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Phase Space Methods for Spin Systems

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N-particle Spin Systems

Consider the Hilbert space $\mathcal{H} = \mathbb{C}^{2N}$, $N \gg 1$, of a system of N spin-$1/2$ particles, and a Hamiltonian matrix $H \in \text{Herm}(\mathcal{H})$ as for example the Heisenberg Hamiltonian:

$$H = \sum_{n,m=1}^{N} \left(J^x_{nm}\sigma^x_n\sigma^y_m + J^y_{nm}\sigma^y_n\sigma^y_m + J^z_{nm}\sigma^z_n\sigma^z_m \right), \tag{1}$$

with constants $J^\mu_{n,m} \in \mathbb{R}$ such that $J^\mu_{nn} = 0$ for all $\mu = x, y, z$, $m, n = 1, \dots, N$ and Pauli-μ operators σ^μ_n acting on site n.

The quantum evolution of an observable $O_{\text{init}} \in \text{Herm}(\mathcal{H})$ is given by the von-Neumann equation

$$\dot{O}(t) = i\left[O(t), H\right], \quad O(t=0) = O_{\text{init}} \tag{2}$$

Consider a density matrix $\rho \in \text{Herm}(\mathcal{H})$ with $\rho \succeq 0$, and $\operatorname{tr}\rho = 1$. The expectation value of $O(t)$ with respect to ρ is

$$\langle O(t) \rangle_\rho := \operatorname{tr}\left[O(t)\,\rho\right]. \tag{3}$$

Numerical simulation of $O(t)$**:** Challenging for $N \gg 1$.

Wigner Functions

Let $N = 1$ and $\mathbb{S}^2 = \{\mathbf{S} = (S^x, S^y, S^z) \in \mathbb{R}^3 \mid \|\mathbf{S}\|_2 = 1\}$. Following [1], we set $\Omega = \mathbb{S}^2$ and consider the map

$$\Delta : \Omega \to \text{Herm}(\mathcal{H}), \quad \Delta(\mathbf{S}) = \tfrac{1}{2}(\mathbb{1} + \mathbf{S}\cdot\sigma),$$

where $\sigma = (\sigma^x, \sigma^y, \sigma^z)$. The **Wigner function** of an operator $O \in \text{Herm}(\mathcal{H})$ is defined as

$$W_O : \Omega \to \mathbb{R}, \quad W_O(\mathbf{S}) = \operatorname{tr}\left[O\Delta(\mathbf{S})\right].$$

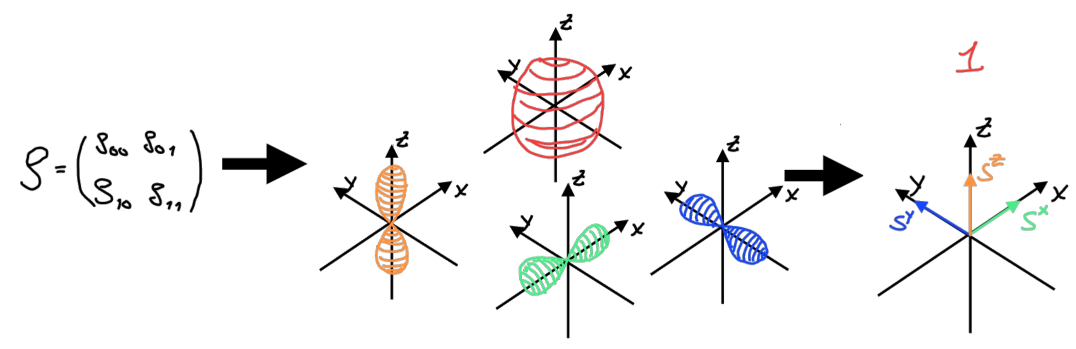

Figure 1. Phase space description for a single spin system ($N = 1$).

Let $N \geq 1$. Let $\Omega = (\mathbb{S}^2)^{\times N}$ and define the Δ-kernel and Wigner transforms as

$$\Delta_N(\mathbf{S}_1, \dots \mathbf{S}_N) = \bigotimes_{n=1}^{N} \Delta(\mathbf{S}_n), \quad W_O(\mathbf{S}_1, \dots, \mathbf{S}_N) = \operatorname{tr}\left[O\Delta_N(\mathbf{S}_1, \dots, \mathbf{S}_N)\right].$$

The expectation value $\langle O \rangle_\rho$ of an observables O wrt. a density matrix ρ satisfies

$$\langle O \rangle_\rho = \int_\Omega W_O(\mathbf{S}_1, \dots, \mathbf{S}_N)\, W_\rho(\mathbf{S}_1, \dots, \mathbf{S}_N)\ \mathsf{d}\mathbf{S}.$$

▷ $\Omega \subset \mathbb{R}^{3N}$ with $N \gg 1$ requires high-dimensional numerical quadrature.

