Quantum Distributions for the Plane Rotator

Marius Grigorescu

Quantum phase-space distributions (Wigner functions) for the plane rotator are defined using wave functions expressed in both angle and angular momentum representations, with emphasis on the quantum superposition between the Fourier dual and the symplectic dual variables. The standard quantization condition for angular momentum appears as necessary for consistency. Signatures of classical behavior are briefly discussed.
1 Introduction

The action-angle coordinates \( \{(J_i, \varphi_i), \ i = 1, N/J_i \in \mathbb{R}, \varphi_i \in [-\pi, \pi]\} \) on the phase-space \( M \) arise in the description of the integrable Hamiltonian systems with periodic orbits [1]. In these variables the Hamilton function depends only on \( J \equiv \{J_i, i = 1, N\} \), such that a submanifold \( \Sigma_J \) of constant \( J \) is a torus parameterized by \( \{\varphi_i, i = 1, N\} \).

In the old quantum mechanics \( J_i \) takes only a discrete set of values, \( J_i = n_i \hbar, n_i \in \mathbb{Z} \), such that the corresponding Lagrangian submanifolds \( \Sigma_{n \hbar} \) provide a partition of \( M \) in "quantum cells" \( q_n \) of volume \( \hbar^N \). However, these cells are not ordered along a complete set of local coordinates on \( M \), and in the limit \( \hbar \to 0 \) they become singular submanifolds of \( M \) rather than points.

Probability distributions of particles on \( M \) may arise from thermal fluctuations, or from an intrinsic "quantum structure", resembling the partition in quantum cells \( q_n \) of finite volume. The quantum structure on \( M = T^*\mathbb{R}^N \) is usually associated with the Wigner transform \( f_\psi \in \mathcal{F}(M) \) of the quantum "wave function" \( \psi \in L^2(\mathbb{R}^N) \), defined in Cartesian coordinates. For the integrable systems the quantum distributions \( f_\psi_n \) provided by the eigenstates \( \psi_n \) of the Hamiltonian operator show an increased localization probability on \( \Sigma_{n \hbar} \subset M \) [3], but despite constant effort, a direct definition of \( f_\psi \) in terms of the action-angle variables is faced with difficulties. Various aspects of the problem are presented in [4, 5, 6, 7].

In this work the quantum distributions for the action-angle variables are discussed on the representative example of the plane rotator \( (M = T^*S^1) \). The treatment is similar to the one applied before to the rigid rotator [8], but instead of discretization here the emphasis is on the quantum superposition between the symplectic dual and Fourier dual variables. The basic elements of the formalism are presented in Section 2, followed in Section 3 by applications to the Wigner functions \( f_\psi \) of the plane rotator using for \( \psi \) both the angle and angular momentum representations. Finite temperature effects, beyond the single particle coherence time, are discussed in Section 4. Concluding remarks are summarized in Section 5.

2 The partial Fourier transform as Hermitian operator

Let \( f(x,y) \) be a real integrable function of \( x,y \in \mathbb{R} \) and \( \tilde{f}(x,k) \) the partial Fourier transform of \( f \) only with respect to \( y \),

\[
\tilde{f}(x,k) = \int dy \ e^{iky} f(x,y) .
\]  

(1)

Because \( \tilde{f}(x,k)^* = \tilde{f}(x,-k) \), we may consider \( \tilde{f}(x,k) \) as a matrix element of a Hermitian operator \( \hat{f} \) on \( L^2(\mathbb{R}) \), having \( x \) and \( k \) as indices not along the rows and columns, but along the diagonals [9]. In the case of \( M = T^*\mathbb{R} \) parameterized by the canonical variables \( (q,p) \), the Fourier transform in momentum \( \tilde{f}(q,k) \) of \( f \in \mathcal{F}(M) \) (the set of smooth functions on

