PHASE-SPACE PATH-INTEGRAL CALCULATION OF THE WIGNER FUNCTION

J H Samson, *Dept Physics*

Loughborough University

It is possible, therefore, that a closer study of the relation of classical and quantum theory might involve us in negative probabilities, and so it does.

R P Feynman (1987)

Can we write expectation values as averages wrt some distribution W in some space Γ?

$$\mathrm{Tr}\left(\hat{A}\hat{\rho}\right) = \int_\Gamma A(x)W(x)\mathrm{d}x \qquad (1)$$

where $A(x)$ depends *only* (and linearly) on the operator $\hat{A}$
and $W(x)$ depends *only* (and linearly) on the density matrix $\hat{\rho}$?
Yes, but…

W exists; no *positive-definite* W exists.

Examples of $W(x)$:

1 Hidden-variable distribution for measurements on entangled state
2 Quantum Monte Carlo sign problem; Γ is sample space
3 Wigner function W, joint distribution of incompatible variables in phase space Γ.
4 Amplitude $W[x] = \exp(-S[x])$ of path in coherent-state path integral; Γ is function space.

We will relate 3 and 4 by showing how the sign oscillations of the Wigner function emerge from interference between Berry phases of paths for

Spin s Wigner function[1]
Phase space Wigner function[2]

This provides a path integral method for evaluation of the Wigner function.

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[1] J H Samson, *J Phys A* **33** 5219–5229 (2000)
[2] J H Samson, *J Phys A* in press and quant-ph/0308119

Wigner function

The Wigner function $W(\mathbf{x})$ characterises a quantum state $\hat{\rho}$ as a distribution over non-commuting variables $\mathbf{x} \in \mathbb{R}$.

- Integration over some variables gives marginal distribution over remaining variables.
- Can be determined tomographically by measurements on ensemble.
- Not in general positive.

N operators $\hat{\mathbf{x}} = \left(\hat{x}_1, \cdots, \hat{x}_N\right)$ e. g., spin components, position and momentum, …

Write the Wigner function as a distribution of the operators

$$W(\mathbf{x}) = \mathrm{Tr}\left\{\hat{\rho}\,\delta(\mathbf{x} - \hat{\mathbf{x}})\right\}, \tag{2}$$

defined with symmetric ordering $\delta(\mathbf{x} - \hat{\mathbf{x}}) = (2\pi)^{-N} \int d^N\lambda\, e^{i\lambda\cdot(\mathbf{x} - \hat{\mathbf{x}})}$ (3)

This recovers the standard Wigner function (14).

Coherent states

Basis $|\lambda\rangle \in \mathcal{H}$ for Hilbert space, where $\lambda \in \mathcal{M}$ is a continuous variable
Overcomplete non-orthogonal basis:

$$\int_{\mathcal{M}} d\lambda\, |\lambda\rangle\langle\lambda| = 1 \tag{4}$$

P-representation of operators as distribution of coherent state projectors:

$$\int_{\mathcal{M}} d\lambda\, P_A(\lambda, \lambda^*)\, |\lambda\rangle\langle\lambda| = \hat{A} \tag{5}$$

P_A may be a singular distribution.

Path integral

E. g., for thermal density matrix.

Insert L copies of completeness relation

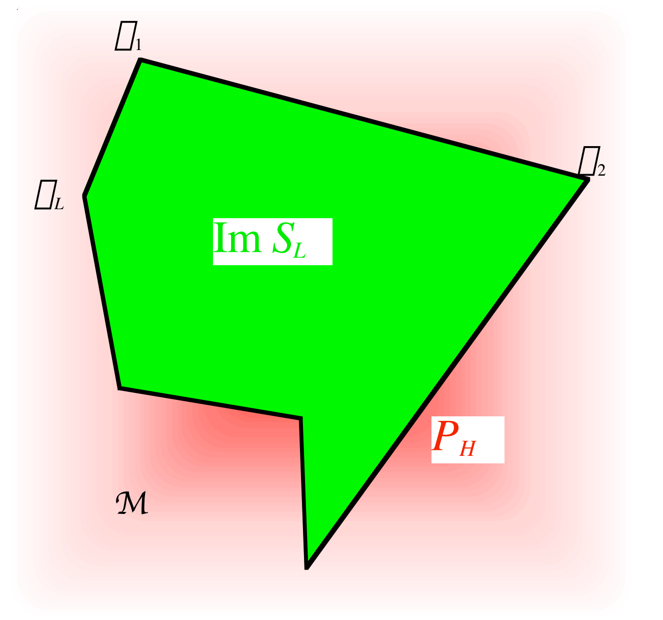
$$e^{-\beta\hat{H}} \approx \left(1-\frac{\beta\hat{H}}{L}\right)^{L} = \prod_{l=1}^{L}\int_{\mathcal{M}} d\alpha_l \left(1-\frac{\beta}{L}P_H\left(\alpha_l,\alpha_l^{*}\right)\right)|\alpha_l\rangle\langle\alpha_l| \qquad (6)$$