Weyl Calculus

Let $A, B \in \text{Herm}(\mathcal{H})$ and define the star product $\star$ such that $W_A \star W_B := W_{AB}$. Based on [1], one can show that for our choice of Ω,

$$W_A \star W_B = W_A \left[\prod_{n=1}^{N} \left(1 + \overleftarrow{\nabla}_n \cdot \overrightarrow{\nabla}_n - (\overleftarrow{\nabla}_n \cdot \mathbf{S}_n)(\mathbf{S}_n \cdot \overrightarrow{\nabla}_n) - i\overleftarrow{\nabla}_n \cdot (\mathbf{S}_n \times \overrightarrow{\nabla}_n) \right) \right] W_B$$

where $\overleftarrow{\nabla}_n$ and $\overrightarrow{\nabla}_n$ act on W_A and W_B, respectively. The Moyal bracket

$$\{W_A, W_B\}_\star := W_A \star W_B - W_B \star W_A$$

can be expanded in terms of differentiation orders, $\{W_A, W_B\}_\star = \sum_{k=1}^{N} \{W_A, W_B\}_k$. The k-bracket has the form

$$\{W_A, W_B\}_k = 2 \sum_{|\mathbf{n}|=k} \sum_{|\alpha|=|\beta|=k} \Gamma^{(\mathbf{n})}_{\alpha,\beta}\ (\partial^\alpha_{\mathbf{n}} W_A)\ (\partial^\beta_{\mathbf{n}} W_B),$$

Here, $\mathbf{n} \in \{1, \dots, N\}^{\times k}$ with $\mathbf{n}_i \neq \mathbf{n}_j$, $\partial^\alpha_{\mathbf{n}} = \partial^{\alpha_1}_{n_1} \dots \partial^{\alpha_k}_{n_k}$ and $\Gamma^{(\mathbf{n})}_{\alpha,\beta}$ is a product of terms like $[I_{n_i}]^{\beta_i}_{\alpha_i} = \delta_{\alpha_i\beta_i} - S^{\alpha_i}_{n_i} S^{\beta_i}_{n_i}$ and $[K_{n_i}]^{\beta_i}_{\alpha_i} = -i\varepsilon_{\alpha_i\gamma\beta_i} S^\gamma_{n_i}$, that contain an **odd** number of K-operators.

Semi-Classical Approximation of Dynamics

Wigner transforming both sides of eq. (2) gives

$$\frac{\mathsf{d}}{\mathsf{d}t} W_O = i\{W_O, W_H\}_\star. \tag{4}$$

The first bracket $\{\cdot,\cdot\}_1$ induces a *Poisson structure* on Ω and a flow map $\Phi^t : \Omega \to \Omega$ defined by

$$\frac{\mathsf{d}}{\mathsf{d}t}[\Phi^t]^\mu_n = i\left\{ S^\mu_n, W_H \right\}_1\big|_{(\mathbf{S}_1, \dots \mathbf{S}_N) = \Phi^t}, \quad \Phi^0 = \mathbb{1}. \tag{5}$$

Using this to approximate the dynamics, expectation values evolve as:

$$\langle O(t) \rangle_\rho \approx \langle O(t) \rangle^{(\text{cl})}_\rho = \int_\Omega W_{O_{\text{init}}}(\Phi^t(\mathbf{S}))\, W_\rho(\mathbf{S})\ \mathsf{d}\mathbf{S}.$$

Two-body Interactions

If the Hamiltonian $H \in \text{Herm}(\mathcal{H})$ **contains only two-body interactions**, then $\{W_A, W_H\}_\star = \{W_A, W_H\}_1 + \{W_A, W_H\}_2$ with

$$\{W_A, W_H\}_1 = 2\sum_{n=1}^{N} (\partial^\mu_n W_A)\, [K_n]^\nu_\mu\, (\partial^\nu_n W_H),$$

$$\{W_A, W_H\}_2 = 2\sum_{\substack{n_1,n_2=1 \\ n_1 \neq n_2}}^{N} (\partial^{\mu_1}_{n_1}\partial^{\mu_2}_{n_2} W_A) \left([I_{n_1}]^{\nu_1}_{\mu_1} [K_{n_2}]^{\nu_2}_{\mu_2} + [K_{n_1}]^{\nu_1}_{\mu_1} [I_{n_2}]^{\nu_2}_{\mu_2} \right) (\partial^{\nu_1}_{n_1}\partial^{\nu_2}_{n_2} W_H).$$

In this case, the error of the semi-classical approximation is given by (see also [2]):

$$\langle O(t) \rangle_\rho - \langle O(t) \rangle^{(\text{cl})}_\rho = \int_\Omega \left(\int_0^t \{W_{O_{\text{init}}} \circ \Phi^\tau, W_H\}_2 \circ \Phi^{t-\tau} \mathsf{d}\tau \right) W_\rho\ \mathsf{d}\mathbf{S} \tag{6}$$

