Physics Letters A 381 (2017) 1129–1133

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Quantum mechanics on phase space and the Coulomb potential

P. Campos [a,b,*], M.G.R. Martins [a], J.D.M. Vianna [a,c]

[a] Instituto de Física, Universidade Federal da Bahia, Campus Ondina, 40210-340 Salvador, Bahia, Brazil
[b] Instituto Federal do Sertão Pernambucano, Campus Petrolina, 56314-520 Petrolina, Pernambuco, Brazil
[c] Instituto de Física, Universidade de Brasília, 70910-900 Brasília, DF, Brazil

ARTICLE INFO

Article history:
Received 3 September 2016
Received in revised form 31 January 2017
Accepted 2 February 2017
Available online 6 February 2017
Communicated by P.R. Holland

Keywords:
Symplectic quantum mechanics
Coulomb potential
Wigner function
Levi-Civita transformation

ABSTRACT

Symplectic quantum mechanics (SMQ) makes possible to derive the Wigner function without the use of the Liouville–von Neumann equation. In this formulation of the quantum theory the Galilei Lie algebra is constructed using the Weyl (or star) product with $\hat{Q} = q\star = q + \frac{i\hbar}{2}\partial_p$, $\hat{P} = p\star = p - \frac{i\hbar}{2}\partial_q$, and the Schrödinger equation is rewritten in phase space; in consequence physical applications involving the Coulomb potential present some specific difficulties. Within this context, in order to treat the Schrödinger equation in phase space, a procedure based on the Levi-Civita (or Bohlin) transformation is presented and applied to two-dimensional (2D) hydrogen atom. Amplitudes of probability in phase space and the correspondent Wigner quasi-distribution functions are derived and discussed.

1. Introduction

There are several alternative ways in order to quantize a micro physical system. One of them refers to the quantum revolution in the twenties of the last century performed by Schrödinger, Heisenberg, Dirac and others, in this standard way we use operators in Hilbert space. Another way is the path integrals, which were conceived by Dirac [1] and formulated by Feynman in 1948 [2,3]. A third way is the formulation of quantum mechanics on phase space (also known as the Moyal quantization or the deformation quantization) which is grounded on Wigner's quasi-distribution function [4] and Weyl's correspondence between ordinary c-number functions in phase space and quantum-mechanical operators in Hilbert space [5,6]. At the ending of the 1970s Bayen et al. [7,8] laid the groundwork for an alternative description of the phase space formulation of quantum mechanics. The roots of this work are found in earlier works of Weyl [5,6], Wigner [4], Groenewold [9], Moyal [10] and Berezin [11–13] on the physical side and of Gerstenhaber and Schack [14–18] on the mathematical side. Since then, many efforts have been made in order to develop the quantum mechanics on phase space, for a comprehensive treatment of the subject the reader may consult Refs. [19–21]. An extensive collection of important papers and list of references can be found in Refs. [22,23].

The phase space representation of quantum mechanics is less well known but is useful in many branches of physics, for example, in quantum optics [24], nuclear physics [25], atomic physics [26–28], condensed matter [29–31], field theory [32–37], M-theory [38–40], noncommutative geometry [41,42] and the noncommutative field theory models [43–48].

The concept of phase space comes naturally from the Hamiltonian formulation of classical mechanics and plays an important role in the relation between quantum and classical mechanics, i.e. the quantum-classical transition. The quantum mechanics on phase space seems to be a result of a generalization of classical Hamiltonian mechanics, in such a way that the phase space formulation of quantum mechanics should smoothly reduce to the formulation of classical Hamiltonian mechanics as the Planck constant $\hbar$ goes to 0, that is $\hbar$ parameterizes the link between classical and quantum mechanics. The interpretation of phase space representation of quantum mechanics is given by considering the Wigner function $f_W(q,p)$, which both the position and momentum variables are c-numbers. A basic advantage of this representation is that it is possible to perform canonical transformations, just as in classical Hamiltonian mechanics [21].

The stationary Wigner phase space distribution function $f_W(q,p)$ in terms of the wave function $\psi(q)$ of the usual time-independent Schrödinger equation $\hat{H}(\hat{q},\hat{p})\psi(q) = E\psi(q)$, is defined through the following expression [4,19]

$$f_W(q,p) = \int e^{\frac{ip\xi}{\hbar}} \psi^\dagger(q+\frac{\xi}{2})\psi(q-\frac{\xi}{2})d\xi, \tag{1}$$

* Corresponding author at: Instituto de Física, Universidade Federal da Bahia, Campus Ondina, 40210-340 Salvador, Bahia, Brazil.
E-mail addresses: pedrodesiqueiracampos@yahoo.com.br (P. Campos), mgraca@ufba.br (M.G.R. Martins), jdavid@fis.unb.br (J.D.M. Vianna).

