5.2), both the momentum and the position spread stabilise to their asymptotic values (5.7). In this case, the Wigner function does not vanish, since $D(t)$ tends to an asymptotic positive value. When the harmonic trap is switched off by putting $\kappa = 0$, we can see that friction is able to stabilise the momentum spread but not the position spread (Fig. 5.3). Consequently, the Wigner function becomes completely spread out in the x direction and, as in the case of Fig. 5.1, tends to vanish ($D(t) \to +\infty$).

In the figures we use arbitrary units, where, in particular, $\tau = 1$. The actual decoherence time depends of course on the considered system (namely, the size and mass of the particle, the scattering properties and the temperature of the environment, and so on). We refer the reader to the accurate discussion contained in Ref. [32].

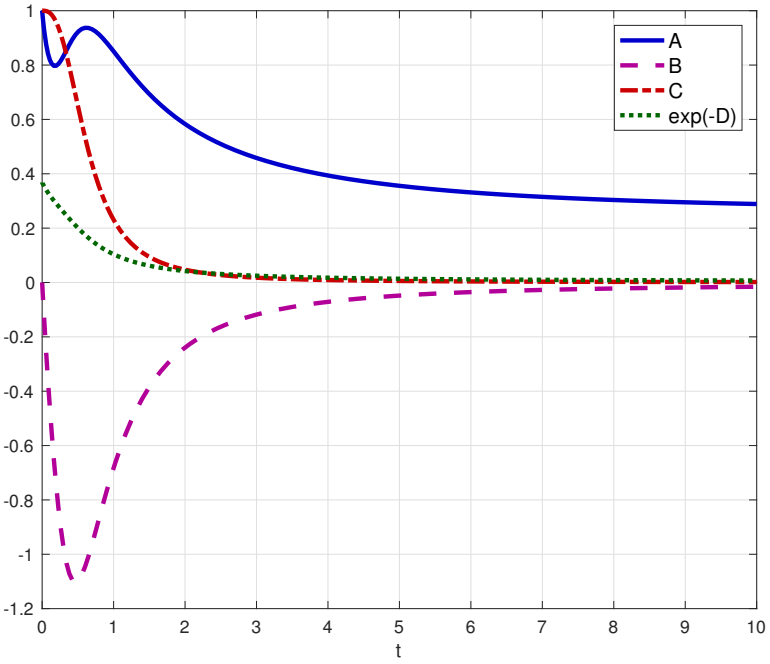


Figure 5.3: The same as in Figure 5.2 but with the harmonic potential removed. The values of the parameters are $m = 0.4$, $\tau = 1$, $\Lambda_0 = 1$, $\kappa = 0$ and $\eta = 0.5$.

The dissipative character of the new term is clearly seen by computing its moments:

$$\int_{\mathbb{R}} \frac{\partial}{\partial p}(pw)\,dp = 0, \qquad \frac{1}{m}\int_{\mathbb{R}} p\frac{\partial}{\partial p}(pw)\,dp = -J, \qquad \frac{1}{2m}\int_{\mathbb{R}} p^2\frac{\partial}{\partial p}(pw)\,dp = -2E.$$

These bring dissipative contributions to the Euler system, which takes the new form

$$\begin{cases} \dfrac{\partial N}{\partial t} + \dfrac{\partial J}{\partial x} = 0, \\ \dfrac{\partial J}{\partial t} + \dfrac{\partial \mathscr{J}_J}{\partial x} + \dfrac{1}{m}V'N = \dfrac{\hbar\Lambda_1}{m\tau}N - \eta J, \\ \dfrac{\partial E}{\partial t} + \dfrac{\partial \mathscr{J}_E}{\partial x} + V'J = \dfrac{\hbar\Lambda_1}{m\tau}J - \dfrac{\hbar^2\Lambda_2}{m\tau}N - 2\eta E. \end{cases} \tag{5.8}$$