Hence partition function is integral over L-gon paths with geometrical action S_L

$$Z = \mathrm{Tr}e^{-\beta\hat{H}} \approx \int_{\mathcal{M}^L}\prod_{l=1}^{L} d\alpha_l \exp\left(-S_L[\alpha]-\frac{\beta}{L}\sum_{l=1}^{L}P_H(\alpha_l,\alpha_l^{*})\right) \qquad (7)$$

$$\exp(-S_L[\alpha]) = \langle\alpha_L|\alpha_{L-1}\rangle\langle\alpha_{L-1}|\alpha_{L-2}\rangle\dots\langle\alpha_1|\alpha_L\rangle \qquad (8)$$

(The P-function of a polynomial Hamiltonian exists, but that of the density matrix may be singular. Hence the advantage of time slicing.)

	Example of path in (7) Paths have complex weight. Re S_L: squares of segment lengths Im S_L: area enclosed by path (Berry phase) P_H: determined by Hamiltonian

We use this to evaluate the Wigner function (2).

Wigner function at **x** □ □ determined by integral over paths associated with *path centroid* **x**. Berry phase of dominant paths □ sign of Wigner function Path integral method of calculating Wigner function

1 Free spin *s* (compact phase space) ref 1

Hilbert space: $\mathcal{H} = \mathbb{C}^{2s+1}$

Coherent state manifold: Bloch sphere $\mathcal{M} = S^2$

Classical spin space: □ = $\mathbb{R}^3$

Density matrix $$\hat{\rho} = \frac{1}{2s+1} \sum_{m=-s}^{s} |m\rangle\langle m| \tag{9}$$

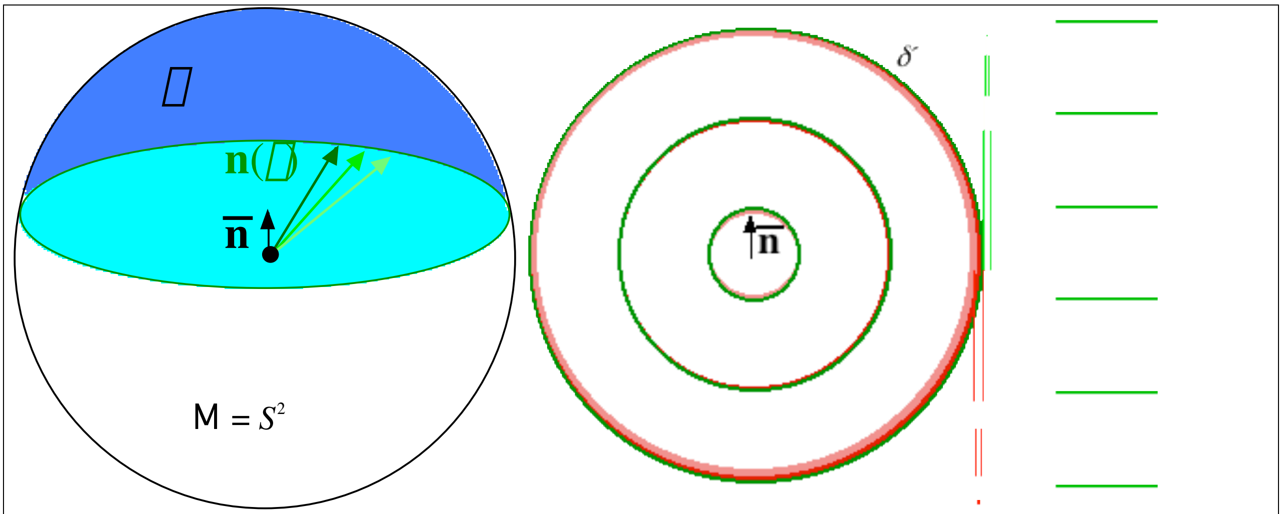
Wigner function from (2)

$$W_s(\mathbf{S}) = \frac{-1}{2s+1} \sum_{m=-s}^{s} \frac{\delta'(S-m)}{2\pi S} \tag{10}$$

