Some notes on: Truncated Wigner approximation for dissipative spin systems

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(Dated: August 16, 2024)

I. PHASE SPACE REPRESENTATION OF THE DENSITY OPERATOR OF SPINS

A. Operator basis and mapping from Hilbert to phase space

1. phase-point operators and Weyl symbols

Any operator $\hat{A}$ in the Hilbert space of a system of N spins (spin 1/2 particles) can be represented in terms of an overcomplete basis of phase-point operators

$$\hat{\boldsymbol{\Delta}}(\boldsymbol{\Omega}) = \prod_{j=1}^{N} \hat{\Delta}_j(\Omega), \tag{1}$$

with $\Omega = (\theta, \phi)$ and $\boldsymbol{\Omega} = (\Omega_1, \Omega_2, \dots, \Omega_N)$

$$\hat{A} = \int d^N\Omega\, \mathcal{A}(\boldsymbol{\Omega})\, \hat{\boldsymbol{\Delta}}(\boldsymbol{\Omega}) \tag{2}$$

where the integration $d^N\Omega = \prod_{j=1}^{N} d\Omega_j$ is over the angles θ_j, ϕ_j

$$\int d\Omega = \frac{1}{2\pi}\int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \tag{3}$$

The c-number function $\mathcal{A}(\boldsymbol{\Omega})$ is called Weyl symbol of the operator $\hat{A}$. Note that with the above normalization $\int d\Omega = 2$, which was chosen in order to have the Weyl symbol of the unit matrix $\mathbf{1}$ to be the number 1. Specifically we chose for the phase-point operators

$$\begin{aligned}\hat{\Delta}(\theta,\phi) =& \frac{1}{2}\left[\mathbb{1}_2 + \boldsymbol{s}(\theta,\phi)\hat{\boldsymbol{\sigma}}\right] \\ =& \frac{1}{2}\begin{pmatrix} 1+\sqrt{3}\cos\theta & \sqrt{3}e^{-i\phi}\sin\theta \\ \sqrt{3}e^{i\phi}\sin\theta & 1-\sqrt{3}\cos\theta \end{pmatrix}. \end{aligned} \tag{4}$$

$$\tag{5}$$

Here the c-number vector

$$\boldsymbol{s}(\theta,\phi) = \sqrt{3}(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)^T \tag{6}$$

is a representation of the surface of the sphere with radius $\sqrt{3}$. Obviously

$$\mathbf{1} = \int d\Omega\, \hat{\Delta}(\Omega). \tag{7}$$

It is useful to decompose the phase-point operators in terms of Pauli matrices and spherical harmonics $\mathrm{Y}_l^m(\theta,\phi)$:

$$\begin{aligned}\hat{\Delta}(\theta,\phi) =& \frac{\sqrt{4\pi}}{2}\mathrm{Y}_0^0(\theta,\phi)\,\mathbf{1} + \frac{\sqrt{4\pi}}{2}\mathrm{Y}_1^0(\theta,\phi)\,\sigma_z \\ &+ \frac{\sqrt{2\pi}}{2}\left(\mathrm{Y}_1^{-1}(\theta,\phi) - Y_1^1(\theta,\phi)\right)\sigma_x \\ &+ \frac{i\sqrt{2\pi}}{2}\left(\mathrm{Y}_1^{-1}(\theta,\phi) + Y_1^1(\theta,\phi)\right)\sigma_y. \end{aligned} \tag{8}$$

Making use of $\mathrm{Y}_1^{-1} = -\left(\mathrm{Y}_1^1\right)^*$ this can be written as

$$\begin{aligned}\hat{\Delta}(\theta,\phi) =& \sqrt{\pi}\mathrm{Y}_0^0(\theta,\phi)\,\mathbf{1} + \sqrt{\pi}\mathrm{Y}_1^0(\theta,\phi)\,\sigma_z \\ &- \sqrt{2\pi}\,\mathrm{Re}\left[\mathrm{Y}_1^1(\theta,\phi)\right]\sigma_x - \sqrt{2\pi}\,\mathrm{Im}\left[\mathrm{Y}_1^1(\theta,\phi)\right]\sigma_y. \end{aligned} \tag{9}$$

The Weyl symbol $\mathcal{A}$ can be obtained from

$$\mathcal{A}(\boldsymbol{\Omega}) = \mathrm{Tr}\left\{\hat{A}\,\hat{\boldsymbol{\Delta}}(\boldsymbol{\Omega})\right\} \tag{10}$$

where the trace is over all N spin degrees.