5.2 The issue of the equilibrium trend

The asymptotic behaviour in non-homogeneous media is not trivial and should require other long efforts, but the x-homogeneous case fits well with standard techniques as entropy methods. At the same time Chapman-Enskog approximations and the diffusive limit would reveal important information about the solution properties. Formal computations follow, starting from an equation like (5.5), where the decoherence dynamics (3.11) is added a friction general term

$$\eta \frac{\partial}{\partial p}(pw). \tag{5.9}$$

Hence, in absence of an external potential, we have

$$\frac{\partial}{\partial t} w + \frac{p}{m}\frac{\partial}{\partial x} w = \eta \frac{\partial}{\partial p}(pw) - \nu\gamma *_p w, \tag{5.10}$$

with $\nu = \frac{1}{\tau}$, as usual. In the x-homogeneous case, $w = w(t,p)$ and Eq. (5.10) becomes simply

$$\frac{\partial}{\partial t} w = \eta \frac{\partial}{\partial p}(pw) - \nu\gamma * w. \tag{5.11}$$

If we Fourier-transform with respect to the p variable and set $u(t,\xi) = \mathscr{F}\{w(t,p)\}$, Eq. (5.11) reads

$$\frac{\partial}{\partial t} u(t,\xi) + \eta\xi \frac{\partial}{\partial \xi} u(t,\xi) = -\mu\,\Lambda(\xi)\,u(t,\xi), \tag{5.12}$$

where $\mu = \nu\sqrt{2\pi}$ and $\Lambda = \mathscr{F}\gamma$. By the characteristic method for linear partial differential equations we are able to find a solution of this kind

$$u(t,\xi) = u_0(\xi e^{\eta t}) e^{-\frac{\mu}{\eta}\int_\xi^{\xi e^{-\eta t}} \frac{\Lambda(k)}{k} dk}, \tag{5.13}$$

where $u_0(\xi e^{-\eta t})$ is the solution of Eq. (5.12), once one has set $\nu = 0$, i.e. $\tau \to \infty$. In the limit $t \to \infty$, $u(t,\xi) \to u_0(0)$ which, translated to w, is nothing but the number density $N_\infty = N(t \to \infty)$ (see (3.20)) for the x-homogeneous case. We get the final form of $u(t,\xi)$ as $t \to \infty$,

$$u_\infty(\xi) = N_\infty e^{-\frac{\mu}{\eta}\int_0^\xi \frac{\Lambda(k)}{k} dk}. \tag{5.14}$$

From this we can outline that when friction is dominating (i.e. $\eta >> \mu$), u_∞ reduces to the constant particle density number N and our function w is therefore a $\delta(p)$ function, corresponding to motionless particles. On the contrary, when $\eta << \mu$, then u_∞ vanishes to zero, confirming the importance of a friction

term in the equation. In the Fokker-Planck approximation $\Lambda(k) = \Lambda_2 k^2$, we obtain a gaussian

$$u_\infty(\xi) = Ne^{-\frac{\mu}{\eta}\frac{\xi^2}{2}},$$

that is consistent with and bring us back to the results gained in the previous Section 5.1. Dealing with the equilibrium issue, we ignore the time evolution and solve the stationary equation

$$\eta \frac{\partial}{\partial p}(pw) = \nu\gamma * w, \tag{5.15}$$

which in terms of u reads as in (5.12)

$$\eta\xi \frac{\partial}{\partial \xi} u(t,\xi) = \mu\,\Lambda(\xi)\,u(t,\xi), \tag{5.16}$$

leading to

$$u(\xi) = u(0)e^{-\frac{\mu}{\eta}\int_0^\xi \frac{\Lambda(k)}{k}dk}. \tag{5.17}$$

The questions we should try to find an answer concern the regularity of $w_\infty = \mathscr{F}^{-1}u_\infty$ which would depend on η and ν, but also on the specific form of the decoherence kernel γ. For instance, similarly to (3.18), if

$$\Lambda(\xi) = \alpha\left(1 - e^{\frac{\xi^2}{2\sigma^2}}\right),$$

the integral in (5.17) is asymptotical to $log(\xi)$ for large values of ξ, and so

$$u_\infty(\xi) \approx |\xi|^{-\frac{\alpha\mu}{\eta}}.$$

This suggests again the relevance of the ratio $\frac{\nu}{\eta}$ in order to make consistent our computation in the sense of the Fourier analysis.

