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Perturbation Theory in Terms of a Generalized Phase-Space Quantization Procedure

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To the memory of Carlo Cercignani

Abstract. – A new approach to perturbation theory in the quantum phase-space formalism is proposed, in order to devise some approximated description of the quantum phase-space dynamics, which is not directly related to the usual semi-classical approximation. A general class of equivalent quasi-distribution functions based on the Wigner-Moyal formalism is considered and a first-order invariant formulation of the dynamics is obtained. The relationship between the various phase-space representations is expressed in term of a pseudo-differential operator defined by the Moyal product. In particular, our theory is applied to the sub-class of representations obtained by a first order perturbation of the Wigner representation. Finally the connection of our approach with some well established gauge-invariant formulations of the Wigner dynamics in the presence of an external magnetic field is investigated.

1. – Introduction.

Since the early studies, the Schrödinger formalism was considered the framework where the perturbative approach to quantum mechanics could been developed in a natural way [1]. In this context, a particular importance was ascribed to the choice of the basis elements used to perform the perturbation expansion. In particular, when the mathematical formalism of quantum mechanics was developed, it was recognized the central role played by the unitary operators. A separable Hilbert space can be characterized by a complete set of basis elements \( \psi_i \), which in turn can be identified by a unitary transformation \( \Theta \) (defined in terms of the projection of the \( \psi_i \) on a reference basis). The class of unitary operators \( \mathcal{C}(\Theta) \) thus defines all the alternative sets of basis elements or “representations” of this Hilbert space. Once a representation is defined, the relevant physical variables and the quantum operator can be explicitly addressed. The use of a suitable unitary transformation can be considered a simple and powerful instrument to investigate equivalent mathematical formulations related to the same physical context. For these reasons a strict connection with the theory of unitary transformations is often found in the context of the quantum perturbation theory.

The phase-space formulation of quantum mechanics [2] offers a framework in which quantum phenomena can be described with a classical language and the
issue of quantum-classical correspondence can be directly investigated. In particular, the visual representation of the quantum motion, represented by quantum-corrected phase-space trajectories, is a valuable aid to a conceptual understanding of the complex quantum dynamics. One of the problems of the description of a quantum system at the kinetic level is that the overall mathematical complexity of the problem increases and, often, the solution of the equation of motion is only available from numerical approximations.

For that reason, it should be very attractive to develop a general procedure where the quantum correction induced by a perturbation of the Hamiltonian can be obtained. In connection with the asymptotic study of quantum systems, the attention is often addressed to the “classical limit” and a huge amount of work has been devoted to derive quantum corrections to a classical system on term of $\hbar$-expansion. Few general results are however available in the phase-space framework concerning the correction of the quantum solution induced by an “external” perturbation of the Hamiltonian. At the same time, it is well known that due to the non-commutativity of quantum mechanical operators, there is no a unique way to describe a quantum system by a phase-space distribution function. In particular, among all the possible definitions of quantum phase-space distribution functions, the Wigner function, the Glauber-Sudarshan $P$ and $Q$ functions, the Kirkwood distribution function and the Husimi distribution have attained a considerable interest (see for example [3] for a complete review).

Even if in principle all these different formulations of the quantum mechanics in the classical phase-space are equivalent, a convenable choice of the representation could strongly simplify the study of a certain class of problems. For example, the Glauber-Sudarshan distribution function has revealed to be particularly convenable to evaluate expectation values of normally-ordered operators used in the quantum optics [4], and in the field of solid state physics, due to the strong similarity with the classical Boltzmann equation, the Wigner formalism is considered as a natural choice to derive quantum corrections to the classical phase-space motion or in the description of the collision processes [5, 6, 7]. Moreover, the choice of the representation is a crucial aspect in deriving the semi-classical limit of the quantum many-body evolution problem. In fact, the Wigner function fails to produce a converging $\hbar$-series in the presence of self-consistent many-particle Hamiltonians, while the convergence of the $\hbar$ expansion can be improved considerably by viewing the semi-classical limit in the Husimi representation [3].

The phase-space representation of quantum mechanics is often considered as a mathematical tool particularly suitable to treat a certain class of physical problems. In particular, based on some general considerations, the choice of the convenient representation is defined a priori, and usually no attempt is done to search for the most convenient representation for the specific problem under study. If we compare this with the description of quantum mechanics based on
the Schrödinger wave function, where the use of the basis rotation is often exploited to obtain simpler mathematical representation of the system, we note that, in general, the use of a fixed phase-space representation, is not the most convenient approach. This is particularly evident in connection with the perturbation theory where the convergence of the series is often improved by using a suitable set of the basis elements.

Despite the progress obtained in this field, a general framework where quantum effects can be easily included in a particle system, where also classical transport plays an important role, is far from being achieved. Different approaches based on the density matrix, non equilibrium Green functions, and the Wigner function have been proposed to achieve a full quantum description of electron transport. Among them, the Wigner-function formalism is the one that bears the closest similarities to the classical Boltzmann equation, which suggests the possibility of using this formalism in order to obtain quantum corrections to the single and multi-band classical phase-space motion [8, 9, 10].

At the Schrödinger level, the “position” and the “momentum” representations are alternative mathematical descriptions of the system, where the position and momentum operators (\(r, p\)), are formally substituted by the operators (\(r, -i\hbar \nabla_r\)) and (\(i\hbar \nabla_p, p\)) respectively. From a mathematical point of view, a clear distinction is made between position and momentum degrees of freedom of a particle (and which are represented by multiplicative or derivative operator). This is in contrast with the classical motion described in the phase-space, where the position and the momentum of a particle are treated equally, and they can be interpreted just as two different degrees of freedom of the system.