We notice that the continuous set of phase point operators is an over-complete set as

$$\begin{aligned}\mathrm{Tr}\left\{\hat{\Delta}(\Omega)\hat{\Delta}(\Omega')\right\} =& 2\pi\Big(\mathrm{Y}_0^0(\Omega)\mathrm{Y}_0^0(\Omega') + \mathrm{Y}_1^0(\Omega)\mathrm{Y}_1^0(\Omega') \\ &+ \mathrm{Y}_1^{1*}(\Omega)\mathrm{Y}_1^1(\Omega') + \mathrm{Y}_1^{-1*}(\Omega)\mathrm{Y}_1^{-1}(\Omega')\Big) \\ &\neq \delta(\Omega-\Omega'). \end{aligned} \tag{11}$$

Eq.(10) is nevertheless correct as one can easily proof for the case of a single-spin operator $\hat{A} = \alpha\mathbf{1} + \beta\sigma_x + \gamma\sigma_y + \lambda\sigma_z$, whose Weyl symbol according to (10) reads:

$$\begin{aligned}\mathcal{A} =& \alpha\sqrt{4\pi}\mathrm{Y}_0^0(\theta,\phi) + (\beta+i\gamma)\sqrt{2\pi}\mathrm{Y}_1^{-1}(\theta,\phi) \\ &+ \lambda\sqrt{4\pi}\mathrm{Y}_1^0(\theta,\phi) - (\beta-i\gamma)\sqrt{2\pi}\mathrm{Y}_1^1(\theta,\phi), \end{aligned}$$

and thus using $\mathrm{Y}_1^{-1} = -\left(\mathrm{Y}_1^1\right)^*$ and the orthogonality of spherical harmonics

$$\int d\Omega\ \mathrm{Y}_l^m(\Omega)^*\mathrm{Y}_{l'}^{m'}(\Omega) = \frac{1}{2\pi}\delta_{ll'}\delta_{mm'} \tag{12}$$

one finds

$$\int d\Omega\, \mathcal{A}(\Omega)\,\hat{\Delta}(\Omega) = \alpha\mathbf{1} + \beta\sigma_x + \gamma\sigma_y + \lambda\sigma_z$$

Alternatively one notices using the completeness relation of spherical harmonics, eq.(64)

$$\mathrm{Tr}\left\{\hat{\Delta}(\Omega)\hat{\Delta}(\Omega')\right\} = \tag{13}$$
$$= \delta(\Omega-\Omega') - 2\pi \sum_{l>1}\sum_{m=-l}^{l} \mathrm{Y}_l^{m*}(\Omega)\mathrm{Y}_l^m(\Omega')$$

that is the trace is equivalent to a Deltafunction up to terms containing only higher-order spherical harmonics both in Ω and in Ω'

2. density matrix and Wigner function

Special importance has the Weyl symbol of the density operator $\hat{\rho}$, which we will call Wigner function for spins

$$\hat{\rho} = \int d\mathbf{\Omega}\, W(\mathbf{\Omega})\, \hat{\mathbf{\Delta}}(\mathbf{\Omega}). \tag{14}$$

3. expectation values

With this expectation values of operators can be expressed in terms of the Wigner function and the Weyl symbol of the operator:

$$\langle \hat{A}\rangle = \mathrm{Tr}\{\hat{A}\hat{\rho}\} = \int d\mathbf{\Omega}\, W(\mathbf{\Omega})\, \mathrm{Tr}\{\hat{A}\hat{\mathbf{\Delta}}(\mathbf{\Omega})\}$$
$$= \int d\mathbf{\Omega}\, W(\mathbf{\Omega})\, \mathcal{A}(\mathbf{\Omega}) \tag{15}$$

