

CLASSICAL-QUANTUM CORRESPONDENCE BY MEANS OF PROBABILITY DENSITIES

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Abstract

Within the frame of the recently introduced phase space representation of non relativistic Quantum Mechanics, we propose a Lagrangian from which the phase space Schrödinger equation can be derived. From that Lagrangian, the associated conservation equations, according to Noether's theorem, are obtained. This shows that one can analyze quantum systems completely in phase space as it is done in coordinate space, without additional complications.

In this paper, we make use of a recently introduced phase space representation of non relativistic Quantum Mechanics[1] which complies with the requirements for a quantum representation. This allows the researcher to investigate quantum dynamics in the same dynamical space in which classical dynamics is commonly studied. Some advantages of this approach is a better comparison between quantum and classical dynamics, a better understanding of quantum effects and the possibility of analyzing quantum systems completely in phase space in the same way as it is done in coordinate space, without the complications found in other approaches.[2, 3]

In this approach to non relativistic Quantum Mechanics in phase space, the operators associated to the momentum and coordinate operators are $\hat{P} \leftrightarrow p/2 - i\hbar\partial/\partial q$ and $\hat{Q} \leftrightarrow q/2 + i\hbar\partial/\partial p$, respectively. As expected, these operators do not commute with each other, in fact, $[\hat{Q}, \hat{P}] = i\hbar$. Then, the phase space Schrödinger equation is given by

$$i\hbar\frac{\partial}{\partial t}\langle\Gamma|\psi_t\rangle = \left[\frac{1}{2m} \left(\frac{p}{2} - i\hbar\frac{\partial}{\partial q} \right)^2 + V \left(\frac{q}{2} + i\hbar\frac{\partial}{\partial p} \right) \right] \langle\Gamma|\psi_t\rangle \quad (1)$$

where $\Gamma = (p, q)$ denotes a point in phase space and $\langle\Gamma|\psi_t\rangle$ denotes the phase space wave function. This is the equation which governs the dynamics of the phase space wave packet and should be solved in order to find eigenfunctions, eigenenergies, etc.

Worth mentioning is the set of phase space eigenfunctions found for the harmonic oscillator, (from here after, we use dimensionless units)

$$\psi_n(\Gamma; \alpha) = \left(\frac{\sqrt{1/4 - \alpha^2}}{2^n \pi n!} \right) \exp \left[- \left(\frac{1}{2} + \alpha \right) \frac{q^2}{2} - \left(\frac{1}{2} - \alpha \right) \frac{p^2}{2} - i\alpha pq \right] H_n(\Gamma; \alpha) \quad , \quad (2)$$

functions which involve the phase space version $H_n(\Gamma; \alpha)$ of Hermite polynomials, with recursion relationship $H_{n+1}(\Gamma; \alpha) = 2u(\Gamma; \alpha)H_n(\Gamma; \alpha) - 4n\alpha H_{n-1}(\Gamma; \alpha)$, where $u(\Gamma; \alpha) = (1/2 + \alpha)q - i(1/2 -$

$\alpha)p$, and $-1/2 \leq \alpha \leq 1/2$. These polynomials have similar properties as the usual one-variable Hermite polynomials but now in phase space. This is in contrast with other sets introduced in previous works.[4]

The wave function in coordinate space $\psi(q)$ can be recovered from the wave function in phase space $\psi(\Gamma; \alpha)$ by means of the projection $\psi(q) = \int_{-\infty}^{+\infty} \exp(ipq/2)\psi(\Gamma; \alpha)dp$, and the wave function in momentum space $\psi(p)$ can be obtained from the wave function in phase space by means of the projection $\psi(p) = \int_{-\infty}^{+\infty} \exp(-ipq/2)\psi(\Gamma; \alpha)dq$