Since the pioneering study of von Neumann [11], considerable interest has been devoted to the study of the relationship between classical and quantum systems and in particular various approach has been developed to establish an appropriate “quantization procedure”. By the term “quantization procedure” we mean a general correspondence between a function \(\mathcal{A}(r, p)\) defined on the classical phase-space, and some well-defined quantum operator \(\hat{\mathcal{A}}(r, p)\) acting on the physical Hilbert space. Due to the non commutativity of the quantum operators \(r\) and \(p\), different choices are possible. In particular in the correspondence \(\mathcal{A}(r, p) \rightarrow \hat{\mathcal{A}}(r, p)\), any other operator that differs from \(\hat{\mathcal{A}}(r, p)\) for the order in which the operators \(r\) and \(p\) appear, can in principle been used equally well to define a new quantum operator. The most common quantization procedures are the standard (anti-standard) Kirkwood ordering, the Weyl (symmetrical) ordering, and the normal (anti-normal) ordering. In particular, standard (anti-standard) ordering refers to a quantization procedure where, given a function \(\mathcal{A}\) admitting Taylor expansion, all of the \(p\) operators appearing in the expansion of \(\hat{\mathcal{A}}(r, p)\) follow (precede) the \(r\) operators. A different choice is made in the Weyl ordering rule where the following association \(e^{i(\eta p + \mu r)} \leftrightarrow e^{i(\eta r + \mu p)}\) holds (here \(\eta, \mu\) are real constants). Following Cohen [12], one can consider a general class of
quantization procedures defined in term of an auxiliary function \( \chi(r,p) \). We restrict to the one-dimensional case for the sake of simplicity (the generalization to the \( n \)-dimensional case being straightforward). The invertible map

\[
A(r,p) \equiv \text{Tr} \left\{ \hat{A}(r,p)e^{i(\mu r + \nu p)}\chi(r,p) \right\}
\]

\[
= \frac{\hbar}{2\pi} \int \left\langle r' + \frac{\eta\hbar}{2} \right| \hat{A} \left| r' - \frac{\eta\hbar}{2} \right\rangle \chi(\mu,\eta) e^{i(r-r')\mu - i\eta p} d\mu d\eta dr'
\]

defines the correspondence \( \hat{A}(r,p) \rightarrow A(r,p) \) and it is referred to as \( \chi \)-transform”. With different choices of the function \( \chi \) we describe different rules of association. In particular if \( \hat{A} \) is the density operator \( \hat{\rho} \) (representing a state of the system), from Eq. (1) we obtain the quantum distribution function \( f^\chi \). One of the main advantage in the application of the definition (1) is that the expectation value of the operator \( \hat{A}(r,p) \) can be obtained by the mean value of the function \( A(r,p) \) under the “measure” of the distribution density \( f^\chi \)

\[
\text{Tr} \left\{ \hat{A}(r,p)\hat{\rho}(r,p,t) \right\} = \int A(r,p)f^\chi(r,p,t) d\rho dr.
\]

As particular cases, it is possible to recover the definition of the most common quasi-probability distribution functions (classification scheme of Cohen). For example for \( \chi = e^{\pm i\frac{\eta^2}{2}} \) we obtain the standard \((-\)) or anti-standard \((+\)) ordered Kirkwood distribution function.

The case of particular interest for our approach is \( \chi = 1 \), which is related to the Weyl ordering rules and where the distribution density \( f^\chi \) becomes the Wigner distribution function

\[
f^W(r,p) \equiv \frac{1}{2\pi} \int \left\langle r + \frac{\eta\hbar}{2} \right| \hat{\rho} \left| r - \frac{\eta\hbar}{2} \right\rangle e^{-i\eta p} d\eta.
\]

We note that, differing from the Schrödinger formalism, where all the possible equivalent mathematical descriptions of a given physical system can be obtained by suitable unitary transformations, it is not clear which class of transformations can be included in this definition of \( \chi \)-transform given in Eq. (1). Even though the definition of \( \chi \)-transform is general enough to include the most relevant quasi-probability distribution densities, it should be desirable to obtain a different class of bilinear phase-space transformations (or quantization procedure) where the connection with the Schrödinger wave function representations can be explicitly investigated. Since at the Schrödinger level the representation of the system is defined by a basis set or, equivalently, by a unitary transformation \( \Theta \), such a procedure should define a bijective map between the representation space \( \mathcal{C}(\Theta) \) and the corresponding phase-space formulation.
In this work we present some results concerning the application of the perturbation theory in the quantum phase-space formalism. Equation (2) is considered as a starting point, in order to derive a general class of quasi-distribution functions, alternative to the Cohen classification. We use this formulation to derive some results based on a perturbation approach.

The rest of the paper is organized as follows. In Section 2 we introduce the $g$-representations of the phase-space description of a quantum system and its dynamics. In Sec. 3 the $g$-representations are exploited in order to find, by means of a variational procedure, the $g$-representation “best suited” to describe a perturbed dynamics. This is translated in Subsection 3.1 into an equation for $g$ and, in Subsection 3.2, the special case of the free-particle perturbation is examined. Then, in Sec. 4, the connections with the phase-space gauge transformations are discussed, which sets the basis for possible extensions of the method. Finally, Sec. 5 is devoted to conclusions.

2. – Representation of the phase-space dynamics.

In this section we present the mathematical ground used in our approach, the starting point being Weyl quantization. For the sake of concreteness hereafter we will consider a spinless quantum particle which can be represented by a wave function $\psi \in \mathbb{H} \equiv L^2(\mathbb{R}^n, \mathbb{C})$. Moreover, we restrict our discussion to the one-dimensional case ($n = 1$) because the extension of the method to a $n$-dimensional system is straightforward.