B. gauge freedom

The Weyl symbol of an operator is not unique. Using the orthonormality relation of spherical harmonics, eq.(12), one notices that one can add any term proportional to spherical harmonics $\mathrm{Y}_{l>1}^m(\theta,\phi)$ to $\mathcal{A}$

$$\mathcal{A} \;\equiv\; \mathcal{A}' = \mathcal{A} + \sum_{l>1,m} c_{lm}\mathrm{Y}_l^m(\theta,\phi) \tag{16}$$

without changing the operator $\hat{A}$, since

$$\int d\Omega\, \mathrm{Y}_{l>1}^m(\theta,\phi)\, \hat{\Delta}(\Omega) = 0. \tag{17}$$

Eq.(16) constitutes a *gauge freedom.*

C. equations of motion of $W(\Omega)$

When discussing open spin systems we consider an ensemble of N spins coupled to reservoirs. In the Schrödinger picture the time evolution of the total density operator $\hat{\chi}$ of the spin system plus the environment is governed by the quantum Liouville equation

$$\partial_t\hat{\chi}(t) = -i\,[H,\hat{\chi}(t)] \tag{18}$$

where H is the total Hamiltonian of system and reservoir and their interaction. The formal solution reads

$$\hat{\chi}(t) = e^{-iHt}\hat{\chi}(0)e^{iHt} \tag{19}$$

Tracing out the reservoir degrees of freedom gives the reduced density operator $\hat{\rho} = \mathrm{Tr}_B\{\hat{\chi}\}$ of the spin system, which obeys the equation of motion

$$\frac{d}{dt}\hat{\rho}(t) = -i\,\mathrm{Tr}_B\big\{[H,\hat{\chi}(t)]\big\}. \tag{20}$$

Making a Born-Markov approximation in the system-bath interaction, which amounts to assumimg that system and reservoir remain uncorrelated, $\hat{\chi}(t) = \hat{\rho}(t)\otimes\hat{\rho}_B(t)$, then gives a Lindblad Master equation

$$\partial_t\hat{\rho}(t) = -i[H_s,\hat{\rho}(t)] + \mathcal{L}_{\mathrm{diss}}\hat{\rho}(t) = \mathcal{L}\hat{\rho}(t) \tag{21}$$

where $\mathcal{L}$ is a Lindblad superoperator including the action of H_s denoting the system Hamiltonian and dissipative couplings $\mathcal{L}_{\mathrm{diss}}$. The formal solution of eq.(21) reads

$$\hat{\rho}(t) = e^{\mathcal{L}t}\hat{\rho}(0) \tag{22}$$

In order to translate the Lindblad equation, eq.(21), into an equation of motion of the Wigner function on has to multiply both sides with $\hat{\mathbf{\Delta}}(\mathbf{\Omega})$ and perform a trace. To this end we note that the product of spin operators with the phase-space operators can be expressed in terms of a complete set of operators in the 2 dimensional spin space, formed by the four operators

$$\hat{\Delta}(\Omega),\;\; \partial_\theta\hat{\Delta}(\Omega),\;\; \partial_\phi\hat{\Delta}(\Omega),\;\; \partial_\phi^2\hat{\Delta}(\Omega). \tag{23}$$

It should be noted that this set of operators is not unique and there may be other choices better suited for particular problems. This then leads to a partial differential equation for the Wigner function

$$\partial_t\hat{\rho}(t) = \int d\mathbf{\Omega}\, \partial_t W(\mathbf{\Omega},t)\hat{\mathbf{\Delta}}(\mathbf{\Omega}) \tag{24}$$
$$= \int d\mathbf{\Omega}\, W(\mathbf{\Omega},t)[\mathcal{L}\hat{\mathbf{\Delta}}(\mathbf{\Omega})] \tag{25}$$