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1 In the standard approach \( J_i \) are considered as coordinates and \( \varphi_i \) as momenta. For systems with symmetry \( J_i \) are provided by the momentum mapping and \( \varphi_i \) are group coordinates.
in a quantum distribution the canonical coordinates (strongly correlated by the implicit dependence of $f$) with the row and column indices $a = q + \hbar k/2$, $b = q - \hbar k/2$ defined using $\hbar$ as a conversion factor from the $k$ to $q$-scale, such that if $f_1, f_2 \in \mathcal{F}(M)$ then

$$(f_1, f_2) = \int_M dq dp \; f_1(q, p) f_2(q, p) = \hbar \int da \int db \; \hat{f}_{1ab} \hat{f}_{2ba} \equiv \hbar Tr(\hat{f}_1 \hat{f}_2) .$$

(2)

The change of integration variables from $(q, p)$ to $(a, b)$ is completely formal and it does not change the physics (classical or quantum) of the observables $f_1, f_2$. However, it distinguishes between a pure quantum distribution $f_\psi \in \mathcal{F}(M)$ and other observables by reducing $\hbar \hat{f}_\psi$ to a projection operator, $h(\hat{f}_\psi)_{ab} = \psi_a^* \psi_b^*$, $\psi \in L^2(\mathbb{R})$, $||\psi|| = 1$. In this case the expectation value of $A \in \mathcal{F}(M)$ with respect to $f_\psi$ is

$$<A>_{f_\psi} = (f_\psi, A) = \hbar Tr(\hat{f}_\psi \hat{A}) = \langle \psi | \hat{A} | \psi \rangle .$$

Similar results can be obtained using the ”momentum representation”, defined by the Fourier transform in coordinate,

$$\hat{f}^\prime(k', p) = \int dq \; e^{ik'q} \; f(q, p) ,$$

(3)

such that $\hat{f}_{1a'b'} \equiv \hbar^{-1} \hat{f}((a'-b')/\hbar, (a'+b')/2)$, with $a' = p+\hbar k'/2$, $b' = p-\hbar k'/2$. It can be shown that if $\hbar \hat{f}$ is separable as $h\hat{f}_{ab} = \psi_a^* \psi_b^*$, then $\hbar \hat{f}'$ is also separable, $h\hat{f}'_{a'b'} = \psi'_a^* (\psi'_a)^*$, with

$$\psi'_p = \frac{1}{\sqrt{2\pi\hbar}} \int dq \; e^{-ipq/\hbar} \psi_q .$$

This result ensures that both marginal distributions are positive definite,

$$F_{\psi}(q) = \int dp f_\psi(q, p) = \psi_q^* \psi_q , \quad F_{\psi}^*(p) = \int dq f_\psi(q, p) = \psi_p^* \psi_p ,$$

and that we may consider $\psi_q$ and $\psi'_p$ as components of the same ”state vector” $|\psi\rangle$ in dual bases, $|q\rangle$ ($\equiv |\hbar k\rangle$), and $|p\rangle$, formally related by Fourier transform,

$$|p\rangle = \frac{1}{2\pi\hbar} \int dq \; e^{ipq/\hbar} |q\rangle .$$

It is interesting to note that the ordering of the matrix indices $a, b$ does not always follow the one of the variables $q, k$. Thus, for variations $\delta a > 0$, $\delta b > 0$ we get also $\delta q > 0$, but $\delta k > 0$ only if $\delta a > 6\delta b$. A related aspect is the sensitivity of $f_\psi$ to the local inversion symmetry of $\psi$, as $f_\psi(q, 0)$ has large negative values at the points $q_n$ where $\psi(q_n + \delta q) = -\psi(q_n - \delta q)$.

Because $F_{\psi}^\prime(q) > 0$ and $F_{\psi}^*(p) > 0$, the negative values of $f_\psi(q, p)$ indicate that in a quantum distribution the canonical coordinates $(q, p)$ are not independent, but strongly correlated by the implicit dependence of $f_\psi$ on the Fourier dual variables, $k$ or $k'$. These correlations are usually described as ”uncertainty”, or ”granularity”, and can be measured by the function $C_\psi(q, p) = f_\psi(q, p) - F_{\psi}^\prime(q) F_{\psi}^*(p)$. 

