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 $H_{\text{eff}}(\{S_i\})$ 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 Feynman

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 $H_{\text{eff}}(x)$ with $c$-number variables $x$ to be used in a classical simulation. A similar non-positivity arises here if the observables described by $x$ are incompatible: the distribution $\exp(-\beta H_{\text{eff}}(x))$ is then a Wigner function, which is not in general positive-definite.

A free spin serves here as a useful toy model to relate the path integral and the Wigner function. 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. 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 $x \in \mathbb{R}^N$ to operators $\hat{x}$. We define the Wigner function $W(x)$ and classical effective Hamiltonian $H_{\text{eff}}(x)$ of these variables as

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

(1)

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

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

(2)

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

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

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

(3)

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

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

(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

$$\sum_{m=-s}^{s} \delta(e \cdot S - m)/(2s + 1)$$

for the normal component of spin. For two coupled spins $1/2$, with Hamiltonian $-J\hat{S}_1 \cdot \hat{S}_2$, a convolution integral of the two single-spin functions $W_{1/2}$ gives (after some manipulations)

$$W(S_1 + S_2) = \frac{3e^{3J/4}W_1(S_1 + S_2) + e^{-3J/4}W_0(S_1 + S_2)}{3e^{3J/4} + e^{-3J/4}}.$$

(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, and the distribution must therefore be non-definite.
3 Coherent-state path integrals

Spin coherent states $|n\rangle$ for spin $s$ are labelled by a unit vector $n$, such that $n \cdot \hat{S}|n\rangle = s|n\rangle$. To relate the Wigner functions just described to the coherent state path integral, we split the exponent of Eq. (3) into $L$ time slices,

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

We now insert a resolution of unity in the form $\frac{2s+1}{4\pi} \int d\lambda |n\rangle\langle n|$ between each slice $i$, represent the spin by its lower symbol $(s+1)n$, and re-exponentiate. The lower symbol is used as the paths (here and in our Monte Carlo calculation) are only piecewise continuous. This gives

$$W_s(S) = \left( \frac{2s+1}{4\pi} \int d\lambda (s+1)n |n\rangle\langle n| \right)^L,$$

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

$$W_s^L(S) = \frac{1}{2s+1} \int \frac{d^3\lambda}{8\pi^3} e^{i\lambda \cdot S} \prod_{i=1}^L \left( \frac{2s+1}{4\pi} d\lambda_i e^{-i(s+1)\lambda_i n_i} \right) \times \langle n_1 | n_2 \rangle \langle n_2 | \cdots | n_L \rangle \langle n_L | n_1 \rangle,$$

where $\bar{n} = \sum_{i=1}^L n_i/L$ is the time-averaged coherent-state label. We therefore have a sequence of well-defined distributions (8) convergent on the Wigner function. For large $L$ the discretised distribution $W_s^L(S)$ can be shown to be asymptotically a smeared Wigner function; for spin $1/2$ we find

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

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 $\bar{n}$. Each path comprises $L$ independent points $n_i, i = 1\ldots L$, 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 $L = 2 \ldots 15$ time slices and $10^7$ Monte Carlo steps.

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

5. J. S. Bell, *Physics* **1**, 195 (1964)