The action of $\mathcal{L}$ on the phase point operators corresponds to evaluating products of spin and phase point operators, which can be expressed in terms of derivatives, eq.(23). By partial integration these derivatives can be transferred to the Wigner function. For products of multiple spin operators this procedure can then be repeated, eventually leading to a partial differential equation for $W(\mathbf{\Omega},t)$. Since conservation of probability demands

$$\int d\mathbf{\Omega}\, W(\mathbf{\Omega},t) = \mathrm{const}_t$$

only terms containing derivatives of $W(\mathbf{\Omega},t)$ occur and the equation of motion reads

$$\frac{\partial}{\partial t}W(\mathbf{\Omega},t) = \sum_j \frac{\partial}{\partial x_j}A_j W(\mathbf{\Omega},t) + \sum_{jl}\frac{\partial^2}{\partial x_j \partial x_l}D_{jl}W(\mathbf{\Omega},t) + \sum_{jlm}\frac{\partial^3}{\partial x_j \partial x_l \partial x_m}G_{jlm}W(\mathbf{\Omega},t) + \cdots \tag{26}$$

where the $x_j \in \{\theta_j, \phi_j\}$ correspond to the angle variables of the spins.

D. Fokker-Planck approximation and stochastic simulations

Under certain conditions eq.(26) can be approximated by a $2N$-dimensional Fokker-Planck equation.

$$\frac{\partial}{\partial t}W(\mathbf{\Omega},t) = -\sum_j \frac{\partial}{\partial x_j}A_j(\mathbf{\Omega}) W(\mathbf{\Omega},t) + \sum_{jl}\frac{\partial^2}{\partial x_j \partial x_l}D_{jl}(\mathbf{\Omega})W(\mathbf{\Omega},t), \tag{27}$$

where the coefficients matrix of second-order derivatives can be decomposed as $\mathbf{D}(\mathbf{\Omega}) = \frac{1}{2}\mathbf{B}(\mathbf{\Omega})^\top \cdot \mathbf{B}(\mathbf{\Omega})$ and with the initial condition $W(\mathbf{\Omega}, t=0) = W_0(\mathbf{\Omega})$ corresponding to the initial density operator. The solution of this equation can be written in terms of the conditional probability $p(\mathbf{\Omega}, t; \mathbf{\Omega}', 0)$

$$W(\mathbf{\Omega},t) = \int d\mathbf{\Omega}'\, p(\mathbf{\Omega}, t; \mathbf{\Omega}', 0)\, W_0(\Omega') \tag{28}$$

$p(\mathbf{\Omega}, t; \mathbf{\Omega}', 0)$ fulfills the same Fokker-Planck equation of motion as W, however with the initial condition

$$p(\mathbf{\Omega}, 0; \mathbf{\Omega}', 0) = \delta(\mathbf{\Omega} - \mathbf{\Omega}'). \tag{29}$$

Thus any expectation value can be calculated in phase space via

$$\langle \hat{A} \rangle = \iint d\mathbf{\Omega}\, d\mathbf{\Omega}' \mathcal{A}(\mathbf{\Omega})\, p(\mathbf{\Omega}, t; \mathbf{\Omega}', 0)\, W_0(\Omega'). \tag{30}$$

which can be efficiently obtained by stochastic simulations.

The time evolution of the conditional probability function under a FPE can be simulated by a set of coupled Ito stochastic differential equations (SDE) for stochastic variables $x_j(t) \in \{\phi_j(t), \theta_j(t)\}$ with initial conditions $\phi_j(0) = \phi_j'$ and $\theta_j(0) = \theta_j'$:

$$dx_j(t) = A_j[\mathbf{\Omega}(t)]\, dt + \sum_l B_{jl}[\mathbf{\Omega}(t)]\, dw_l \tag{31}$$

where dw_l is a differential Wiener process. This provides an efficient way to (approximately) calculate integrals of the type

$$\int d\mathbf{\Omega}\, f(\mathbf{\Omega})\, W(\mathbf{\Omega},t) = = \iint d\mathbf{\Omega}\, d\mathbf{\Omega}' f(\mathbf{\Omega})\, p(\mathbf{\Omega}, t; \mathbf{\Omega}', 0) W_0(\Omega') \tag{32}$$

if W_0 is positive and can be interpreted as probability distribution by the following procedure:

(i) choose an initial value Ω' for all spin variables with probability weight $W_0(\Omega')$.

(ii) solve the Ito SDE's (31) to obtain $\Omega(t)$ with these initial values

(iii) calculate $f(\Omega(t))$

(iv) average over many trajectories (if the SDE's have noise terms) and the initial distribution $W_0(\Omega')$.

