

EXACT CLASSICAL EFFECTIVE POTENTIALS

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A quantum spin system can be modelled by an equivalent classical system, with an effective Hamiltonian obtained by integrating all non-zero frequency modes out of the path integral. The effective Hamiltonian $H_{\text{eff}}(\{\mathbf{S}_i\})$ derived from the coherent-state integral is highly singular: the quasiprobability density $\exp(-\beta H_{\text{eff}})$, a Wigner function, imposes quantisation through derivatives of delta functions. This quasiprobability is the distribution of the time-averaged lower symbol of the spin in the coherent-state integral. We relate the quantum Monte Carlo minus-sign problem to the non-positivity of this quasiprobability, both analytically and by Monte Carlo integration.

1 Introduction

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 Feynman¹

One may distinguish two broad numerical approaches to quantum statistical mechanics. One can evaluate a path integral by direct Monte Carlo methods. Here the notorious *minus-sign problem* (or *phase problem*) often hinders direct evaluation of the path integral: this refers to a rapid oscillation of the integrand in sign or phase, and the resulting intolerably slow convergence of integrals evaluated by random sampling. Alternatively, one can integrate out the quantum fluctuations, leaving an effective Hamiltonian $H_{\text{eff}}(\mathbf{x})$ with c -number variables \mathbf{x} to be used in a *classical* simulation². A similar non-positivity arises here if the observables described by \mathbf{x} are incompatible: the distribution $\exp(-\beta H_{\text{eff}}(\mathbf{x}))$ is then a Wigner function, which is not in general positive-definite.

A free spin s serves here as a useful toy model to relate the path integral and the Wigner function³. The spin coherent-state path integral, a poor starting point for numerical simulations, presents the worst case of the sign problem: for continuous paths the integrand is a pure Berry phase factor. The spin Wigner function is highly singular, consisting of derivatives of delta functions supported on concentric spheres of quantised radius^{3,4}. We demonstrate the common origin of these non-positivities both analytically and numerically.

2 Classical effective Hamiltonian

We consider a system with density matrix $\hat{\rho} \equiv \exp(-\beta\hat{H})$, and assign c -number variables $\mathbf{x} \in \mathbb{R}^N$ to operators $\hat{\mathbf{x}}$. We define the *Wigner function* $W(\mathbf{x})$ and *classical effective Hamiltonian* $H_{\text{eff}}(\mathbf{x})$ of these variables as

$$W(\mathbf{x}) \equiv \exp(-\beta H_{\text{eff}}(\mathbf{x})) = \text{Tr}(\hat{\rho} \delta_N(\mathbf{x} - \hat{\mathbf{x}})), \quad (1)$$

where δ_N is the N -dimensional delta function. To remove operator-ordering ambiguity, we define

$$\delta_N(\mathbf{x} - \hat{\mathbf{x}}) \equiv \int \frac{d^N \lambda}{(2\pi)^N} \exp(i\lambda \cdot (\mathbf{x} - \hat{\mathbf{x}})). \quad (2)$$

If the components of $\hat{\mathbf{x}}$ do not commute, the delta operator need not be positive.

Here we restrict consideration to the spin operator $\hat{\mathbf{x}} = \hat{\mathbf{S}}$ in the spin- s representation. The distribution is the spin Wigner function $W_s(\mathbf{S})$. For a single spin with vanishing Hamiltonian the trace of Eq. (2) is easily evaluated^{3,4} to give derivatives of delta functions supported on concentric spheres of quantised radius:

$$W_s(\mathbf{S}) = \langle \delta_3(\mathbf{S} - \hat{\mathbf{S}}) \rangle = \frac{-1}{2s+1} \sum_{m=-s}^s \frac{1}{2\pi S} \frac{d}{dS} \delta(S - m), \quad (3)$$

where $S = |\mathbf{S}|$ and $\hat{\mathbf{S}}^2 = s(s+1)$. The spheres with $m < 0$ do not contribute and for *integer* spin there is a positive delta function at the origin of weight

$$\frac{-\delta'(S)}{2\pi S(2s+1)} = \frac{\delta_3(\mathbf{S})}{(2s+1)}. \quad (4)$$

To motivate this form, we need to verify that the correct marginal distributions are obtained. Integrating W_s over a plane yields the expected distribution $\sum_{m=-s}^s \delta(\mathbf{e} \cdot \mathbf{S} - m)/(2s+1)$ for the normal component of spin³. For two coupled spins $1/2$, with Hamiltonian $-J\mathbf{S}_1 \cdot \mathbf{S}_2$, a convolution integral of the two single-spin functions $W_{1/2}$ gives (after some manipulations)

$$W(\mathbf{S}_1 + \mathbf{S}_2) = \frac{3e^{\beta J/4} W_1(\mathbf{S}_1 + \mathbf{S}_2) + e^{-3\beta J/4} W_0(\mathbf{S}_1 + \mathbf{S}_2)}{3e^{\beta J/4} + e^{-3\beta J/4}}. \quad (5)$$

This is the correct thermal average of triplet and singlet distributions, in line with the effective-Hamiltonian interpretation. Eq. (5) can be further interpreted as a local hidden variable distribution, which must give the correct correlations for spin measurements on two electrons. No positive definite distribution exists for a singlet state^{4,5}, and the distribution must therefore be non-definite.