http://dx.doi.org/10.1016/j.physleta.2017.02.005
0375-9601/

where all integral runs from $-\infty$ to $-\infty$. The Wigner function is identified as a quasi-distribution in the sense that $f_W(q,p)$, where (q,p) are the coordinates of a phase space manifold Γ, is real but not positive definite, and as such cannot be interpreted as probability. However, the integrals $\rho(q)=\int f_W(q,p)\,dp$ and $\rho(p)=\int f_W(q,p)\,dq$ are (true) distribution functions. In the Wigner formalism, each operator, say A, defined in the Hilbert space, $\mathbb{H}$, is associated with a function, say $a_W(q,p)$, in Γ. Then there is an application $\Omega_W: A\mapsto a_W(q,p)$, such that, the associative algebra of operators defined in $\mathbb{H}$ turns out to be an associative (but not commutative) algebra in Γ, given by $\Omega_W: AB\mapsto a_W\star b_W$, where the star-product $\star$ is defined by

$$a_W\star b_W=a_W(q,p)\exp\left[\frac{i\hbar}{2}\left(\frac{\overleftarrow{\partial}}{\partial q}\frac{\overrightarrow{\partial}}{\partial p}-\frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial q}\right)\right]b_W(q,p), \quad (2)$$

and the arrows over the vector fields ∂_q,∂_p denote that a given vector field acts only the function standing on the left or on the right side of the vector field. Studies of the representation of the Galilei group in a manifold with phase space content have been developed since long ago [49–56]. This type of representation, called symplectic unitary representation, has been used by several authors [5,10,19,21]; in particular Oliveira et al. [57] in order to explore the algebraic structure of the Wigner formalism have considered unitary representations based on operators of the type $a_W\star$ and shown that the operators

$$\widehat{Q}=q\star=q+\frac{i\hbar}{2}\partial_p, \quad \widehat{P}=p\star=p-\frac{i\hbar}{2}\partial_q, \quad (3)$$

$$\widehat{K}=k\star=mq\star-tp\star=m\widehat{Q}-t\widehat{P}, \quad (4)$$

$$\widehat{\mathfrak{L}}_i=\epsilon_{ijk}\widehat{Q}_j\widehat{P}_k=\epsilon_{ijk}q_jp_k-\frac{i\hbar}{2}\epsilon_{ijk}q_j\frac{\partial}{\partial q_k}+\frac{i\hbar}{2}\epsilon_{ijk}p_j\frac{\partial}{\partial q_k}+\frac{\hbar^2}{4}\epsilon_{ijk}\frac{\partial^2}{\partial q_j\partial p_k}, \quad (5)$$

and

$$\widehat{H}=h\star=\frac{\widehat{P}^2}{2m}=\frac{1}{2m}\sum_{i=1}^{3}\widehat{P}_i^2=\frac{1}{2m}\sum_{i=1}^{3}\left(p_i-\frac{i\hbar}{2}\frac{\partial}{\partial q_i}\right)^2, \quad (6)$$

satisfy the Lie algebra for the Galilean symmetry with a central extension characterized by m. Furthermore Oliveira et al. have introduced a pair of multiplicative operators $\underline{Q}$ (coordinates) and $\underline{P}$ (momenta) which allows us to endow $\mathbb{H}(\Gamma)$, the Hilbert space over Γ, with basis $|q,p\rangle$ in which $\underline{Q}$ and $\underline{P}$ are diagonal operators. It follows that in this formulation, called Symplectic Quantum Mechanics (SQM), the time-independent Schrödinger equation in phase space is written as

$$H\left(\widehat{Q},\widehat{P}\right)\Psi(q,p)=E\Psi(q,p). \quad (7)$$

Here $H\left(\widehat{Q},\widehat{P}\right)=\frac{\widehat{P}^2}{2m}+V\left(\widehat{Q}\right)$ with $\widehat{P}=p\star$, $\widehat{Q}=q\star$, and the Wigner function is defined by $\boldsymbol{f}_W=\Psi(q,p)\star\Psi^\dagger(q,p)$. Eq. (7) is symplectically covariant [58,59] and for a complete understanding of this equation the reader may consult Refs. [57–61]. This approach provides satisfactory interpretation for numerous aspects of the phase space quantum theory and, although associated with the Wigner formalism, has a Hamiltonian, not a Liouvillian, operator as generator of time translation; from Eq. (7) it follows, for example, that $H\left(\widehat{P},\widehat{Q}\right)\Psi\star\Psi^\dagger=E\Psi\star\Psi^\dagger$ or $H\left(\widehat{P},\widehat{Q}\right)f_W=Ef_W$. SQM has been applied to some quantum systems: states of linear oscillator, nonlinear oscillator [57], one dimensional hydrogen atom [62] have been obtained in terms of amplitudes of probability in phase space $\Psi(q,p)$. However, for two and three dimensional Coulomb potential there are some specific difficulties and it is not known the correspondent $\Psi(q,p)$. In this work in order to solve the Schrödinger equation (7) for the 2D hydrogen atom we present a procedure based on the Levi-Civita (or Bohlin) transformation [63–65].