Alternatively

(i) choose random initial value Ω' uniformly distributed on the unit sphere

(ii) solve the Ito SDE's (31) to obtain $\Omega(t)$ with these initial values

(iii) calculate $f(\Omega(t))W_0(\Omega')$

(iv) average over many trajectories (if the SDE's have noise terms) and the initial flat distribution of Ω'.

II. TWO-TIME CORRELATIONS

A. quantum regression theorem

Let us now discuss how two-time correlations can be calculated in the phase-space representation. For the calculation of two-time correlations the knowledge of the density operator is not enough and thus the translation into a phase-space representation is not straight forward.

Two-time correlations are defined in the Heisenberg picture:

$$\langle \hat{A}(t+\tau)\hat{B}(t)\rangle = \mathrm{Tr}\left\{\hat{A}_H(t+\tau)\hat{B}_H(t)\hat{\chi}\right\} \tag{33}$$

where $\chi = \mathrm{const}_t$ is the time-independent density operator of the total system consisting of spins and reservoir, and

$$\hat{A}_H(t+\tau) = e^{iH(t+\tau)}\hat{A}e^{-iH(t+\tau)}, \tag{34}$$

$$\hat{B}_H(t) = e^{iHt}\hat{B}e^{-iHt}. \tag{35}$$

Thus

$$\langle \hat{A}(t+\tau)\hat{B}(t)\rangle = \mathrm{Tr}\left\{e^{iH\tau}\hat{A}e^{-iH\tau}\hat{B}\hat{\chi}(t)\right\} \tag{36}$$

where

$$\hat{\chi}(t) = e^{-iHt}\,\hat{\chi}\,e^{iHt} \tag{37}$$

Since $\hat{A}$ and $\hat{B}$ are operators acting only in the Hilbert space of spins, we can carry out the trace over the reservoir degrees of freedom

$$\langle \hat{A}(t+\tau)\hat{B}(t)\rangle = \mathrm{Tr}_S\left\{\hat{A}\,\mathrm{Tr}_B\left\{e^{-iH\tau}\hat{B}\hat{\chi}(t)e^{iH\tau}\right\}\right\} \quad (38)$$

We now define the operator $\hat{Y}(\tau,t)$

$$\hat{Y}(\tau,t) = e^{-iH\tau}\hat{B}\hat{\chi}(t)e^{iH\tau}, \quad \hat{Y}(0,t) = \hat{B}\chi(t), \quad (39)$$

which takes over the role of the total (system + reservoir) density operator in simple expectation values. Tracing over the reservoir degrees of freedom gives an operator in the Hilbert space of the spins, which takes over the role of the reduced density operator in simple expectation values $\hat{X}(\tau,t) = \mathrm{Tr}_B\left\{\hat{Y}(\tau,t)\right\}$ which fulfills the equation of motion with respect to the difference time τ:

$$\frac{d}{d\tau}\hat{X}(\tau,t) = -i\,\mathrm{Tr}_B\big\{[H,\hat{Y}]\big\}. \quad (40)$$

This equation has exactly the same structure as eq.(20), which is basis of the quantum regression theorem. Now making again a Born-Markov approximation in the system-reservoir coupling, which amounts to $\hat{\chi}(t) = \hat{\rho}(t)\otimes\hat{\rho}_B(t)$ leads to the Lindblad equation (21) for $\hat{X}(\tau,t)$ in τ

$$\frac{\partial}{\partial\tau}\hat{X}(\tau,t) = \mathcal{L}\hat{X}(\tau,t) \quad (41)$$

with the solution

$$\hat{X}(\tau,t) = e^{\mathcal{L}\tau}\hat{X}(0,t) = e^{\mathcal{L}\tau}\left[\hat{B}\hat{\rho}(t)\right]. \quad (42)$$

In terms of $\hat{X}(\tau,t)$ the two time correlation can be expressed as

$$\langle \hat{A}(t+\tau)\hat{B}(t)\rangle = \mathrm{Tr}\left\{\hat{A}\,\hat{X}(\tau,t)\right\} \quad (43)$$