Let us consider, formally, an operator $\hat{A}$ acting on $\mathbb{H}$. The Weyl quantization procedure establishes a unique correspondence between $\hat{A}$ and a function $A(r, p)$, called the symbol of the operator [13]. We denote this map as $\mathcal{W}[A] = \hat{A}$. We have

$$\hat{A}h(x) = \mathcal{W}[A]h(x) = \frac{1}{2\pi\hbar} \int A\left(\frac{x + y}{2}, p\right) h(y) e^{i\pi(x-y)p} \, dy \, dp .$$

The inverse of $\mathcal{W}$ is given by the Wigner transform

$$A(r, p) = \mathcal{W}^{-1}\left[\hat{A}\right](r, p) = \int \mathcal{K}_A\left(r + \frac{\eta}{2}, r - \frac{\eta}{2}\right) e^{-i\eta p} \, d\eta ,$$

where $\mathcal{K}_A(x, y)$ is the kernel of the operator $\hat{A}$. Let us now fix an orthonormal basis $\mathbb{V} = \{v_i \mid i = 1, 2, \ldots\}$. A mixed state is defined by its density operator $\hat{S}_\psi$

$$\left(\hat{S}_\psi \right)(x) = \int \rho_\psi(x, x') h(x') \, dx'$$

whose kernel is the density matrix, identified by the coefficients with respect to
the basis $\psi$:
\[
\rho_{\psi}(x, x') = \sum_{i,j} \rho_{ij} \psi_i(x) \overline{\psi}_j(x').
\]

The von Neumann equation gives the evolution of the density operator $\hat{\mathcal{S}}_{\psi} = \hat{\mathcal{S}}_{\psi}(t)$ for a system with Hamiltonian operator $\hat{\mathcal{H}}$:
\[
i\hbar \frac{\partial \hat{\mathcal{S}}_{\psi}}{\partial t} = [\hat{\mathcal{H}}, \hat{\mathcal{S}}_{\psi}]
\]

where, as usual, the brackets denote the commutator. Eq. (6) gives the evolution of the system expressed in operatorial form. The equivalent Wigner evolution equation can be obtained by applying the Wigner transform, obtaining
\[
i\hbar \frac{\partial f_{\psi}}{\partial t} = [\mathcal{H}, f_{\psi}] = \mathcal{H} * f_{\psi} - f_{\psi} * \mathcal{H}
\]

where the symbol $2\pi f_{\psi} = \mathcal{W}^{-1} \left[ \hat{\mathcal{S}}_{\psi} \right]$ is the Wigner transform of the function $\rho_{\psi}(x, x')$
\[
f_{\psi}(r, p) = \frac{1}{2\pi} \int \rho_{\psi} \left( r + \frac{\eta}{2}, r - \frac{\eta}{2} \right) e^{-i \eta \cdot \eta} \, d\eta.
\]

The symbol $*$ in Eq. (7) denotes the Moyal product. When two phase-space functions $A$ and $B$ are smooth enough, the Moyal product between $A$ and $B$ admits the following $\hbar$-expansion
\[
A * B = \sum_{k=0}^{\infty} \frac{\hbar^k}{(2i)^k} \sum_{|a| + |b| = k} \frac{(-1)^{|a|}}{a! b!} \left( \partial_{\rho}^a \partial_{p}^b A \right) \left( \partial_{\rho}^a \partial_{p}^b B \right)
\]

and
\[
[A, B]_* = \sum_{k=1,3,5,\ldots} \frac{\hbar^k}{(2i)^k} \sum_{0 < \beta < k/2} \frac{2(-1)^{\beta+1}}{(k - \beta)! \beta!} \left[ \left( \partial_{\rho}^{k-\beta} \partial_{p}^{\beta} A \right) \left( \partial_{\rho}^{k-\beta} \partial_{p}^{\beta} B \right)
\]
\[ - \left( \partial_{\rho}^{k-\beta} \partial_{p}^{\beta} B \right) \left( \partial_{\rho}^{k-\beta} \partial_{p}^{\beta} A \right) \right].
\]

Let us now consider a spinless quantum particle of mass $m$ in the presence of a potential $U$. In this case, the Hamiltonian operator has the standard form
\[
\hat{\mathcal{H}} = -\hbar^2 \frac{\partial}{\partial x} + U(x),
\]

corresponding to the classical symbol $\mathcal{H}(r, p) = \frac{p^2}{2m} + U(r)$.

In the remaining part of this section, we study the modification of the explicit form of the Hamiltonian $\mathcal{H}$ (and thus of the equation of motion (7)), induced by a unitary transformation. We consider a unitary operator $\hat{\Theta}$ and the “rotated” orthonormal basis $\varphi = \{ \varphi_i \mid i = 1, 2, \ldots \}$, where $\varphi_i = \hat{\Theta} \psi_i$. It is easy to verify
that the following property

\[ \Theta^{-1}(r, p) = \Theta(r, p), \]

holds, where, according to Eq. (4), \( \Theta \Theta^{-1} \) is the Weyl symbol of \( \Theta \Theta^{-1} \). Eq. (9) suggests to put

\[ \Theta(r, p) = e^{ig(r, p)}, \]

where \( g \) is a real function. In accordance with the previously introduced notations, the phase-space representation of the state under the unitary transformation \( \Theta \) will be denoted by \( f_{\Phi} \equiv \mathcal{W}^{-1}\left[ \tilde{S}_{\Phi} \right] \), where \( \tilde{S}_{\Phi} \) is the new density operator of the system:

\[ \tilde{S}_{\Phi} = \Theta \tilde{S}_{\Phi} \Theta^\dagger, \]

where \( \Theta^\dagger \) denotes the adjoint operator. By using Eq. (9) it is immediate to verify that the equation of motion for \( f_{\Phi} \) is still expressed by Eq. (7) with the Hamiltonian \( \mathcal{H}' = \Theta \mathcal{H} \Theta^{-1} \). After some algebra it is possible to show that \( \mathcal{H}' \equiv \mathcal{W}^{-1}\left[ \Theta \mathcal{H} \Theta^\dagger \right] \) is explicitly given by

\[
\mathcal{H}'(r, p) = \int \Theta \left( \frac{r + r' + r''}{2}, \frac{p + p' + p''}{2} \right) \Theta^{-1} \left( \frac{r + r' - r''}{2}, \frac{p + p' - p''}{2} \right) \times
\left[U(r') + \frac{p^2}{2m}\right] e^{i\phi(r-r'p''-(p-p')r'')} \frac{dr' dp' dr'' dp''}{(2\pi \hbar)^2},
\]

which, by introducing the phase-space variable

\[ \zeta \equiv (r, p), \]

can be simplified into

\[
\mathcal{H}'(\zeta) = \int \Theta \left( \frac{\zeta + \zeta' + \eta}{2} \right) \Theta^{-1} \left( \frac{\zeta + \zeta' - \eta}{2} \right) \mathcal{H}(\zeta') e^{i\phi(\zeta-\zeta')} \frac{d\zeta'}{2\pi \hbar} \frac{d\eta}{(2\pi \hbar)^2},
\]

where

\[ \{a, b\} \equiv a_1 b_2 - a_2 b_1, \text{ with } a \equiv (a_1, a_2) \text{ and } b \equiv (b_1, b_2). \]