(singular distribution in $\mathbb{R}^3$ supported on quantised spheres)

Marginals give correct distribution for any spin component:

$$W_s(S_z) = \int\int dS_x dS_y W_s(\mathbf{S}) = \frac{1}{2s+1} \sum_{m=-s}^{s} \delta(S-m) \tag{11}$$



Path integral over paths on S^2 □ Wigner function $W(\boldsymbol{S})$ in $\mathbb{R}^3$ □ Marginals $W(S_z)$

Main result: the Wigner function is the distribution of the path centroid of the *P*-symbol of the operators. Equivalence class of all paths with centroid $\bar{\mathbf{n}} = \int_0^1 \mathbf{n}(□)\, d□$ contribute to Wigner function at that point (s+1)$\bar{\mathbf{n}}$.

Typical path has non-zero phase.

Interference of paths □ sign oscillations of Wigner function.

2 Particle in one dimension (flat phase space) ref 2

Hilbert space: $\mathcal{H} = L^2(\mathbb{R})$, with harmonic oscillator basis

Coherent state manifold = classical phase space $\mathcal{M} = \mathbb{C}$, □ = $\mathbb{R}^2$

Coherent states

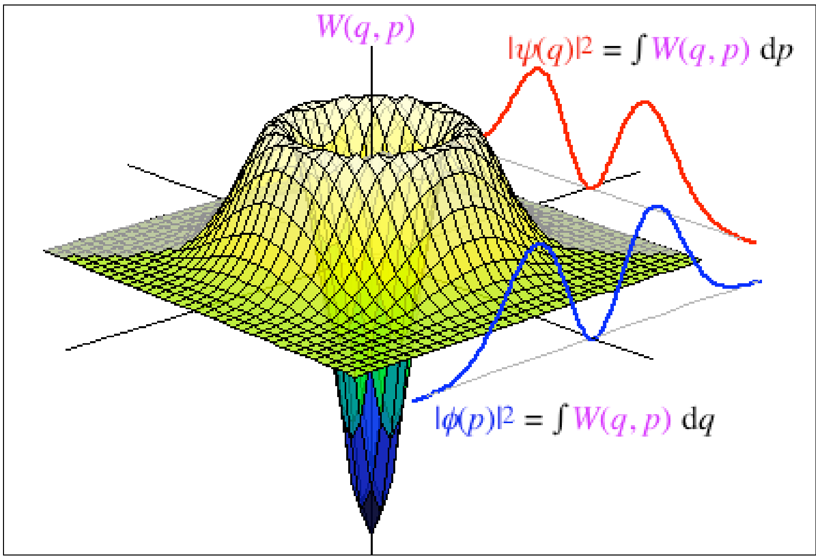
$$|\alpha\rangle \equiv e^{\alpha \hat{a}^\dagger - \alpha^* \hat{a}}|0\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}}|n\rangle \tag{12}$$

correspond to minimum-uncertainty states centred at phase space point (q, p):

$$\alpha = \sqrt{\frac{m\omega}{2\hbar}}q + \frac{i}{\sqrt{2m\hbar\omega}}p \tag{13}$$

Wigner function $W(q, p)$ or $W(□, □^*)$ joint distribution of position and momentum in phase space □. For a pure state

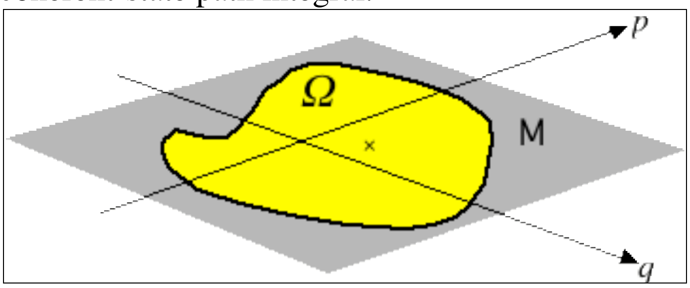
$$W(q, p) = \frac{1}{\pi\hbar}\int_{-\infty}^{\infty} \psi^*(q-y)\psi(q+y)e^{-2ipy/\hbar}\,\mathrm{d}y \tag{14}$$



Wigner function for first excited state of harmonic oscillator, showing recovery of position and momentum distributions as marginals

Amplitude $\exp(-S[x])$ of path in coherent-state path integral.

$$S_{\text{geom}} = \int_0^1 \left\langle \psi \right| \frac{\partial}{\partial t} \left| \psi \right\rangle \mathrm{d}t \quad i□$$



We wish to understand the sign oscillations of the Wigner function in terms of interference between phases of paths of associated with that point.