Conclusions

We have seen how Wigner equation can be endowed with terms describing a dynamical decoherence mechanism. This is not a novelty, of course, but, as far as we know, this is the first time that the decoherence term has a fairly general form, coming from basic quantum mechanics. In particular, we started from the single-collision decoherence model derived in Ref. [3], which describes the decoherence of a "heavy" particle as a consequence of the collision with a much lighter one. By assuming the heavy particle to undergo multiple random collisions in an environment of light particles, we (formally) derived the Wigner equation (3.11). The latter admits two contributions from the collisions with the environment: a Hamiltonian part, represented by the function Γ, and a true decoherence part, represented by the function Λ, which is nothing but the inverse Fourier transform of the convolution kernel γ appearing in the right-hand side of Eq. (3.11). This picture allows for the interesting interpretation that decoherence smooths out the oscillations of the Wigner function, due to quantum interference, so that the Wigner function tends to a classical distribution in phase-space.

Then, we have seen that when Λ assumes particular forms, our model reduces to existing decoherence models. In particular, the largely-used Wigner-Fokker-Planck equation (3.17) corresponds to the quadratic approximation of Λ. Moreover, when $1-\Lambda$ is assumed to be a decaying exponential function, our model shows analogies with the Jacoboni-Bordone model [31], in which the exponential decay of the coherence length is embedded *ab initio* in the definition of the Wigner function. Our analysis, however, allows us to deduce some general features of decoherence (or, at least, of this kind of decoherence), as for example its effects on the dynamics of the macroscopic quantities N, J and E, i.e. the number, current and energy spatial densities (see Eq. (3.25)).

A big issue, already addressed in the classical paper by Joos and Zeh [32] is the long time behaviour of decoherence. In Section 5.1 we have considered the special case of a gaussian Wigner function, for which the Wigner equation (3.11), in the particular form (5.1), comes down to an equivalent system if

ODEs. In this way we realized that the addition of a Caldeira-Legget quantum friction term [13] produces a physically meaningful behaviour in the long run, since the momentum spread of the particle is stabilised to an asymptotic value. Equivalently, the coherence length, reaches a corresponding asymptotic value.

The addition of the quantum friction fixes the issue of the long-time behaviour, yet it is not completely satisfactory. In fact, as remarked by Arnold et al. [5,4], the friction + diffusion term (i.e. the right-hand side of Eq. (5.5)) is not quantum mechanically "correct" (unless $\eta = 0$), since it does not satisfy the Lindblad condition, assuring the complete positivity of the evolution [17]. We believe, however, that our analysis indicates the right direction to search for a model that is compatible with the fundamental laws of quantum mechanics and keeps its validity for asymptotically long times. We have sketched few ideas about this in Section 5.2 .

In Chapter 4 we had instead a satisfactory result from a physical point of view. Indeed, by the means of very basic numerical schemes, it turned out that decoherence, inhibiting reflection, favours transmission of low energy electrons through the potential barrier in the scattering process. Not by chance the effect is much weaker in a transmission-dominated regime.

The appropriateness of the language of mathematics for the formulation of the laws of physics is a wonderful gift which we neither understand nor deserve. We should be grateful for it and hope that it will remain valid in future research and that it will extend, for better or for worse, to our pleasure even though perhaps also to our bafflement, to wide branches of learning,

Eugene Wigner, [59].