2. 2D hydrogen atom

For the 2D hydrogen atom, the potential energy is $V_c(q)=-e^2q^{-1}$, with $q=\sqrt{q_1^2+q_2^2}$. There is a great interest in this system due to its applications in condensed matter physics [66–69] and in atomic and molecular physics [70], in particular, in the branch of atomic spectroscopy, the 2D hydrogen atom was regarded as a simplified model of the ionization process of the highly excited 3D hydrogen atom by circular-polarized microwaves [70]. For simplicity of presentation, we suppose units are selected in such a way that both the charge e and the mass m have unit value. With this choice of units, the corresponding classical Hamiltonian for the system is

$$H_c=(2^{-1}p^2-kq^{-1}), \quad (8)$$

where $p^2=p_1^2+p_2^2$ and k is a positive constant. In the SQM picture for the $H_c(q,p)$ we have

$$H\left(\widehat{Q},\widehat{P}\right)=\frac{1}{2}\sum_{i=1}^{2}\left(p_i-\frac{i}{2}\frac{\partial}{\partial q_i}\right)^2+V(q_1\star,q_2\star) \quad (9)$$

and in consequence it is difficult to determine solutions of the Schrödinger equation (7). To solve this problem we propose a procedure where the connection between the Coulomb problem in a plane in parabolic coordinates and the 2D harmonic oscillator in Cartesian coordinates is used [71]. Specifically, with our notation, let now $\mathbb{U}=\mathbb{R}^2$, $\mathbb{X}=\mathbb{R}^2$, $\mathbb{U}^*=\mathbb{U}\setminus\{0\}$, $\mathbb{X}^*=\mathbb{X}\setminus\{0\}$ and

$$T(u):=\frac{1}{2}\begin{pmatrix}u_1 & -u_2\\ u_2 & u_1\end{pmatrix},\ u\in\mathbb{U}^*. \quad (10)$$

The Levi-Civita (or Bohlin) transformation [63–65] is given by $f:\mathbb{U}^*\to\mathbb{X}^*$, $x=f(u)=T(u)u$. The columns of $T(u)$ form analytic orthogonal frame for $\mathbb{U}^*$. A theorem of Hurwitz [72,73] states that square matrix $T(u)$ satisfies the three properties of which can be shown by straightforward calculations: $T(u)$ is orthogonal for all $u\neq 0$, $T(u)$ is linear in u, and one of the columns of $T(u)$ is u. Therefore we have the transformation

$$x=T(u)u=\begin{pmatrix}\frac{1}{2}\left(u_1^2-u_2^2\right)\\ u_1u_2\end{pmatrix}=\begin{pmatrix}q_1\\ q_2\end{pmatrix}, \quad (11)$$

with $q=u^2$, $q=\sqrt{q_1^2+q_2^2}$, and $u^2=u_1^2+u_2^2$. Thus according to the Levi-Civita transformation [74,75] the plan (u_1,u_2) is the double covering of the plan (q_1,q_2). Therefore, the points (u_1,u_2) and $(-u_1,-u_2)$ represent the same point of the plane and the wavefunctions must satisfy $\psi(u_1,u_2)=\psi(-u_1,-u_2)$. We note here the rather obvious fact that the Levi-Civita mapping, which is simply a transformation to parabolic coordinates, carries the flat q space into a flat u space. The "inverse" transformation is given by $u_1=\pm\left[\frac{(q_1+2q)}{4}\right]^{\frac{1}{2}}$ and $u_2=\frac{q_2}{u_1}$, giving the parabolic coordinates u_i in terms of the Cartesian coordinates. By developing $dq^tdq=4du^tT^tTdu$, we obtain $dq_1{}^2+dq_2{}^2=q\left(du_1{}^2+du_2{}^2\right)$. The reader will verify that $\frac{\partial}{\partial u}=2T^t\frac{\partial}{\partial q}$, this can be inverted to give $\frac{\partial}{\partial q}=\frac{2}{q}T\frac{\partial}{\partial u}$. Applied to classical Hamiltonian (8), H_c in terms of parabolic coordinates u_1,u_2 defined by $q_1=\frac{1}{2}\left(u_1^2-u_2^2\right)$ and $q_2=u_1u_2$ is