Example

Consider one-parameter family of density matrices

$$\hat{\rho}_L(N), \text{ with } L \in \mathbb{Z}^+ \text{ and } N \in \mathbb{R}^+ \tag{15}$$

interpolating between a Poisson state of mean occupation N for $L = 1$ and a number state $|n\rangle\langle n|$ (where n is the largest integer $< N$) for $L = \infty$:

$$\hat{\rho}_1(N) = \int_0^{2\pi} \frac{d\theta}{2\pi} \left|\sqrt{N}e^{i\theta}\right\rangle \left\langle \sqrt{N}e^{i\theta}\right| = e^{-N} \sum_{n=0}^{\infty} \frac{N^n}{n!} |n\rangle\langle n| \tag{16}$$

$$\hat{\rho}_L(N) = \frac{(\hat{\rho}_1(N))^L}{Z_L(N)} = \frac{\prod_{l=1}^{L}\left(\int_0^{2\pi} \frac{d\theta_l}{2\pi} |\sqrt{N}e^{i\theta_l}\rangle\langle\sqrt{N}e^{i\theta_l}|\right)}{Z_L(N)} = \frac{e^{-LN}}{Z_L(N)} \sum_{n=0}^{\infty} \left(\frac{N^n}{n!}\right)^L |n\rangle\langle n| \tag{17}$$

where $Z_L(N) = \mathrm{Tr}\,(\hat{\rho}_1(N))^L$.

(18)

This is a sequence of physically realizable density matrices, corresponding to the Hamiltonian

$$\hat{H}(N) = N + \ln \hat{n}! - \hat{n} \ln N = N + \ln \int_0^{\infty} e^{-x + \hat{n}\ln(x/N)} dx \tag{19}$$

at inverse temperature $\beta = L$.

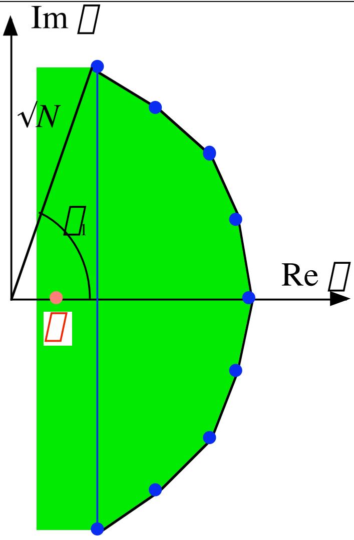
Lowest energy levels for large N might model, e.g., charging energy of Cooper pair box:

$$\hat{H}(N) \approx \frac{\ln 2\pi N}{2} + \frac{\left(\hat{n} + \frac{1}{2} - N\right)^2}{2N} \tag{20}$$

Wigner function of $\hat{\rho}_L(N)$ now given by exact path integral over L-gon:

$$W_L(\alpha, \alpha^*; N) = \frac{1}{Z_L(N)} \prod_{l=1}^{L} \left(\int_0^{2\pi} \frac{d\theta_l}{2\pi}\right) e^{-S_L[\theta,\alpha]} \tag{21}$$

$$S_L[\theta, \alpha] = LN + 2|\alpha|^2 - N \sum_{l=1}^{L} e^{i(\theta_{l-1}-\theta_l)} + 2Ne^{i(\theta_L-\theta_1)} - 2\sqrt{N}|\alpha|(e^{-i\theta_1} + e^{i\theta_L}) \tag{22}$$



Dominant (real) path in integral (21) contributing to $W_L(\alpha, \alpha^*; N)$ for $L = 9$.

The paths associated with α have the mid-point of the ends close to α.

The phase of the path is proportional to the green shaded area, resulting in the sign oscillations of the Wigner function.