B. phase-space representation of two-time correlations

The two-time correlation, eq.(43), can be expressed in terms of phase space variables

$$\begin{aligned}\langle \hat{A}(t+\tau)\hat{B}(t)\rangle &= \mathrm{Tr}\left\{\hat{A}\,\hat{X}(\tau,t)\right\} \\ &= \int d\mathbf{\Omega}\,\mathcal{A}(\mathbf{\Omega})\mathrm{Tr}\left\{\hat{\mathbf{\Delta}}(\mathbf{\Omega})\,\hat{X}(\tau,t)\right\} \quad (44)\\ &= \int d\mathbf{\Omega}\,\mathcal{A}(\mathbf{\Omega})\mathcal{X}(\mathbf{\Omega},\tau,t),\end{aligned}$$

where in the last step we have introduced the Weyl symbol $\mathcal{X}$ of $\hat{X}$.

Since the equation of motion of $\hat{X}(\tau,t)$ with respect to τ is exactly the same as the Lindblad equation of $\hat{\rho}(t)$, its Weyl symbol $\mathcal{X}(\mathbf{\Omega},\tau,t)$ at relative time τ obeys

$$\mathcal{X}(\mathbf{\Omega},\tau,t) = \int d\mathbf{\Omega}'\,p(\mathbf{\Omega},\tau;\mathbf{\Omega}',0)\,\mathcal{X}(\mathbf{\Omega}',0,t). \quad (45)$$

The remaining task is to determine $\mathcal{X}(\mathbf{\Omega}',0,t)$. To this end we note that $\hat{X}(0,t) = \hat{B}\hat{\rho}(t)$

$$\begin{aligned}\mathcal{X}(\mathbf{\Omega}',0,t) &= \mathrm{Tr}\left\{\hat{B}\hat{\rho}(t)\hat{\mathbf{\Delta}}(\mathbf{\Omega}')\right\} = \mathrm{Tr}\left\{\hat{\mathbf{\Delta}}(\mathbf{\Omega}')\hat{B}\hat{\rho}(t)\right\} \quad (46)\\ &= \int d\mathbf{\Omega}''\,W(\mathbf{\Omega}'',t)\,\mathrm{Tr}\big\{\hat{\mathbf{\Delta}}(\mathbf{\Omega}')\hat{B}\hat{\mathbf{\Delta}}(\mathbf{\Omega}'')\big\}\end{aligned}$$

The function

$$f(\hat{B},\mathbf{\Omega}',\mathbf{\Omega}'') = \mathrm{Tr}\Big\{\hat{\mathbf{\Delta}}(\mathbf{\Omega}')\hat{B}\hat{\mathbf{\Delta}}(\mathbf{\Omega}'')\Big\} \quad (47)$$

can be explicitly evaluated for every operator $\hat{B}$. Thus we eventualy end up at the following phase space representation for a two-time correlator

$$\begin{aligned}&\langle \hat{A}(t+\tau)\hat{B}(t)\rangle = \quad (48)\\ &= \iiiint d\mathbf{\Omega}\,d\mathbf{\Omega}'d\mathbf{\Omega}''d\mathbf{\Omega}'''\,\mathcal{A}(\mathbf{\Omega})\,p(\mathbf{\Omega},\tau;\mathbf{\Omega}',0)\times\\ &\times\ f(\hat{B},\mathbf{\Omega}',\mathbf{\Omega}'')\,p(\mathbf{\Omega}'',t;\mathbf{\Omega}''',0)\,W_0(\mathbf{\Omega}''')\end{aligned}$$

This expression can be stochastically simulated by the following procedure:

(i) choose an initial value Ω''' for all spin variables with probability weight $W_0(\Omega''')$.

(ii) solve the Ito SDE's (31) to obtain $\Omega''(t)$ with the initial value $\Omega''(t=0) = \Omega'''$.

(iii) To calculate the second time evolution, choose an arbitrary value of Ω' on the unit sphere as new initial value for the second time evolution.

(iv) Solve the Ito SDE's (31) to obtain $\Omega(t+\tau)$ with the initial values $\Omega(t) = \Omega'$ from (iii).