Example: Ising Model

The **Ising model** is a special case of eq. (1) where $J^x_{nm} = 0 = J^y_{nm}$. Using eq. (5) with $W_H = \sum_{nm} J^z_{nm} S^z_n S^z_m$, the corresponding classical flow is:

$$[\Phi^t(\mathbf{S}_1, \dots \mathbf{S}_N)]^\mu_n = \begin{cases} S^x_n \cos(2\omega_n t) + S^y_n \sin(2\omega_n t), & \mu = x, \\ S^y_n \cos(2\omega_n t) - S^x_n \sin(2\omega_n t), & \mu = y, \\ S^z_n, & \mu = z. \end{cases}$$

with $\omega_n = \sum_m J^z_{nm} S^z_m$. If the initial state is $\rho = (|+\rangle\langle+|)^{\times N}$ and $O_{\text{init}} = \sigma^x_n$, then

$$\langle \sigma^x_n(t) \rangle_\rho = \prod_{m=1}^{N} \cos(2J_{nm}t) \neq \langle \sigma^x_n(t) \rangle^{(\text{cl})}_\rho = \prod_{m \neq n}^{N} \frac{\sin(2J_{nl}t)}{tJ_{nm}}. \tag{7}$$

Discrete Phase Space

Following [4], define the phase space $\Omega^{(D)} = \{(0,0), (0,1), (1,0), (1,1)\}^{\times N}$ and the corresponding Wigner transform of ρ:

$$\rho \mapsto w_a = \operatorname{tr}\left[\rho A_a\right], \quad A_a = \bigotimes_{n=1}^{N} \frac{1}{2}\left[\mathbb{1} + \mathbf{r}_{a_n} \cdot \sigma\right], \quad a = (a_1, \dots, a_n) \in \Omega^{(D)}.$$

where $\{\mathbf{r}_{a_n}\}$ are four distinct points on $\mathbb{S}^2$. Using this (first done in [3]), we find

$$\langle O \rangle_\rho = \int_\Omega W_O(\mathbf{S})\, W_\rho(\mathbf{S})\ \mathsf{d}\mathbf{S} = \sum_{a \in \Omega^{(D)}} w_a W_O(\mathbf{r}_{a_1}, \dots \mathbf{r}_{a_N}).$$

Ising model:

▷ One-site observables are exact, $\langle \sigma^\mu_n(t) \rangle_\rho = \langle \sigma^\mu_n(t) \rangle^{(\text{cl})}_\rho$.

▷ Correlations are not captured exactly, $\langle (\sigma^\mu_n \sigma^\nu_m)(t) \rangle_\rho \neq \langle (\sigma^\mu_n \sigma^\nu_m)(t) \rangle^{(\text{cl})}_\rho$.

Evolution of Observables in the Ising Model

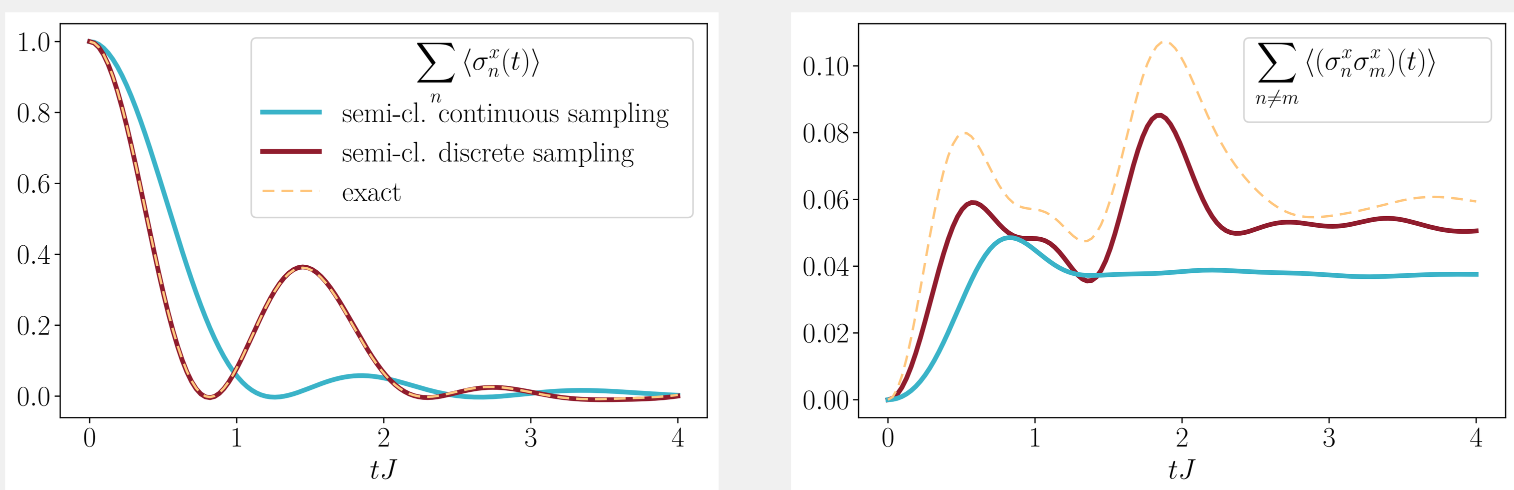

Figure 2. Time evolution in the 1D Ising model. $J_{nm} = |n - m|^{-3}$ and $N = 100$.

Outlook

- Analyse semi-classical time-evolution beyond the Ising model.
- Improve accuracy by exploiting Poisson structure in numerical time integration.
- Use Weyl calculus for beyond semi-classical approximations.

References

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