Appendix 1

The following code is the one implemented to obtain Figure 3.2 in Matlab.

```
global xmax nx dx

%variables and domain
t = 0;
T = 1;
dt=T/50;

nx = 170;
np = nx;
nk = np;
xmax = 7;
x = linspace(-xmax,xmax,nx);
dx = 2*xmax/(nx-1);
y = x;
r = x;

[X,Y] = meshgrid(x,y);

p = linspace(-10,10,np);
[RR,P] = meshgrid(r,p);

k = linspace(-10,10,nk);
k = k';
[R,K] = meshgrid(r,k);

%parameters
p0 = 5;
x0 = 2;
sigma = .7;
tau = .005;
lam = 7;    % <----- this parameter is the major responsible for the fringes
            %       damping velocity

% density matrix definition
```

```
phipX = exp(-(X-x0).^2/(4*sigma^2)).*exp(-1i*p0*X)/((2*pi)^(1/4)*sigma);
phimX = exp(-(X+x0).^2/(4*sigma^2)).*exp(+1i*p0*X)/((2*pi)^(1/4)*sigma);
phipY = exp(-(Y-x0).^2/(4*sigma^2)).*exp(+1i*p0*Y)/((2*pi)^(1/4)*sigma);
phimY = exp(-(Y+x0).^2/(4*sigma^2)).*exp(-1i*p0*Y)/((2*pi)^(1/4)*sigma);

N = sqrt(2)*(1 + exp(-x0^2/(2*sigma^2))*exp(2*sigma^2)*p0^2);
N=1/N;

rho = (N^2)*(phipX + phimX).*(phipY + phimY);

% rotation R of the superposition initial state rho
etapX = exp(-(R+K/2-x0).^2/(4*sigma^2)).*exp(-1i*p0*(R+K/2))/((2*pi)^(1/4)*sigma);
etamX = exp(-(R+K/2+x0).^2/(4*sigma^2)).*exp(+1i*p0*(R+K/2))/((2*pi)^(1/4)*sigma);
etapY = exp(-(R-K/2-x0).^2/(4*sigma^2)).*exp(+1i*p0*(R-K/2))/((2*pi)^(1/4)*sigma);
etamY = exp(-(R-K/2+x0).^2/(4*sigma^2)).*exp(-1i*p0*(R-K/2))/((2*pi)^(1/4)*sigma);

eta = N^2*(etapX + etamX).*(etapY + etamY);

%decoherence operator I definition
I = exp(-K.^2/(2*(lam^2)));

%%%%%% let's start %%%%%

W0 = zeros(np,nx);
W = zeros(np,nx);
G = W;

lettera=1;
while t<T+dt
    % decoherence step for eta function
    eta = exp((I-1)*dt/tau).*eta;

    % Wignerization
    for j = 1:nx
        for i = 1:np
            f = eta(:,j);
            phas = exp(-1i*k*p(i));
            w = (1/2/pi)*trapz(k,f.*phas);
            W(i,j) = w;
         end
    end

    % Free transport step on Wigner function
    for j = 1:nx
        for i = 1:np
            xtrasl = x(j) - dt*p(i);
            jfloor = indj(xtrasl);
```

```
            alpha = (xtrasl - x(jfloor))/dx;
            G(i,j) = W(i,jfloor)*(1-alpha) + W(i,jfloor+1)*alpha;
        end
    end
    W = G;

    % Coming back step to eta function
     for j = 1:nx
        for i = 1:nk
            phas = exp(1i*k(i)*p);
            g = G(:,j);
            h = trapz(p,g'.*phas);
            eta(i,j) = h;
         end
     end

    % graphics
    set(gcf,'color','white')
    surfl(RR,P,real(W))
    axis([-5,5,-10,10,-0.07,0.07]);
    colormap(winter)
    shading interp
    axis on
    box off
    grid off
    xlabel('x')
    ylabel('p')
    zlabel('w')
    title(['w(x,p,t)    t = ' num2str(t,2)])
    shg
    drawnow
    saveas(gcf,strcat('immaginedeco',num2str(lettera),'.png'));
   lettera=lettera+1;
    t=t+dt;
end

function j = indj(x)
global xmax nx dx
r = floor((x+xmax)/dx +1);
if r < 1
    j = 1;
elseif r > nx-1
    j = nx-1;
else
    j = r;
end
end
```