(v) Evaluate the expression $\mathcal{A}(\Omega(t))f(\hat{B},\Omega',\Omega''(t))$.

(vi) Average over many trajectories (if the SDE's have noise terms) and the initial distribution $W_0(\Omega''')$.

Thus two-time correlations can in principle be simulated!

The apparent problem is that in the above given form the number of trajectories explodes. Say for the faithful evaluation of $\Omega''(t)$ from initial values Ω''' with the SDE's it is required to simulate n trajectories. The same then applies to the evaluation of the SDE's for the second time evolution to obtain $\Omega(t+\tau)$ from the (random) initial values $\Omega(t) = \Omega'$. Thus naively n^2 trajectories would be needed. A potential way out is to make use of the fact that the operator $\hat{B}$ is typically only an operator of a single spin, say j, i.e. $\hat{B} = \hat{B}_j$, so

$$\begin{aligned}&f(\hat{B}_j,\mathbf{\Omega}',\mathbf{\Omega}'') = \quad (49)\\ &= \mathrm{Tr}_j\{\hat{\Delta}_j(\Omega')\hat{B}_j\hat{\Delta}_j(\Omega'')\}\prod_{k\neq j}\mathrm{Tr}_k\{\hat{\Delta}_k(\Omega')\hat{\Delta}_k(\Omega'')\}\end{aligned}$$

and thus one can have the hope that only trajectories for one spin variable would have to be calculated in addition, but this needs still to be worked out, as the last factors are not Delta-functions, see eq.(11).

However from eq.(48) one recognizes that $f(\hat{B}_j, \mathbf{\Omega}', \mathbf{\Omega}'')$ is integrated over the Wigner function at time t, i.e. there is term proportional to

$$\begin{aligned}
&\int d\mathbf{\Omega}'' \int d\mathbf{\Omega}''' f(\hat{B}_j, \mathbf{\Omega}', \mathbf{\Omega}'') p(\mathbf{\Omega}'', t; \mathbf{\Omega}''', 0) W_0(\mathbf{\Omega}''') = \\
&= \int d\mathbf{\Omega}'' f(\hat{B}, \mathbf{\Omega}', \mathbf{\Omega}'') W(\mathbf{\Omega}'', t) \qquad (50) \\
&= \int d\mathbf{\Omega}'' f(\hat{B}_j, \mathbf{\Omega}', \mathbf{\Omega}'') \mathrm{Tr}\{\hat{\rho}(t) \hat{\mathbf{\Delta}}(\mathbf{\Omega}'')\}
\end{aligned}$$

The last term contains however only spherical harmonics $\mathrm{Y}_l^m(\Omega'')$ with $l = 0, 1$. Thus all terms in $f(\hat{B}_j, \mathbf{\Omega}', \mathbf{\Omega}'')$ proportional to higher-order spherical harmonics vanish after integration $d\Omega''$. Thus we are allowed to set

$$\begin{aligned}
&f(\hat{B}_j, \mathbf{\Omega}', \mathbf{\Omega}'') = \qquad (51) \\
&\quad = \mathrm{Tr}_j\{\hat{\Delta}_j(\Omega') \hat{B}_j \hat{\Delta}_j(\Omega'')\} \prod_{k \neq j} \delta(\Omega_k - \Omega'_k)
\end{aligned}$$

This represents a **significant improvement** as only for the one spin "j" new trajectories need to be simulated. Namely in eq.(48) we have to sample a new initial value Ω'_j at time t from the unit sphere and propagate it with the SDE's to time $t + \tau$. The trajectories for all other spins are just continued from t to $t + \tau$.

With this we can estimate the simulation effort: Say that for any spin we need to simulate m trajectories to get faithful averages. This means that $n = Nm$ is the total number of trajectories needed to simulate a single-time expectation value. Thus for a single-spin two-time correlation function we need only $n_2 = (N+1)m$ trajectories, which is much less than n^2 !! For collective correlations we may need two-time correlations for *all* spins, i.e. $j = 1, 2, \ldots N$. In this case the number of trajectories needed changes from Nm to $2Nm$.