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3 Distributions for the plane rotator

A distribution function $f(\varphi, J)$ of angle ($\varphi$) and orbital angular momentum ($J \equiv L_z$) on $M = T^*S^1 \simeq S^1 \times \mathbb{R}$ may describe an ensemble of beads on a circle, and can be regarded as a constrained distribution on $T^*\mathbb{R}^2$ (Appendix 1). Along the lines of Section 2 we may also start with the Fourier transform

$$\tilde{f}(\varphi, k) = \int dJ \, e^{ikJ} f(\varphi, J).$$

To proceed towards the one-particle quantum distributions one should note that if we let $k \in \mathbb{R}$ and $\varphi \in [-\pi, \pi]$ then $\alpha = \varphi + \hbar k/2$, $\beta = \varphi - \hbar k/2$ are not well defined as indices for a matrix element $\bar{f}_{\alpha\beta} = h^{-1/2}f((\alpha + \beta)/2, (\alpha - \beta)/\hbar)$ of a Hermitian operator $\hat{f}$ on the quantum Hilbert space $\mathcal{H} = L^2(S^1)$. Therefore, following the example of the rigid rotator $[3]$, quantum distributions $f_\psi$ can be defined using a separable expression $f_\psi(\varphi, k) \equiv \psi_\alpha \psi_\beta^*$, only if the range of $\gamma = \hbar k$ is restricted to the first "Brillouin zone", $\gamma \in [-\pi, \pi]$. In this case one obtains

$$f_\psi(\varphi, J) = \frac{1}{2\pi h} \int_{-\pi}^{\pi} d\gamma \, e^{-i\gamma J/\hbar} \psi(\varphi + \frac{\gamma}{2}) \psi^*(\varphi - \frac{\gamma}{2}),$$

in agreement with $V_\psi(\theta, p)$ of [4]. The overlap between two such functions is

$$(f_\psi, f_{\psi'}) = \int_{-\infty}^{\infty} dJ \int_{-\pi}^{\pi} d\varphi \, f_\psi f_{\psi'} = h \text{Tr}(\hat{f}_\psi \hat{f}_{\psi'}) = \frac{|\langle \psi_1 | \psi_2 \rangle|^2}{2\pi h},$$

where $\langle \psi_1 | \psi_2 \rangle \equiv \oint d\varphi \psi_1^* \psi_2$ is the scalar product between $\psi_1$ and $\psi_2$ as elements of $\mathcal{H}$. The marginal distributions provided by (5) are

$$F^{\psi}_\psi(\varphi) = \int dJ f_\psi(\varphi, J) = \psi_\varphi \psi_\varphi^*,$$

positive definite, and

$$F^{\text{ms}}_\psi(J) = \oint d\varphi f_\psi(\varphi, J) = \frac{1}{\hbar} \langle \psi | \hat{P}_J | \psi \rangle,$$

where $(\partial_\varphi \equiv \partial/\partial \varphi)$,

$$\hat{P}_J = \frac{1}{2\pi} \oint d\gamma e^{i\gamma (J-J)/\hbar}, \quad \hat{J} = -i\hbar \partial_\varphi.$$

If $\psi_n(\varphi) = e^{in\varphi}/\sqrt{2\pi}$ is an eigenstate\footnote{For the harmonic oscillator Hamiltonian $H$ on $T^*\mathbb{R}$ the action variable $J = H/\omega$ is positive, $(\sqrt{2J}, \varphi)$ are polar coordinates on $T^*\mathbb{R}$, $(dp \wedge dq = dJ \wedge d\varphi)$, and the eigenstates of $\hat{J}$ are real.} of $\hat{J}$, ($\hat{J} \psi_n = n\hbar \psi_n$), then $\langle \psi_n | \hat{P}_J | \psi_n \rangle = j_0(\pi(n - J/\hbar))$, $j_0(x) = \sin(x)/x$. This shows that $F^{\text{ms}}_\psi(J)$ is not positive definite if $J/\hbar \in \mathbb{R}$, but if $J/\hbar \in \mathbb{Z}$ then $P_{nh}$, $n \in \mathbb{Z}$ becomes a projection operator on $\psi_n$, $P_{nh} = |\psi_n \rangle \langle \psi_n|$, and
\[ F_{\psi}^{ms}(n\hbar) = |\langle \psi | \psi_n \rangle|^2 / \hbar \geq 0. \] Moreover, if \( J/\hbar \in \mathbb{Z} \) and \( \psi \) is a function of good parity, \( \psi(\varphi + \pi) = \pm \psi(\varphi) \), then the integral (11) becomes intrinsic on \( S^1 \), namely invariant to a change of parameter \( \gamma \to \gamma + 2\pi \).