By using the “representation function” \( g \) (see Eq. (10)), the previous expression can be rewritten as

\[ \mathcal{H}'(\zeta) = \int \exp \left[ ig \left( \frac{\zeta + \zeta' + \eta}{2} \right) - ig \left( \frac{\zeta + \zeta' - \eta}{2} \right) \right] \mathcal{H}(\zeta') e^{i\phi(\zeta-\zeta')} \frac{d\zeta'}{(2\pi \hbar)^2}. \]

When passing from the position representation (where the basis elements in the
Schrödinger formalism are the Dirac delta distributions and where \( \hat{\Theta} \) is the identity operator), to another possible representation, the Hamiltonian operator which governs the evolution of the system modifies according to formula (12). Despite the mathematical structure of the equation of motion can be strongly affected by such basis rotation, from the definition of the function \( f_\varphi \) and from Eq. (7) we have that the distribution function is always defined in terms of the classical conjugated variables position and momentum.

In our approach, in analogy with the Schrödinger formalism, we use the class of unitary operators in order to “rotate” the Hilbert space \( \mathcal{H} \) and we define, accordingly, a class of equivalent quasi-distribution functions, or \( g \)-representations. Differing from the Cohen classification, the generality of our approach is ensured by the injective correspondence between a generical unitary transformation (describing all the physical relevant basis transformations) and a framework where the description of the problem is a priori in the phase-space.

3. – The perturbative procedure.

In this section we present an alternative approach to perturbation theory in the quantum phase-space framework. We rewrite the total Hamiltonian as

\[
\mathcal{H}(r, p) = \mathcal{H}_0(r, p) + \delta \mathcal{H}(r, p),
\]

where \( \mathcal{H}_0(r, p) \) represents the unperturbed system and \( \delta \mathcal{H}(r, p) \) is the perturbation, considered “small” compared to \( \mathcal{H}_0(r, p) \). Our method is based on the application of a variational procedure in order to relate the representation function \( g \), appearing in Eq. (12), and the perturbation \( \delta \mathcal{H} \). To this aim, a wide class of formulations of quantum mechanics in phase-space is exploited, and the function \( g(r, p) \) is considered as a new available degree of freedom. In particular, the \( g \)-representation can be used to “adapt” the phase-space formulation to the specific problem under consideration.

We define the evolution operator

\[
\mathcal{W}_g^{\mathcal{H}}[f] \equiv [\mathcal{H}', f]_*,
\]

where the symbol \( \mathcal{H}' \) is obtained from Eq. (12) with the substitution \( \mathcal{H} \rightarrow \mathcal{H}_0 + \delta \mathcal{H} \). Since the symbol \( \mathcal{H}' \) depends, through Eq. (12), both on the original Hamiltonian symbol \( \mathcal{H} \) and on the representation function \( g \), then we have indicate explicitly the dependence of the operator \( \mathcal{W}_g^{\mathcal{H}} \) on \( g \) and \( \mathcal{H} \). Note that

\[
(i \hbar \frac{\partial}{\partial t} = \mathcal{W}_g^{\mathcal{H}}[f]
\]

is the phase-space equation of motion in the \( g \)-representation for a system with Hamiltonian \( \mathcal{H} \).
We adopt the following strategy: we consider $g$ to be a functional of the total Hamiltonian $\mathcal{H}$ and, by using a variational procedure, we impose some constraint on the form of the equation of motion (13). Thus, we derive an equation for the function $g(r, p, \mathcal{H})$, for which the constraint is fulfilled. In this way, we implicitly define a map between the Hamiltonian of the system and the $g$-representation in the phase-space. In particular, in the present work, we shall restrict our attention to the subclass of the $g$-representations whose difference with the Wigner representation ($g = 0$) is of the first order with respect to the Hamiltonian perturbation $\delta \mathcal{H}$, i.e. \(^{(1)}\)

$$g(\mathcal{H}_0) = 0.$$  

Then, up to the first order in $\delta \mathcal{H}$, we have

$$\mathcal{H}^{\mathcal{H}}_{g(\mathcal{H})} = \mathcal{H}^{\mathcal{H}}_{g(\mathcal{H}_0)} + \delta \mathcal{H}^{\mathcal{H}}_{g(\mathcal{H}_0)} + o(\delta \mathcal{H})$$

with

\[
\delta \mathcal{H}^{\mathcal{H}}_{g(\mathcal{H}_0)} = \mathcal{H} \left( \frac{\partial \mathcal{H}}{\partial g} \frac{\delta g}{\delta \mathcal{H}} + \frac{\partial \mathcal{H}}{\partial \mathcal{H}} \right)_{g(\mathcal{H}_0)},
\]

where $\frac{\partial \mathcal{H}}{\partial g}$ and $\frac{\partial \mathcal{H}}{\partial \mathcal{H}}$ denote Fréchet derivatives. The constraint we are going to impose is that $g$ is chosen in such a way that (at least at first order in $\delta \mathcal{H}$) the evolution equation for the perturbed problem (13) takes the simplest possible form, namely the same of the “free” case:

\[
i \hbar \frac{\partial f}{\partial \mathcal{H}} = \mathcal{H}^{\mathcal{H}}_{g(\mathcal{H}_0)} [f].
\]

This amounts to solve the following problem: **find a representation function $g = g(\mathcal{H})$ such that**

\[
\delta \mathcal{H}^{\mathcal{H}}_{g(\mathcal{H}_0)} [f] = 0
\]

(for all $f$ in a suitable regularity domain), where $\delta \mathcal{H}^{\mathcal{H}}_{g(\mathcal{H}_0)}$ is given by (14) and $g(\mathcal{H}_0) = 0$. In other words, if such a function $g(\mathcal{H})$ exists, then the equation of motion is an invariant of the infinitesimal transformation $\mathcal{H}_0 \rightarrow \mathcal{H}$.