The diagonal matrix element of the quantum probability conservation equation is

$$\frac{\partial}{\partial t} \langle \Gamma | \hat{\rho} | \Gamma \rangle = -\frac{\partial}{\partial q} \frac{1}{2} \left[\langle \Gamma | \hat{P} \hat{\rho} | \Gamma \rangle + \langle \Gamma | \hat{\rho} \hat{P} | \Gamma \rangle \right] + \frac{\partial}{\partial p} \sum_{n=1}^{\infty} V_n \sum_{l=0}^{n-1} \langle \Gamma | \hat{Q}^l \hat{\rho} \hat{Q}^{n-l-1} | \Gamma \rangle \quad , \quad (3)$$

where $\hat{\rho}$ denotes the density operator, and where we have assumed that the potential function can be written as a power series in its argument, $V(q) = \sum_{n=0}^{\infty} V_n q^n$. Note that Eq. (3) is a combination of the corresponding equations in coordinate

$$\frac{\partial}{\partial t} \langle q | \hat{\rho} | q \rangle = -\frac{\partial}{\partial q} \frac{1}{2} \left[\langle q | \hat{P} \hat{\rho} | q \rangle + \langle q | \hat{\rho} \hat{P} | q \rangle \right] \quad , \quad (4)$$

and momentum

$$\frac{\partial}{\partial t} \langle p | \hat{\rho} | p \rangle = \frac{\partial}{\partial p} \sum_{n=1}^{\infty} V_n \sum_{l=0}^{n-1} \langle p | \hat{Q}^l \hat{\rho} \hat{Q}^{n-l-1} | p \rangle \quad , \quad (5)$$

spaces, providing an alternative description of quantum dynamics.

For a density operator of the form $\hat{\rho} = \sum_{\psi, \chi} P(\psi, \chi) | \psi \rangle \langle \chi |$, we introduce the Lagrangian

$$L = \sum_{\psi, \chi} P(\psi, \chi) \frac{1}{2} \left\{ \chi^* \hat{E} \psi + \psi (\hat{E} \chi)^* - \chi^* \hat{V}(\hat{Q}) \psi - \psi [\hat{V}(\hat{Q}) \chi]^* - \frac{1}{2} \chi^* \hat{P}^2 \psi - \frac{1}{2} \psi [\hat{P}^2 \chi]^* \right\} \quad , \quad (6)$$

where ψ and χ are wave functions in phase space. By means of the methods used for continuous systems,[5] this Lagrangian leads to the Euler-Lagrange equations

$$\frac{\delta L}{\delta \psi} + \hat{E}^* \frac{\partial L}{\partial \hat{E} \psi} + \hat{P}^2 \frac{\partial L}{\partial \hat{P}^2 \psi} + \hat{V}^*(\hat{Q}) \frac{\partial L}{\partial \hat{V}(\hat{Q}) \psi} = 0 \quad , \quad (7)$$

and

$$\frac{\partial L}{\partial \chi^*} + \hat{E}^* \frac{\partial L}{\partial (\hat{E} \chi)^*} + \hat{P}^2 \frac{\partial L}{\partial (\hat{P}^2 \chi)^*} + \hat{V}^*(\hat{Q}) \frac{\partial L}{\partial [\hat{V}(\hat{Q}) \chi]^*} = 0 \quad , \quad (8)$$

equations from which the Schrödinger equation and its complex conjugate in phase space are obtained.

In order to obtain the conservation equations derived from this Lagrangian, we make use of Noether's theorem,[5] which leads to