Appendix 2

The following code is the one adopted for obtaining Tables 4.1, 4.2,4.3 in Chapter 4.

```
global hbar tau ;
hbar=0.5;
tau = 1000;
Lambda=[3,4,7,10,12,15,40,100,900];
Energies = [.5, 1, 1.5, 2];
LL=length(Lambda);
LE=length(Energies);


tabellaTC = zeros(LE,LL);
for a=1:LE
        for b= 1:LL
        tabellaTC(a,b) = trasmcoeff(Lambda(b),Energies(a))
    end
end



function TC = trasmcoeff(lambda,EK)

%Global Variables
global sigma0 x0 p0;
global kx kp;
global norm pav dx dp;
global tau hbar;
global filter;

%Quantities
    sigma0 = 0.1*EK;
    p0 = sqrt(2.0*EK);

%Domain and discretization
tinf=60.0;
```

```
tf=60.0;
x0=-0.5*p0*tinf;
n=1024;
m=1024;
dt=0.02;
dtm=0.5*dt;
xmax=150;
pmax=10.0;
dx=2*xmax/n;
dp=2*pmax/m;
x=-xmax+(0:(n-1))*dx;
p=-pmax+(0:(m-1))*dp;
Fx=2*pi/dx;
Fp=2*pi/dp;
kx=(Fx/n)*(0:n/2);
kp=(Fp/m)*(0:m/2);

%barrier
filter=zeros(1,m);
for j= 1 : m/2+1
    filter(j)=(1-ffilter(kp(j)/lambda))/tau;
end
for j= m/2+2 : m
    filter(j)=filter(m-j+2);
end

%initialization
t=0.0;
it=1;
tt(it)=t;
f=zeros(n,m);
for i=1:n
    for j=1:m
        f(i,j)=finit(x(i),p(j));
    end
end
dens=moments(p,f,n,m);
pavt(it)=pav;
normt(it)=norm;
% figure
% plot(x,dens);
plot(tt,pavt);
% hold on
%contours=[0.0005, 0.001, 0.02,0.2,0.4];
% contours=[0.02 0.2 0.4];
% figure;
% contour(x,p,f',contours,'k');
```

```
% hold on;
[X,P]=meshgrid(x,p);
F=f';
% figure
% surfl(X,P,F);
% shading interp;
% grid off;
% hold on
w=hshift(f, p, n, m, dtm);
dtprint=tf/5;
tprint=dtprint;
ifig=1;
tic
f=w;
while t <= tf
    w=pshift(f, x, p, n, m, dt,lambda);
    f=hshift(w, p, n, m, dt);
    t=t+dt;
    it=it+1;
    tt(it)=t;
    dens=moments(p,f,n,m);
    pavt(it)=pav;
    normt(it)=norm;
%     if t>=tprint
%         figure
%         plot(x,dens);
%         hold on
%         figure;
%         contour(x,p,f',contours,'r');
%         hold on;
%         F=f';
%         figure
%         surfl(X,P,F);
%         shading interp;
%         grid off;
%         hold on
%         tprint=tprint+dtprint
%         ifig=ifig+1
%     end
end
% figure
% plot(x,dens);
% hold on
% figure;
% contour(x,p,f',contours);
% hold on;
F=f';
```

```
% figure
% surfl(X,P,F);
% shading interp;
% grid off;
% hold on
% figure
% plot(tt,pavt);
% hold on;
% figure
% plot(tt,normt);
% axis([0 tf 0 1.2]);
% hold on;
toc


%calculus transmission coefficients

integranda=zeros(1,m);
for jj = 1:m
    integranda(jj) = trapz(x,F(:,jj));
end
p_average=trapz(p,p.*integranda);
TC=(1+p_average/p0)/2;

end

function w=finit(x,p) %funzione initiale
    global hbar sigma0 x0 p0;
    arg=sigma0*(x-x0)^2+hbar^2*(p-p0)^2/(4*sigma0);
    w=exp(-2*arg/hbar^2)/(pi*hbar);
end

function w=moments(p,f,n,m)
    global norm pav dx dp;
    w=zeros(1,n);
    sum1=0.0;
    sum2=0.0;
    for i=1:n
        sum=0.0;
        for j=1:m
            sum=sum+f(i,j);
            sum1=sum1+p(j)*f(i,j);
            sum2=sum2+f(i,j);
        end
        w(i)=sum*dx;
    end
    norm=sum2*dp*dx;
```

```
    pav=sum1*dp*dx/norm;
end
function f=ffilter (x)   %potential
    f=1/cosh(x);
end


function w=hshift(f, p, n, m, dt)
    global kx;
    w=zeros(n,m);
    for j=1:m
        y=zeros(1,n);
        zr=zeros(1,n);
        zi=zeros(1,n);
        for i=1:n
            y(i)=f(i,j);
        end
        z=fft(y);
        pdt=p(j)*dt;
        for i=1:n/2+1
            kpdt=kx(i)*pdt;
            tempr=real(z(i))/n;