Equation (15) has the same form of a Wigner equation for the free Hamiltonian $\mathcal{H}_0$. However, $f$ is not the Wigner function of the system but it is the phase-space function in the $g$-representation. From Eq. (11) it easily follows that

\((1)\) The choice of the Wigner representation for the unperturbed problem is motivated only by simplicity, since the Wigner formulation leads to the simplest model for a free particle.
\(f\) is related to the Wigner function \(f_0\) by the transformation \(f = M_g[f_0]\), where

\[
M_g[f_0](\tilde{\xi}) = \int \exp \left[ i \left( \frac{\tilde{\eta} + \eta'}{2} \right) + i \left( \frac{\tilde{\eta} - \eta'}{2} \right) \right] f_0(\eta') e^{i \tilde{\xi} \cdot (\eta - \eta')} \frac{d \eta'}{(2\pi \hbar)^2},
\]

where we used phase-space variables as in (12). Thus, if we assume that the initial Wigner function \(f_0^{\text{in}}\) is known, then Eq. (15) has to be supplemented with the initial condition

\[f(t_0) = M_g[f_0^{\text{in}}].\]

Note that, somehow, all the effects of the perturbation have been concentrated in the initial datum. In other words, our procedure results into an extreme simplification of the evolution equation, which is paid by a complication in the initial datum. Also the physical interpretation becomes more involved since the relevant physical quantities of the system (such as density of particles, mean momentum, etc.) have simple expressions in terms of \(f_0\), but usually not in terms of \(f\). However, \(f_0\) can always be recovered from \(f\) by inverting the relation (17).

To summarize, our procedure leads to the following problem:

\[
\begin{cases}
  i\hbar \frac{\partial f}{\partial t} = \mathcal{W}_g^{\mathcal{H}_0}[f], \\
  f(t_0) = M_g[f_0^{\text{in}}], \quad g \text{ solves Eq. (16)},
\end{cases}
\]

where we recall that \(g(\mathcal{H}_0) = 0\). Finally, by using the linearity of \(\mathcal{W}_g^{\mathcal{H}}[f]\) with respect to \(f\), we note that the solution \(f\), up to the first order in the perturbation, can also be obtained as \(f = f_0 + \delta f\), where \(f_0\) is the Wigner function (satisfying the free Wigner equation) and \(\delta f\) satisfies

\[
\begin{cases}
  i\hbar \frac{\partial \delta f}{\partial t} = \mathcal{W}_g^{\mathcal{H}_0}[\delta f] \\
  \delta f(t_0) = M_g[f^{\text{in}}] - f^{\text{in}}.
\end{cases}
\]

As before, the description of the “frame rotation” \(g\) only affects the initial condition \(\delta f(t_0)\).

3.1 – The equation for \(g\).

In this section we derive an explicit equation for the representation function \(g\) such that it satisfies Eq. (16). i.e. \(\delta \mathcal{W}_g^{\mathcal{H}_0} = 0\). We can assume, rather generically, that \(g\) has an integral dependence of \(\mathcal{H}\) through some kernel \(\mathcal{K}_g\):

\[
g(r, p; \mathcal{H}) = \int \mathcal{K}_g(r, p, \tilde{r}, \tilde{p}, \mathcal{H}(\tilde{r}, \tilde{p})) \, d\tilde{r} \, d\tilde{p}
\]
or, using phase-space variables,

\begin{equation}
(20) \quad g(\xi; \mathcal{H}) = \int \mathcal{K}_g(\xi, \xi'; \mathcal{H}(\xi')) \, d\xi'.
\end{equation}

Moreover, according to the preceding discussion, we assume that

\begin{equation}
(21) \quad g(\xi; \mathcal{H}_0) = 0.
\end{equation}

for the unperturbed Hamiltonian \( \mathcal{H}_0 \). Our variational problem, given by Eq. (16), equivalent to \( \delta \mathcal{H}' = 0 \), requires the evaluation of the total variation of the Hamiltonian \( \mathcal{H}' \), defined by Eq. (12), which takes the form

\begin{equation}
(22) \quad \mathcal{H}'(\xi; \mathcal{H}) = \int \exp \left[ ig(\xi^+; \mathcal{H}) - ig(\xi^-; \mathcal{H}) \right] \mathcal{H}(\xi') \, e^{i(\xi' - \xi) / (2\pi \hbar)} \, \frac{d\xi'}{d\eta (2\pi \hbar)^2} \frac{d\xi'}{d\eta (2\pi \hbar)^2}
\end{equation}

where we introduced the shorthands

\[ \xi^+ = \xi' + \eta. \]

The variation of \( \mathcal{H}' \) with respect to \( \mathcal{H} \) at \( \mathcal{H}_0 \) is therefore given by

\[ \delta \mathcal{H}'(\xi, \mathcal{H}_0) = \int \exp \left[ ig(\xi^+; \mathcal{H}) - ig(\xi^-; \mathcal{H}) \right] i \left[ \delta g(\xi^+; \mathcal{H}) - \delta g(\xi^-; \mathcal{H}) \right] \frac{d\xi'}{d\eta (2\pi \hbar)^2} \]

\[ \times \mathcal{H}_0(\xi') \, e^{i(\xi' - \xi) / (2\pi \hbar)} \, \frac{d\xi'}{d\eta (2\pi \hbar)^2} + \int \exp \left[ ig(\xi^+; \mathcal{H}) - ig(\xi^-; \mathcal{H}) \right] \delta \mathcal{H}(\xi') \, e^{i(\xi' - \xi) / (2\pi \hbar)} \, \frac{d\xi'}{d\eta (2\pi \hbar)^2}, \]

where (21) is exploited and, recalling (20), the variation of \( g(\xi^\pm; \mathcal{H}) \) at \( \mathcal{H} = \mathcal{H}_0 \) is

\[ \delta g(\xi^\pm; \mathcal{H}) \bigg|_{\mathcal{H} = \mathcal{H}_0} = \int \frac{\partial K_g}{\partial \zeta}(\xi^\pm, \zeta, z) \bigg|_{z = \mathcal{H}_0(\xi)} \delta \mathcal{H}(\xi) \, d\zeta. \]