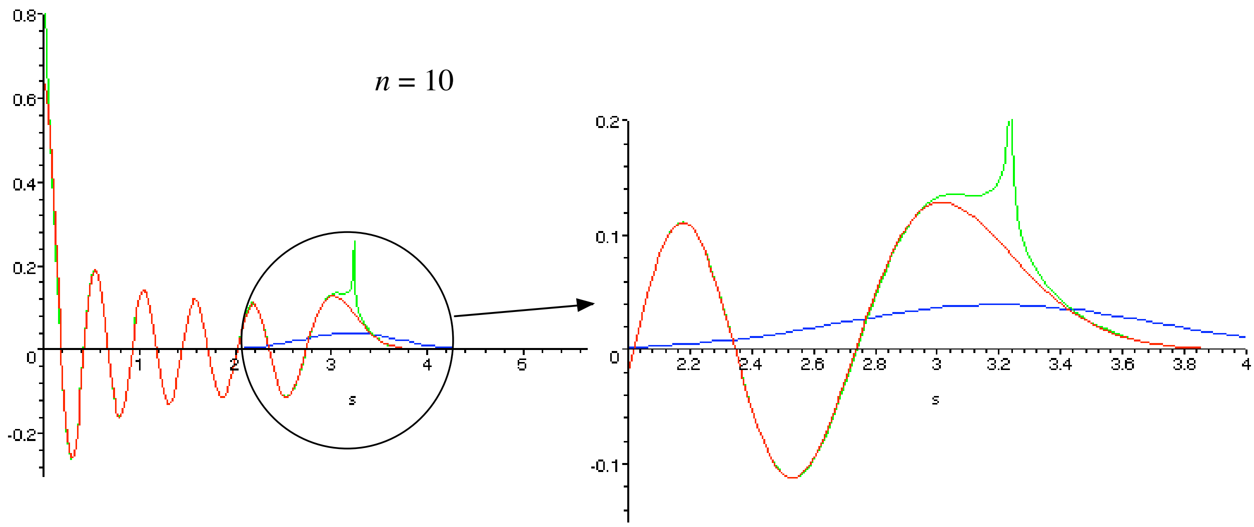
Dominant path for points $|\alpha| > \sqrt{N}$ outside the energy surface encloses zero area and gives positive Wigner function.

Saddle-point expansion of (21) to second-order for $N = n + 1/2$ in the limit $L \to \infty$ is

$$W_L^{\rm sp}(\alpha,\alpha^*;n+\tfrac{1}{2}) \sim \begin{cases} \dfrac{\cos\left(2|\alpha|\sqrt{n+1/2-|\alpha|^2}-(2n+1)\cos^{-1}\left(\frac{|\alpha|}{\sqrt{n+\frac{1}{2}}}\right)+\pi/4\right)}{L^{1/2}\left(1+\frac{1}{24n}\right)^L\left[\frac{|\alpha|^2}{n+\frac{1}{2}}\left(1-\frac{|\alpha|^2}{n+\frac{1}{2}}\right)\right]^{1/4}}, & |\alpha| < \sqrt{n+\frac{1}{2}} \\ \dfrac{\exp\left((2n+1)\cosh^{-1}\left(\frac{|\alpha|}{\sqrt{n+1/2}}\right)-2|\alpha|\sqrt{|\alpha|^2-n-\frac{1}{2}}\right)}{2L^{1/2}\left(1+\frac{1}{24n}\right)^L\left[\frac{|\alpha|^2}{n+\frac{1}{2}}\left(\frac{|\alpha|^2}{n+\frac{1}{2}}-1\right)\right]^{1/4}}, & |\alpha| > \sqrt{n+\frac{1}{2}} \end{cases} \qquad (23)$$

which (apart from a normalization factor) is identical to the WKB approximation of Berry and reproduces the oscillations of the exact Wigner function

$$W_\infty(\alpha,\alpha^*;N) = \frac{2}{\pi}(-1)^n e^{-2|\alpha|^2} L_n(4|\alpha|^2) \qquad (24)$$



The exact number-state Wigner function W_∞ (red, eq 24), the present saddle-point approximation $W^{\rm sp}_\infty$ (green, eq 23, with amplitude fitted), and the exact Wigner function W_1 for the Poisson state (blue, eq 16) for n=10 (N = 10.5). Horizontal axis is $|\alpha|$.