$$\begin{aligned} -\frac{\partial L}{\partial x} &= \sum_{\psi, \chi} P(\psi, \chi) \left\{ \frac{\partial}{\partial t} \left(\frac{i}{2} \chi^* \frac{\partial \psi}{\partial x} - \frac{i}{2} \psi \frac{\partial \chi^*}{\partial x} \right) \right. \\ &+ \frac{1}{4} \left[\frac{\partial \psi}{\partial x} (\hat{P}^2 \chi)^* - \chi^* \frac{\partial \hat{P}^2 \psi}{\partial x} + \frac{\partial \chi^*}{\partial x} \hat{P}^2 \psi - \psi \frac{\partial (\hat{P}^2 \chi)^*}{\partial x} \right] \\ &+ \left. \frac{1}{2} \left[\frac{\partial \psi}{\partial x} (\hat{V} \chi)^* - \chi^* \frac{\partial \hat{V} \psi}{\partial x} + \frac{\partial \chi^*}{\partial x} \hat{V} \psi - \psi \frac{\partial (\hat{V} \chi)^*}{\partial x} \right] \right\} - \frac{dL}{dx} \quad , \quad (9) \end{aligned}$$

where x is any of the variables t , q or p .

Now, Eq. (9), for $x = t$, leads to

$$\begin{aligned} & \frac{\partial}{\partial t} \Re \langle \Gamma | \hat{H} \hat{\rho} | \Gamma \rangle + \frac{\partial}{\partial q} \frac{1}{2} \Re \langle \Gamma | \hat{P} (\hat{H} \hat{\rho} + \hat{\rho} \hat{H}) | \Gamma \rangle \\ & - \frac{\partial}{\partial p} \sum_{n=1}^{\infty} V_n \sum_{l=0}^{n-1} \Re \langle \Gamma | \hat{Q}^l \hat{H} \hat{\rho} \hat{Q}^{n-l-1} | \Gamma \rangle = \Re \langle \Gamma | \frac{\partial \hat{V}(t)}{\partial t} \hat{\rho} | \Gamma \rangle \quad . \end{aligned} \quad (10)$$

For $x = q$, Eq. (9) leads to

$$\begin{aligned} & \frac{\partial}{\partial t} \Re \langle \Gamma | (\hat{P} - \hat{P}^*) \hat{\rho} | \Gamma \rangle + \frac{\partial}{\partial q} \frac{1}{2} \Re \langle \Gamma | \hat{P} [(\hat{P} - \hat{P}^*) \hat{\rho} + \hat{\rho} (\hat{P} - \hat{P}^*)] | \Gamma \rangle \\ & - \frac{\partial}{\partial p} \sum_{n=1}^{\infty} V_n \sum_{l=0}^{n-1} \Re \langle \Gamma | \hat{Q}^l (\hat{P} - \hat{P}^*) \hat{\rho} \hat{Q}^{n-l-1} | \Gamma \rangle = 2 \Re \langle \Gamma | \hat{F}(\hat{Q}) \hat{\rho} | \Gamma \rangle \quad , \end{aligned} \quad (11)$$

and, for $x = p$, Eq. (9) leads to

$$\begin{aligned} & \frac{\partial}{\partial t} \Re \langle \Gamma | (\hat{Q} - \hat{Q}^*) \hat{\rho} | \Gamma \rangle + \frac{\partial}{\partial q} \frac{1}{2} \Re \langle \Gamma | \hat{P} [(\hat{Q} - \hat{Q}^*) \hat{\rho} + \hat{\rho} (\hat{Q} - \hat{Q}^*)] | \Gamma \rangle \\ & - \frac{\partial}{\partial p} \sum_{n=1}^{\infty} V_n \sum_{l=0}^{n-1} \Re \langle \Gamma | \hat{Q}^l (\hat{Q} - \hat{Q}^*) \hat{\rho} \hat{Q}^{n-l-1} | \Gamma \rangle = 2 \Re \langle \Gamma | \hat{P} \hat{\rho} | \Gamma \rangle \quad . \end{aligned} \quad (12)$$