Thus we can write

\[ \delta \mathcal{H}'(\xi, \mathcal{H}_0) = \int \left\{ i \left[ g(\xi^+; \mathcal{H}) - g(\xi^-; \mathcal{H}) \right] \mathcal{H}_0(\xi') + \delta^D(\xi' - \xi) \right\} \delta \mathcal{H}(\xi) \, e^{i(\xi' - \xi) / (2\pi \hbar)} \, \frac{d\xi'}{d\eta (2\pi \hbar)^2}, \]

where \( \delta^D \) is the Dirac delta and

\begin{equation}
(23) \quad g(\xi^\pm, \mathcal{H}) \equiv \frac{\partial K_g}{\partial \zeta}(\xi^\pm, \zeta, z) \bigg|_{z = \mathcal{H}_0(\xi)}. \]
In the first part of the expression for $\delta \mathcal{H}'(\xi, \mathcal{H}_0)$ it is not difficult to identify a Moyal bracket of $g(\xi^\pm, \bar{\xi})$ (as a function of $\xi$) with the unperturbed Hamiltonian $\mathcal{H}_0$:

$$\int i\left[g(\xi^+, \bar{\xi}) - g(\xi^-, \bar{\xi})\right] \mathcal{H}_0(\xi^\prime) e^{\frac{i}{\hbar}(\xi - \xi^\prime) \eta} \frac{d\xi^\prime d\eta}{(2\pi\hbar)^2} = i[\mathcal{H}_0, g]_\times(\xi, \bar{\xi}).$$

Thus, by using also

$$\int \delta^D(\xi - \xi^\prime) e^{\frac{i}{\hbar}(\xi - \xi^\prime) \eta} \frac{d\xi^\prime d\eta}{(2\pi\hbar)^2} = \delta^D(\xi - \xi),$$

we arrive at

$$\delta \mathcal{H}'(\xi, \mathcal{H}_0) = \int \left\{i[\mathcal{H}_0, g]_\times(\xi, \bar{\xi}) + \delta^D(\xi - \xi)\right\} \delta \mathcal{H}(\xi) d\xi.$$  

(24)

In conclusion, the variational problem $\delta \mathcal{H}' = 0$ (or equivalently $\delta \mathcal{H}'_{\mathcal{H}_0} = 0$) is reformulated in terms of the following Green equation for the unknown $g = g(\xi, \bar{\xi})$:

$$i[\mathcal{H}_0, g]_\times = -\delta^D(\xi - \xi).$$

(25)

For an Hamiltonian of the form $\mathcal{H}_0(r, p) = \frac{p^2}{2m} + U(r)$ (and coming back to explicit phase-space variables), the previous equation takes the explicit form

$$\frac{\hbar}{m} \frac{\partial}{\partial r} g - i\Theta_U[g] = \delta^D(\bar{r} - r)\delta^D(\bar{p} - p),$$

(26)

where $g = g(r, p, \bar{r}, \bar{p})$ and

$$\Theta_U[g](r, p, \bar{r}, \bar{p}) = \frac{1}{2\pi} \int \left[U\left(r + \frac{\hbar}{2} \eta\right) - U\left(r - \frac{\hbar}{2} \eta\right)\right] g(r, p', \bar{r}, \bar{p}) e^{i(p - p') \eta} d\eta d\eta'. $$

3.2 – A particular case: the free particle.

As a simple example, we apply our procedure to a free particle, where $\mathcal{H}_0 = \frac{p^2}{2m}$ (i.e. $U = 0$). Furthermore, we limit ourselves to consider a potential-like perturbation $\delta \mathcal{H}(r, p) = \delta U(r)$. Since the perturbation does not depend on the momentum of the particle, it is possible to show that Eq. (26) simplifies into

$$\frac{\hbar}{m} \frac{\partial}{\partial r} g = \delta^D(r - \bar{r}),$$

(27)
which admits the solution
\[ g = g(r, p, \tilde{r}) = \frac{m}{\hbar p} \theta(r - \tilde{r}) + \gamma_0, \]
where \( \theta \) is the Heaviside step function and \( \gamma_0 \) is the integration constant. Since, from the previous subsection, \( g \) and \( \tilde{g} \) are related by
\[ \delta g(\xi, \mathcal{H}) |_{\mathcal{H} = \mathcal{H}_0} = \int g(\xi, \tilde{\xi}) \delta \mathcal{H}(\tilde{\xi}) \, d\tilde{\xi}, \]
then, in the particular case under consideration, we have that the first order contribution to the \( g \)-representation function is
\[ \delta g(r, p; U) = \int g(r, p, \tilde{r}) \delta U(\tilde{r}) \, d\tilde{r} = \int \left[ \frac{m}{\hbar p} \theta(r - \tilde{r}) + \gamma_0 \right] \delta U(\tilde{r}) \, d\tilde{r}. \]

4. – Connection with the Green gauge-invariant approach.

In this section we illustrate the connection of our theory with some gauge-invariant approach to the Wigner dynamics, by considering a single particle (in a three-dimensional space) in the presence of a static magnetic field. The formulae obtained in the previous sections have a straightforward generalization to the three dimensional case. In order to avoid confusion, three dimensional variables and vectors will be indicated in bold letters.