To obtain quantum distributions using the angular momentum representation the approach is similar, but also faced with difficulties. Because \( \varphi \) has a finite range a function \( f \in \mathcal{F}(M) \) can be expanded in a Fourier series,

\[ f(\varphi, J) = \frac{1}{2\pi \hbar} \sum_{m \in \mathbb{Z}} e^{-im\varphi} \tilde{f}^j(m, J/\hbar) , \tag{10} \]

but with \( J/\hbar \in \mathbb{R} \) and \( m \in \mathbb{Z} \) we cannot take \( a = J/\hbar + m/2 \) and \( b = J/\hbar - m/2 \) as indices of a matrix element. However, if \( J/\hbar \in \mathbb{Z} \) and \( f^j(\varphi, J) \) has the form (15) with \( \psi \) of good parity, then \( a, b \in \mathbb{Z} \) too, and \( f^j' \psi^j(\varphi, J) = \psi^j(\varphi, J/\hbar) \) with

\[ \psi^j_{n} = \frac{1}{\sqrt{2\pi}} \oint d\varphi \ e^{-in\varphi} \psi(\varphi) . \tag{11} \]

In this representation

\[ F_{\psi}^{cs}(\varphi) = \hbar \sum_{n \in \mathbb{Z}} f^j' \psi^j(\varphi, n\hbar) = \psi(\varphi)\psi^\ast_{\varphi} , \tag{12} \]

(considering \( \int dJ = \hbar \sum_{n=J/\hbar} \), and

\[ F_{\psi}^{ms}(J) = \oint d\varphi f^j_{\psi^j}(\varphi, J) = \psi^j(\varphi, J/\hbar) \) . \tag{13} \]

Moreover, for \( f_1, f_2 \in \mathcal{F}(M) \) we get \( (f_1, f_2) = \hbar Tr'(f_1^j f_2^j) \), where \( Tr' = \sum_{a,b \in \mathbb{Z}} \) and \( \tilde{f}^j_{ba} = \tilde{f}^j(m, J/\hbar)/\hbar, m = a - b, J = \hbar(a + b)/2 \). In particular, \( \hat{1}_{ba} = \delta_{ba}, \hat{J}_{ba} = \hbar a\delta_{ba}, \) and

\[ \hat{\varphi}_{ba} = -\frac{i}{a-b} (-1)^{a-b}(1-\delta_{ab}) . \tag{14} \]

The angle operator \( \hat{\varphi}' \) coincides with \( \langle \hat{\phi} - \pi \rangle_p \) from [10], and corresponds to the series expansion

\[ \varphi = -\sum_{m \neq 0} \frac{(-1)^m}{m} \sin m\varphi . \]

One should consider though \( \varphi \) only as a local coordinate, because at the points of discontinuity \( \varphi = \pm \pi \) this series contains \( \pm \sin m\pi = 0 \), while instead of \( \pi \), as is \( \lim_{n \to \infty} (\pi - \varphi/n) \), the limit

\[ \lim_{n \to \infty} 2 \sum_{m=1}^{n} \frac{\sin(m\varphi/n)}{m} \]

yields 1.08949\( \pi \) (the "Gibbs phenomenon")

\[ ^3 \text{This means that } m \text{ is an even integer. The odd values of } m \text{ enlarge the domain } a = n \in \mathbb{Z} \text{ of } \psi_a \text{ by new points, } a = n + 1/2, n \in \mathbb{Z}. \]
4 Coherence properties and temperature effects

Similarly to the case of the free particle on the \( \mathbb{R} \)-axis [11], also for the free plane rotator the quantum distribution \( f_\psi(\varphi, J) \) is coherent, in the sense that if \( f_\psi \) is a solution of the classical Liouville equation,

\[
\partial_t f_\psi + \frac{J}{I} \partial_\varphi f_\psi = 0 ,
\]

then \( \psi \) is a solution of the Schrödinger equation, \( i\hbar \partial_t \psi = \hat{H} \psi, \hat{H} = J^2 / 2I \), by \( I \) denoting the moment of inertia.