It has been pointed out[1] that the classical analog to the quantum density $\langle \Gamma | \hat{\rho} | \Gamma \rangle$ is the classical density $\rho(\Gamma; t)$, so, we can ask for the classical analogs to the quantum conservation equations derived previously. These classical analogs are obtained by taking the time derivative of the densities of interest and combining the resulting equation with Hamilton's $\dot{p} = -\partial H/\partial q$, $\dot{q} = \partial H/\partial p$, and Liouville's $\partial \rho/\partial t = -p \partial \rho/\partial q - F(q) \partial \rho/\partial p$, equations. The classical energy conservation equation so obtained is

$$\frac{\partial}{\partial t} H \rho(\Gamma; t) + \frac{\partial}{\partial q} p H \rho(\Gamma; t) + \frac{\partial}{\partial p} F(q) H \rho(\Gamma; t) = \frac{\partial V(q; t)}{\partial t} \rho(\Gamma; t) \quad . \quad (13)$$

Note the close resemblance that the above equation has with Eq. (10), the difference being the symmetrization of the classical products $H \rho(\Gamma; t)$, $p H \rho(\Gamma; t)$, $F(q) H \rho(\Gamma; t)$, with $F(q) = -\sum_{n=1}^{\infty} n V_n q^{n-1}$, and $[\partial V(q, t)/\partial t] \rho(\Gamma; t)$

The conservation equation for the momentum density $p \rho(\Gamma; t)$ is

$$\frac{\partial}{\partial t} p \rho(\Gamma; t) + \frac{\partial}{\partial q} p^2 \rho(\Gamma; t) + \frac{\partial}{\partial p} F(q) p \rho(\Gamma; t) = 2 F(q) \rho(\Gamma; t) \quad , \quad (14)$$

which is the classical analog to Eq. (11). Note that the quantum density corresponding to $p \rho(\Gamma; t)$ is $\Re \langle \Gamma | (\hat{P} - \hat{P}^*) \hat{\rho} | \Gamma \rangle$, the quantum density corresponding to $p^2 \rho(\Gamma; t)$ is $\Re \langle \Gamma | \hat{P} [(\hat{P} - \hat{P}^*) \hat{\rho} + \hat{\rho} (\hat{P} - \hat{P}^*)] | \Gamma \rangle / 2$ and $\sum_{n=1}^{\infty} V_n \sum_{l=0}^{n-1} \Re \langle \Gamma | \hat{Q}^l (\hat{P} - \hat{P}^*) \hat{\rho} \hat{Q}^{n-l-1} | \Gamma \rangle$ is the quantum analog corresponding to $F(q) p \rho(\Gamma; t)$. It would be very difficult to guess the correct quantum densities without the help of a Lagrangian and Noether's theorem.

The conservation equation for $q\rho(\Gamma; t)$ is given by

$$\frac{\partial}{\partial t}q\rho(\Gamma; t) + \frac{\partial}{\partial q}pq\rho(\Gamma; t) + \frac{\partial}{\partial p}F(q)q\rho(\Gamma; t) = 2p\rho(\Gamma; t) \quad , \quad (15)$$

which is the classical analog to Eq. (12). Note that the quantum density corresponding to $q\rho(\Gamma; t)$ is $\Re\langle\Gamma | (\hat{Q} - \hat{Q}^*)\hat{\rho} | \Gamma\rangle$, the quantum density corresponding to $pq\rho(\Gamma; t)$ is $\Re\langle\Gamma | \hat{P} [(\hat{Q} - \hat{Q}^*)\hat{\rho} + \hat{\rho}(\hat{Q} - \hat{Q}^*)] | \Gamma\rangle/2$ and $\sum_{n=1}^{\infty} V_n \sum_{l=0}^{n-1} \Re\langle\Gamma | \hat{Q}^l(\hat{Q} - \hat{Q}^*)\hat{\rho}\hat{Q}^{n-l-1} | \Gamma\rangle$ is the quantum analog corresponding to $F(q)q\rho(\Gamma; t)$. It would be very difficult to guess the correct quantum densities without the help of a Lagrangian and Noether's theorem.

With these results, we can see that one can analyze quantum systems completely in phase space and in the same way as it is done in coordinate space, without the need of further complications, increasing our confidence in this representaton.

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