The magnetic field is described by a vector potential \( A(r) \) and, following the canonical substitution \( p \rightarrow p - \frac{e}{c} A(r) \), we have that the Hamiltonian of the system becomes
\[ \tilde{\mathcal{H}}(\nabla_x, x) = \frac{1}{2m} \left( -i \hbar \nabla_x - \frac{e}{c} A(x) \right)^2. \]
It is not difficult to show that the corresponding Hamiltonian symbol is \(^(2)^\)
\[ \mathcal{H}(r, p) = \mathcal{W}^{-1} \left[ \frac{1}{2m} \left( -i \hbar \nabla_x - \frac{e}{c} A(x) \right)^2 \right] = \frac{1}{2m} \left( p - \frac{e}{c} A(r) \right)^2. \]
It is well known that the vector potential \( A(r) \) can be perturbed by adding the gradient of a function, \( \nabla_r \chi \), without changing the physics of the problem. However, the formal substitution \( A(r) \rightarrow A(r) + \nabla_r \chi(r) \) modifies the form of the

\(^{(2)^}\) It is enough to notice that the Hamiltonian operator of Eq. (29) is the square of a sum of \( p \)-like and \( x \)-like operators, which guarantee the symmetric ordering of the operators, so that the correspondence between operators and functions becomes trivial.
equation of motion. A gauge-invariant transformation is a transformation allowing the definition of a new set of unknowns for which also the equation of motion is unaffected by the presence of the function \( \chi \). Our method applied to the perturbed Hamiltonian

\[
\mathcal{H}'(\mathbf{r}, \mathbf{p}) = \frac{1}{2m} \left[ \mathbf{p} - \frac{e}{c} \left( \mathbf{A}(\mathbf{r}) + \nabla_{\mathbf{r}} \chi(\mathbf{r}) \right) \right]^2 ,
\]

where the function \( \nabla_{\mathbf{r}} \chi \) plays the role of the perturbation, directly provides a gauge-invariant formulation of the Wigner dynamics (see Section 3). For sake of simplicity we shall limit ourselves to the case of a uniform magnetic field \( \mathbf{B} \), so that \( \mathbf{A} = \frac{1}{2} \mathbf{B} \times \mathbf{r} \).

The starting point is Eq. (25). Multiplying both sides by \( \delta \mathcal{H}'(\tilde{\xi}) \), integrating over \( \tilde{\xi} \) and using Eq. (28), we obtain an equation for \( \delta g \):

\[
i [\mathcal{H}_0, \delta g] = -\delta \mathcal{H}'.
\]

In our case, \( \mathcal{H}_0 = \frac{1}{2m} (\mathbf{p} - \frac{e}{c} \mathbf{A})^2 \) and \( \delta \mathcal{H}' = \frac{e}{mc} (\mathbf{p} - \frac{e}{c} \mathbf{A}) \nabla_{\mathbf{r}} \chi \) (which is easily obtained by expanding (30) with respect to \( \nabla_{\mathbf{r}} \chi \)) and then, after a little algebra, Eq. (31) yields

\[
(\mathbf{p} - \frac{e}{c} \mathbf{A}) \cdot \nabla_{\mathbf{r}} \delta g + \frac{e}{2c} \left[ (\mathbf{p} - \frac{e}{c} \mathbf{A}) \times \mathbf{B} \right] \cdot \nabla_{\mathbf{p}} \delta g = \frac{e}{\hbar c} (\mathbf{p} - \frac{e}{c} \mathbf{A}) \cdot \nabla_{\mathbf{r}} \chi .
\]

which admits the solution \( \delta g = \frac{e}{\hbar c} \chi \). Thus, recalling that the perturbed representation function is \( g = g_0 + \delta g \), with \( g_0 = 0 \), we get

\[
g = \frac{e}{\hbar c} \chi .
\]

Now, the perturbed, gauge-invariant, phase-space function \( f' \) is given by (the three-dimensional version of) Eq. (17) which, for \( g(\mathbf{r}, \mathbf{p}) = \frac{e}{\hbar c} \chi(\mathbf{r}) \), reads as follows:

\[
f'(\mathbf{r}, \mathbf{p}) = \int e^{i\frac{\hbar}{2} \left[ \chi(\mathbf{r} + \mathbf{s}) - \chi(\mathbf{r} - \mathbf{s}) \right]} e^{i \mathbf{p} \cdot \mathbf{s}} f_0(\mathbf{r}', \mathbf{p}') \frac{d\mathbf{r}' d\mathbf{p}' d\mathbf{s} d\mathbf{q}}{(2\pi \hbar)^6}
\]

\[
= \int e^{i\frac{\hbar}{2} \chi(\mathbf{r} + \mathbf{s} - 2\mathbf{r})} e^{i \mathbf{p} \cdot \mathbf{s}} f_0(\mathbf{r}, \mathbf{p}') \frac{d\mathbf{p}' d\mathbf{s}}{(2\pi \hbar)^3} .
\]

This expression can be clearly understood if we consider the Wigner function \( f_0 \) for a pure state defined by a wave function \( \psi \). It is well known that for the gauge transformation \( \mathbf{A}'(\mathbf{r}) = \mathbf{A}(\mathbf{r}) + \nabla_{\mathbf{r}} \chi(\mathbf{r}) \), the gauge-invariant wave function is \( \psi' = \psi e^{i\frac{\hbar}{2} \chi} \). It is immediate to verify that the corresponding Wigner function \( f' \) is related to \( f_0 \) exactly by Eq. (32).
We can now analyze the connections between our methodology and the standard Wigner-Green gauge theory [14, 15]. The gauge invariant Green function $G$ in the presence of an external vector potential $A(r)$ is usually defined in terms of the free Green function $G_0$ as follows:

$$G(r, p, t, \omega) = \int e^{-i \frac{p \cdot \delta x}{\hbar} + \frac{i}{\hbar} \int_{-1/2}^{1/2} s \cdot A(r + \delta s, t + \delta t) d\lambda} G_0(r, p', t, \omega') \times e^{i (\omega - \omega') + \frac{i}{\hbar} s \cdot (p' - p)} \frac{ds \, dp'}{(2\pi\hbar)^3} \frac{d\tau \, d\omega}{2\pi} .$$