APPENDIX

Spherical Harmonics

1. definition

Here we summarize some properties of spherical harmonics and list the definitions used in this paper. For $l = 0, 1, 2, \ldots$ and $m = -l, -(l-1), \ldots, (l-1), l$

$$\mathrm{Y}_l^m(\theta, \phi) \equiv \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} P_l^m(\cos\theta)\, e^{im\phi}, \qquad (52)$$

with $P_l^m(x)$ being the generalized Legendre functions with $m \leq 0$

$$P_l^m(x) = (-1)^m (1-x^2)^{m/2} \frac{d^m}{dx^m} P_l(x), \qquad |x| \leq 1 \quad (53)$$

and $P_l(x)$ are the Legendre polynomials.

$$\mathrm{Y}_l^{-m}(\Omega) = (-1)^m\, \mathrm{Y}_l^{m*}(\Omega) \qquad (54)$$

2. explicit expressions

Te lowest spherical harmonics read

$$\mathrm{Y}_0^0(\Omega) = \frac{1}{\sqrt{4\pi}}, \qquad (55)$$

$$\mathrm{Y}_1^0(\Omega) = \sqrt{\frac{3}{4\pi}} \cos\theta, \qquad (56)$$

$$\mathrm{Y}_1^{-1}(\Omega) = \sqrt{\frac{3}{8\pi}} \sin\theta\, e^{-i\phi}, \qquad (57)$$

$$\mathrm{Y}_1^1(\Omega) = -\sqrt{\frac{3}{8\pi}} \sin\theta\, e^{i\phi}. \qquad (58)$$

The inverse relations are also useful

$$\cos\theta = \sqrt{\frac{4\pi}{3}} \mathrm{Y}_1^0(\Omega), \qquad (59)$$

$$\begin{aligned}
\sin\theta\cos\phi &= \frac{1}{2}\sqrt{\frac{8\pi}{3}} \left(\mathrm{Y}_1^{-1} - \mathrm{Y}_1^1\right) \\
&= \frac{1}{2}\sqrt{\frac{8\pi}{3}} \left(\mathrm{Y}_1^{-1} + \mathrm{Y}_1^{-1*}\right) \qquad (60) \\
&= \sqrt{\frac{8\pi}{3}} \mathrm{Re}\left[\mathrm{Y}_1^{-1}(\Omega)\right] = -\sqrt{\frac{8\pi}{3}} \mathrm{Re}\left[\mathrm{Y}_1^1(\Omega)\right]
\end{aligned}$$

$$\begin{aligned}
\sin\theta\sin\phi &= -\frac{1}{2i}\sqrt{\frac{8\pi}{3}} \left(\mathrm{Y}_1^{-1} + \mathrm{Y}_1^1\right) \\
&= -\frac{1}{2i}\sqrt{\frac{8\pi}{3}} \left(\mathrm{Y}_1^{-1} - \mathrm{Y}_1^{-1*}\right) \qquad (61) \\
&= -\sqrt{\frac{8\pi}{3}} \mathrm{Im}\left[\mathrm{Y}_1^{-1}(\Omega)\right] = -\sqrt{\frac{8\pi}{3}} \mathrm{Im}\left[\mathrm{Y}_1^1(\Omega)\right]
\end{aligned}$$

3. orthogonality and completeness

With the definition used in this paper

$$\int d\Omega = \frac{1}{2\pi} \int_0^{2\pi} d\phi \int_0^{\pi} d\theta\, \sin\theta \qquad (62)$$

it holds

$$\int d\Omega\, \mathrm{Y}_l^{m*}(\Omega) \mathrm{Y}_{l'}^{m'}(\Omega) = \frac{1}{2\pi} \delta_{ll'} \delta_{mm'}. \qquad (63)$$

Moreover for functions on the unit sphere the completeness relation

$$\begin{aligned}
\sum_{l=0}^{\infty} \sum_{m=-l}^{l} \mathrm{Y}_l^{m*}(\Omega) \mathrm{Y}_l^m(\Omega') &= \delta(\phi - \phi') \delta(\cos\theta - \cos\theta') \\
&= \frac{1}{2\pi} \delta(\Omega - \Omega') \qquad (64)
\end{aligned}$$

holds