At finite temperature we may consider the thermal average over distributions (10),

\[
f_T(\varphi, J) = \frac{1}{2\pi\hbar} \sum_{m \in \mathbb{Z}} e^{-im\varphi} \tilde{f}_T(m, J/\hbar) ,
\]

where \( \tilde{f}_T(m, J/\hbar) = \sum_{s \in \mathcal{S}} w_{s,T} \psi_b^*(\psi_a^s)^* \), \( a = J/\hbar + m/2 \), \( b = J/\hbar - m/2 \), and \( w_{s,T} \) is the thermal distribution function at the temperature \( T \), (e.g. \( w_{s,T} \sim e^{-E_s/k_B T} \), over a set of one-particle states \( \mathcal{S} \) with energy \( E_s \) and average angular momentum \( J_s \).

At thermal equilibrium, during a small single-particle coherence time \( \tau \) [12], a quantum wave function \( \psi_s(J/\hbar + \mu, t), \mu = \pm m/2 \), will become

\[
\psi_s(J/\hbar + \mu, t + \tau) = e^{-i(E_s - \mu\hbar J_s / I)\tau} \psi_s(J/\hbar + \mu, t) ,
\]

such that \( \tilde{f}_T \) changes into

\[
\tilde{f}_T(m, J/\hbar, t + \tau) = \sum_{s \in \mathcal{S}} w_{s,T} e^{-irmJ_s / I} \psi_b^*(\psi_a^s)^* .
\]

Presuming that in the sum above we can approximate \( w_{s,T}(J_s^2 - <J^2>_T) \approx 0 \), with \( <J^2>_T = \sum_s w_{s,T} J_s^2 \), we get

\[
\partial_t^2 \tilde{f}_T(m, J/\hbar, t) = \partial_t^2 \tilde{f}_T(m, J/\hbar, t + \tau)|_{\tau=0} \approx -m^2 \Omega_T^2 \tilde{f}_T(m, J/\hbar, t) ,
\]

where \( \Omega_T^2 = <J^2>_T / I^2 \). In this approximation we find the transition presumed in [11], from the complex wave functions \( \psi^s \) to real classical waves, because for a time \( t >> \tau, f_T \) of [10] is a solution of the classical wave equation \( \partial_t^2 f_T = \Omega_T^2 \partial_t^2 f_T \). The result is independent of \( \hbar \) and should hold also in a classical ensemble, with the condition of constructive interference along the circle providing a discrete spectrum of "angular wavelengths".

5 Concluding remarks

Quasiprobability distributions (Wigner functions) for the angle \( \varphi \) and orbital angular momentum \( J \) of the plane rotator have been defined using quantum wave functions expressed in both representations, \( \psi_\varphi \) and \( \psi_{J/\hbar} \). It is shown that the "quantum" identification between the symplectic dual and the Fourier dual \((x\hbar)\) introduces constraints,
and the integrality condition $J/\hbar \in \mathbb{Z}$ appears as necessary for consistency.

It is interesting to note that the Titius-Bode law for the planetary system suggests a constraint resembling a form of "entropy quantization", such as

$$\log_2\left( \frac{J}{J_G} \right)^3 = n \ , \ n = 0, 1, 2, \ldots \tag{17}$$

where $J_G = M c R_G$ with $R_G = 2\gamma G M_0/c^2$ denoting the Schwarzschild radius of the central body (the Sun for the planets or Jupiter for its satellites), (Appendix 2). At the atomic scale a constraint of this type is unlikely, but for the high circular Rydberg levels under active investigation \cite{13, 14}, a mixed state with a Poisson distribution \cite{19} could be regarded as a signature for localization along the orbit.