By using the general relation between a Wigner function $f$ and a Green function $G$,

$$f(r, p, t) = \int G(r, p, t, \omega) \, d\omega ,$$

from (33) we obtain

$$f(r, p, t) = \int e^{-i \frac{p \cdot \delta x}{\hbar} + \frac{i}{\hbar} \int_{-1/2}^{1/2} s \cdot A(r + \delta s, t) d\lambda} f_0(r, p', t) e^{i \frac{s \cdot (p' - p)}{\hbar}} \frac{ds \, dp'}{(2\pi\hbar)^3} ,$$

where, of course, $f_0$ denotes the Wigner function corresponding to $G_0$. After the gauge “perturbation” $A(r) \rightarrow A(r) + \nabla r' \chi(r)$, the preceding relation, for the new Wigner function $f'$, becomes

$$f'(r, p, t) = \int e^{-i \frac{p \cdot \delta x}{\hbar} + \frac{i}{\hbar} \int_{-1/2}^{1/2} s \cdot A(r + \delta s, t) d\lambda + \chi \left( \frac{r + \delta s}{\hbar} \right) - \chi \left( \frac{r - \delta s}{\hbar} \right)} f_0(r, p', t) e^{i \frac{s \cdot (p' - p)}{\hbar}} \frac{ds \, dp'}{(2\pi\hbar)^3} .$$

We remark that, since in our theory the unitary transformations are assumed to be time-independent, it is evident that no time-dependent gauge transformation (including, for example, the relativistic-invariant ones) can be obtained. In order to compare the gauge transformation defined by Eq. (36) with the unitary transformation defined by Eq. (17) we shall restrict the gauge transformation to a time independent magnetic field. We shall show that, even in this case, the gauge transformations cannot be recast in the form (17) and, therefore, the class of unitary transformation is not large enough to include them.

To see this, since in (36) the $g$-function does not depend on $p$, we can restrict the discussion to a $\Theta$-transformation for which the $g$-function only depends on $r$. In this case Eq. (17) simplifies into

$$f'(r, p) = \int e^{i \left[ g \left( r + \frac{\delta x}{\hbar} \right) - g \left( r - \frac{\delta x}{\hbar} \right) \right]} f_0(r, p') e^{i \frac{s \cdot (p' - p)}{\hbar}} \frac{ds \, dp'}{(2\pi\hbar)^3} .$$

In order to compare this transformation with the gauge transformation (36), it is
convenient to look for a $g$ function of the (generic) form

$$g(r) = -\frac{e}{\hbar} \int_{\Gamma(r)} A(y) \cdot dy + \frac{e}{\hbar} \chi(r) + b(r)$$

where $b$ is a real function and $\Gamma(r)$ the straight-line integration path connecting a generic point O (that may be assumed to be the origin of the spatial axes) with $r$. By comparing (37) with (36) we see that we have to impose

$$g\left(r + \frac{s}{2}\right) - g\left(r - \frac{s}{2}\right) = -\frac{e}{\hbar} s \cdot \int_{-1/2}^{1/2} A(r + is) d\lambda - \frac{e}{\hbar} \int_{S(r,s)} B \cdot n \, d\sigma$$

$$+ \frac{e}{\hbar} \left[ \chi\left(r + \frac{s}{2}\right) - \chi\left(r - \frac{s}{2}\right) \right] + b\left(r + \frac{s}{2}\right) - b\left(r - \frac{s}{2}\right)$$

where $B = \nabla \wedge A$ is the magnetic field, the integration surface $S(r,s)$ is the triangle with vertices $\left(0, r + \frac{s}{2}, r - \frac{s}{2}\right)$ and $n$ is the (suitably oriented) unit vector normal to the surface $S(r,s)$. It is evident that the transformation (36) can be recast into the form (37) if and only if

$$b\left(r + \frac{s}{2}\right) - b\left(r - \frac{s}{2}\right) = \frac{e}{\hbar} \int_{S(r,s)} B \cdot n \, d\sigma$$

for all $r, s \in \mathbb{R}^3$. This equation, in general, has no solution. In fact when $r$ is parallel to $s$ the integral vanishes (the surface $S(r,s)$ degenerates on a line) and, since the equality must hold for any $r, s \in \mathbb{R}^3$, we conclude that the function $b$ is a constant independent on $B$, which makes Eq. (39) impossible to be satisfied for $B \neq 0$. Thus, in spite of the generality of our approach, there are some important transformations that cannot be expressed by (17). Such “negative” result should be considered as a useful guideline in view of possible extensions of our formalism that include more general transformations, still preserving the advantage of our approach (in particular, the possibility of deriving a systematic procedure that automatically guarantees the gauge-invariant formulation of the system).

5. – Conclusions.

In this contribution, a new approach to the perturbation theory in the quantum phase-space formalism has been proposed. In analogy with the Schrödinger formalism, the class of unitary operators $\Theta$ has been exploited in order to define a class of equivalent quasi-distribution functions ($g$-representations). The relationship between the various phase-space representations can be
then expressed by means of a pseudo-differential operator, defined in terms of the Moyal product, and the generality of our approach is ensured by a correspondence between the $g$-representation and the class of unitary transformations of the original Hilbert space. In particular, our theory has been developed by focusing on the subclass of $g$-representations obtained as a first order perturbation of the Wigner representation. For these representations, a variational procedure has been proposed that leads to the simplest possible phase-space dynamics description for a perturbed Hamiltonian. Finally, the connection of our approach with some well established gauge-invariant formulation of the Wigner dynamics in the presence of an external magnetic field has been investigated. However, as remarked at the end of Sec. 4, our methodology deserves a deeper investigation in order to include more general transformation, still preserving the advantages of our original approach. This will be the subject of a future work.

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