            tempi=imag(z(i))/n;
            zr(i)=tempr*cos(kpdt)+tempi*sin(kpdt);
            zi(i)=tempi*cos(kpdt)-tempr*sin(kpdt);
        end
        for i=n/2+2:n
            zr(i)=zr(n-i+2);
            zi(i)=-zi(n-i+2);
        end
        zi(n/2+1)=0.0;
        z=complex(zr,zi);
        y1=ifft(z*n);
        w(1:n,j)=y1';
    end
end


function w=pshift(f, x, p, n, m, dt,lambda)
    global kp filter;
    global hbar;
    global tau;
    w=zeros(n,m);
    for i=1:n
        y=zeros(1,m);
        for j=1:m
            y(j)=f(i,j);
```

```
        end
        z=fft(y);
        zr=real(z(1:m/2+1))/m;
        zi=imag(z(1:m/2+1))/m;
        for j=1:m/2+1
            tempr=zr(j);
            tempi=zi(j);
            sym=(pot(x(i)+0.5*hbar*kp(j))-pot(x(i)-0.5*hbar*kp(j)))/hbar;
            zr(j)=exp(-filter(j))*(tempr*cos(sym*dt)-tempi*sin(sym*dt));
            zi(j)=exp(-filter(j))*(tempi*cos(sym*dt)+tempr*sin(sym*dt));
        end
        for j=m/2+2:m
            zr(j)=zr(m-j+2);
            zi(j)=-zi(m-j+2);
        end
        zi(m/2+1)=0.0;
        z=complex(zr,zi);
        y1=ifft(z*m);
        w(i,1:m)=y1';
    end
end
function f=pot(x)
    f=exp(-x^2);
end
```

```
%density in time

%Global Variables
global hbar tau ;
global sigma0 x0 p0;
global kx kp;
global norm pav dx dp;
global filter;
hbar=0.5;
tau = 10;

tinf=60.0;
tf=60.0;

Lambda=[4,7,10,12,15,40,100];
Energies = [.5, 1, 1.5];
LL=length(Lambda);
LE=length(Energies);
```

```
%Domain and discretization
n=1024*2;
m=1024*2;
dt=0.02;
dtm=0.5*dt;
xmax=550; %350
pmax=15.0; %10
dx=2*xmax/n;
dp=2*pmax/m;
x=-xmax+(0:(n-1))*dx;
p=-pmax+(0:(m-1))*dp;
Fx=2*pi/dx;
Fp=2*pi/dp;
kx=(Fx/n)*(0:n/2);
kp=(Fp/m)*(0:m/2);


for a=1:LE
    EK=Energies(a);
    figure
    for b= 1:LL
    lambda= Lambda(b);
    %Quantities
    sigma0 = 0.1*EK;
    p0 = sqrt(2.0*EK);
    x0=-0.5*p0*tinf;

%barrier
filter=zeros(1,m);
for j= 1 : m/2+1
    filter(j)=(1-ffilter(kp(j)/lambda))/tau;
end
for j= m/2+2 : m
    filter(j)=filter(m-j+2);
end

%initialization
t=0.0;
it=1;
tt(it)=t;
f=zeros(n,m);
for i=1:n
    for j=1:m
        f(i,j)=finit(x(i),p(j));
    end
end
```

```
dens=moments(p,f,n,m);
pavt(it)=pav;
normt(it)=norm;

w=hshift(f, p, n, m, dtm);
dtprint=tinf/5;
tprint=dtprint;
ifig=1;
tic
f=w;
while t <= tf
    w=pshift(f, x, p, n, m, dt,lambda);
    f=hshift(w, p, n, m, dt);
    t=t+dt;
    it=it+1;
    tt(it)=t;
    dens=moments(p,f,n,m);
    pavt(it)=pav;
    normt(it)=norm;

end
F=f';
figure((a-1)*2+1)
plot(x,dens);
title (['density profile with \tau=10, E_K=' num2str(EK,2)])
legend('\lambda = 4','\lambda = 7','\lambda = 10','\lambda = 12','\lambda = 15','\lambda = 40','\l
hold on
figure(a*2)
plot(tt,normt);
axis([0 tf 0 1.2]);

hold on
toc
 end
end
function w=finit(x,p) %funzione initiale
    global hbar sigma0 x0 p0;
    arg=sigma0*(x-x0)^2+hbar^2*(p-p0)^2/(4*sigma0);
    w=exp(-2*arg/hbar^2)/(pi*hbar);
end
function w=moments(p,f,n,m)
    global norm pav dx dp;
    w=zeros(1,n);
    sum1=0.0;
    sum2=0.0;
    for i=1:n
        sum=0.0;
```

```
        for j=1:m
            sum=sum+f(i,j);
            sum1=sum1+p(j)*f(i,j);   %rettangoli
            sum2=sum2+f(i,j);
        end
        w(i)=sum*dx;
    end
    norm=sum2*dp*dx;
    pav=sum1*dp*dx/norm;
end
function f=ffilter (x)   %potential
    f=1/cosh(x);
end
```

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