3 Coherent-state path integrals

Spin coherent states $|\mathbf{n}\rangle$ for spin s are labelled by a unit vector \mathbf{n} , such that $\mathbf{n} \cdot \hat{\mathbf{S}}|\mathbf{n}\rangle = s|\mathbf{n}\rangle$. To relate the Wigner functions just described to the coherent state path integral, we split the exponent of Eq. (2) into L time slices,

$$W_s(\mathbf{S}) = \langle \delta_3(\mathbf{S} - \hat{\mathbf{S}}) \rangle = \int \frac{d^3\lambda}{8\pi^3} e^{i\lambda \cdot \mathbf{S}} \left\langle \left(1 - i\lambda \cdot \hat{\mathbf{S}}/L + O(L^{-2}) \right)^L \right\rangle. \quad (6)$$

We now insert a resolution of unity in the form $\frac{2s+1}{4\pi} \int d\mathbf{n} |\mathbf{n}\rangle \langle \mathbf{n}|$ between each slice⁶, represent the spin by its *lower* symbol $(s+1)\mathbf{n}$ ^{7,8},

$$\hat{\mathbf{S}} = \frac{2s+1}{4\pi} \int d\mathbf{n} (s+1)\mathbf{n} |\mathbf{n}\rangle \langle \mathbf{n}|, \quad (7)$$

and re-exponentiate. The lower symbol is used as the paths (here and in our Monte Carlo calculation) are only piecewise continuous. This gives

$$W_s(\mathbf{S}) = \lim_{L \rightarrow \infty} W_s^L(\mathbf{S}), \quad (8)$$

the limit defined in the sense of a distribution, with approximants

$$\begin{aligned} W_s^L(\mathbf{S}) &= \frac{1}{2s+1} \int \frac{d^3\lambda}{8\pi^3} e^{i\lambda \cdot \mathbf{S}} \int \prod_{i=1}^L \left(\frac{2s+1}{4\pi} d\mathbf{n}_i e^{-i(s+1)\lambda \cdot \mathbf{n}_i} \right) \times \\ &\quad \times \langle \mathbf{n}_1 | \mathbf{n}_2 \rangle \langle \mathbf{n}_2 | \dots | \mathbf{n}_L \rangle \langle \mathbf{n}_L | \mathbf{n}_1 \rangle \\ &= \frac{1}{2s+1} \int \prod_{i=1}^L \left(\frac{2s+1}{4\pi} d\mathbf{n}_i \right) \delta_3(\mathbf{S} - (s+1)\bar{\mathbf{n}}) \langle \mathbf{n}_1 | \mathbf{n}_2 \rangle \dots \langle \mathbf{n}_L | \mathbf{n}_1 \rangle, \end{aligned} \quad (9)$$

where $\bar{\mathbf{n}} = \sum_{i=1}^L \mathbf{n}_i / L$ is the time-averaged coherent-state label. We therefore have a sequence of well-defined distributions (9) convergent on the Wigner function. For large L the discretised distribution $W_s^L(\mathbf{S})$ can be shown to be asymptotically a smeared Wigner function; for spin 1/2 we find

$$W_{1/2}^L(\mathbf{S}) \approx \left(\frac{L}{\pi} \right)^{3/2} \int d^3\mathbf{x} e^{-L(\mathbf{x}-\mathbf{S})^2} W_{1/2}(\mathbf{S}). \quad (10)$$

In order to verify this result and investigate the importance of the sign problem, we have computed the discretised Wigner function (9) by direct Monte Carlo sampling of the histogram for $\bar{\mathbf{n}}$. Each path comprises L independent points $\mathbf{n}_i, i = 1 \dots L$, taken from a uniform distribution on the sphere. Since the product of overlaps in Eq. 9 is complex for $L > 2$, a phase problem arises. For the results shown in Fig. 1, 10^7 independent paths were generated for each L from 2 to 15. Further analysis shows the numerical distributions converging to the Wigner

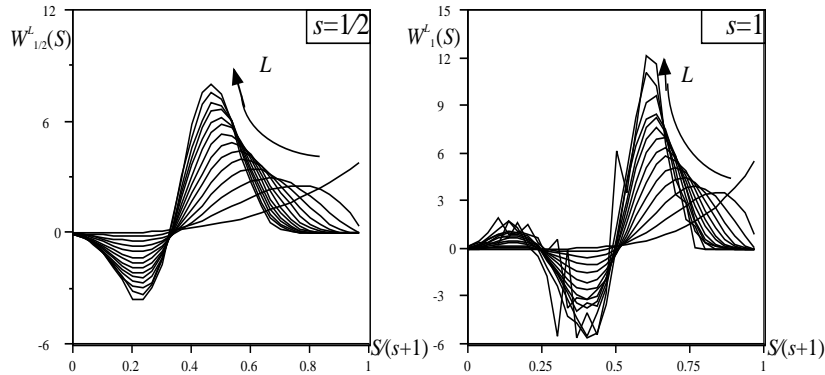


Figure 1. Discretised Wigner function for spin 1/2 and 1 with $L = 2 \dots 15$ time slices and 10^7 Monte Carlo steps.

function (3) according to Eq. (10). We also see how the phase fluctuations lead to numerical instabilities. The correct distribution would be obtained if the the number of Monte Carlo steps were taken to infinity before the number of time slices. It is clear from the figure that 10^7 steps are insufficient for convergence for spin 1; results for higher spin show still slower convergence.

We have thus demonstrated the emergence of a non-positive quasiprobability (the spin Wigner function) from the Berry phases of the integral. Numerical calculations are however rapidly overwhelmed by the sign problem.

References

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