**Appendix 1: Rotational coherent states**

Let us consider a particle of mass $M$, in uniform rotation with the angular frequency $\omega > 0$, around the Z-axis, on a circle of radius $R$ in the XY plane. Thus, if $u = (u_x, u_y)$ and $v = (v_x, v_y)$ are the position and momentum vectors, then $u = (R \cos \varphi, R \sin \varphi)$, $v = (-P \sin \varphi, P \cos \varphi)$, with $P = M \omega R$ and $\varphi = \varphi_0 + \omega t$. It can be shown that a Gaussian distribution on $T^* \mathbb{R}^2$, centered on $u$ and $v$, of the form

$$f_{u,v}(q,p) = \frac{1}{\pi^2 \ell^2} e^{-(q-u)^2/\ell^2-(p-v)^2/\ell^2}, \ a = \ell^2/\hbar = \hbar/M \omega$$

can be obtained by a standard Wigner transform of the rotational coherent state ("symmetry breaking vacuum"),

$$|Z\rangle = e^{\frac{\ell^2}{\hbar}z^* b_u |0\rangle} \ , \tag{18}$$

where $z = \sqrt{J/\hbar} e^{-i\varphi}$, $J = M a R^2$, and $\hat{b}_u = (\hat{b}_x + i \hat{b}_y)/\sqrt{2}$, with $\hat{b}_q = \sqrt{M \omega/2\hbar}(\hat{q} + i \hat{p}_q/M \omega)$, $\hat{b}_q |0\rangle = 0$, $q = x, y$. Moreover, the average of $f_{u,v}$ over $\varphi \in [-\pi, \pi]$ at constant $J$ is the Wigner transform of the density operator

$$\hat{\rho}_\omega = \sum_{n=0}^{\infty} w_n |n\rangle \langle n| \ , \ |n\rangle = \frac{1}{\sqrt{n!}} (\hat{b}_u^\dagger)^n |0\rangle \ , \tag{19}$$

expressed by a Poisson (non-thermal) distribution $w_n = e^{-J/\hbar} (J/\hbar)^n / n!$ of quantum entropy \cite{8} $S_n = -\sum_n w_n \ln w_n$ \cite{9}, over the eigenstates $|n\rangle$ of the angular momentum operator $L_z = \hbar (\hat{b}_z^\dagger \hat{b}_u - \hat{b}_u^\dagger \hat{b}_d), \hat{b}_d^\dagger = (\hat{b}_x - i \hat{b}_y)/\sqrt{2}$.

**Appendix 2: Comparison with astronomical data**

The condition \cite{17} and the third law of J. Kepler (May 15 1618) yield for the n’th circular orbit the radius $r_n = R_G 2^{1+2n/3}$, $n = 0, 1, 2, \ldots$ . In the case of Jupiter $R_G = 2.82$ m, and for $n = 39, 40, 41, 42$ we get values ($r_n$) close to the ones observed ($r_{obs}$) for its largest satellites: Io, Europa, Ganimede, Callisto, discovered by G. Galilei in 1610.

\footnote{A Gaussian distribution on $\mathbb{R}$ with the same mean and variance as $\{w_n\}$ has the entropy $S_J = [1 + \ln(2\pi J/\hbar)]/2$.}
Table 1. Comparison between the observed orbital radius \( (r_{\text{obs}}) \) of the Jupiter satellites and the calculated value \( (r_n) \).

| Satellite/n | Io/39 | Eu/40 | Ga/41 | Ca/42 |
|-------------|-------|-------|-------|-------|
| \( r_{\text{obs}} \) (10^3 km) | 421.6 | 670.8 | 1070  | 1882  |
| \( r_n \) (10^3 km)    | 378.5 | 600.8 | 953.7 | 1514  |
| \( r_{\text{obs}}/r_n \) | 1.11  | 1.12  | 1.12  | 1.24  |

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