Perspectives on the truncated Wigner approximation

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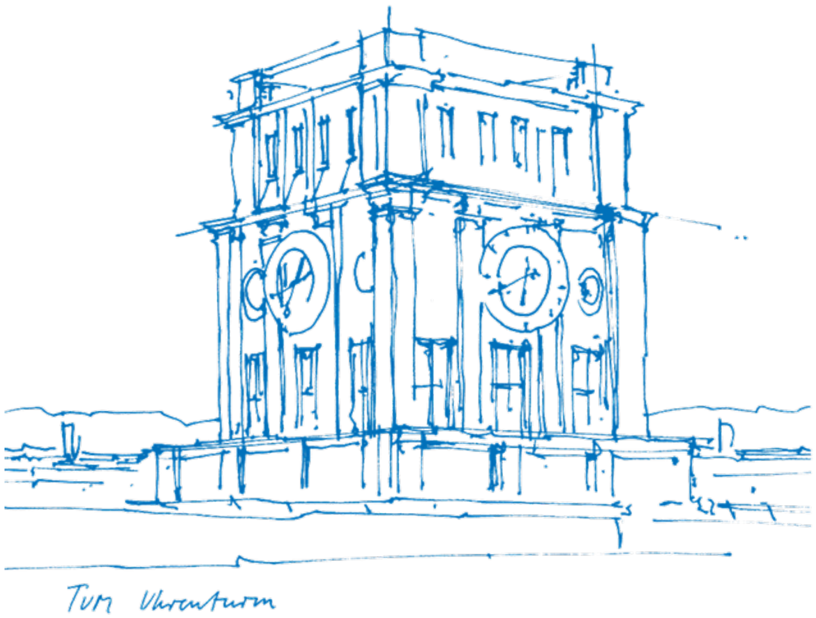

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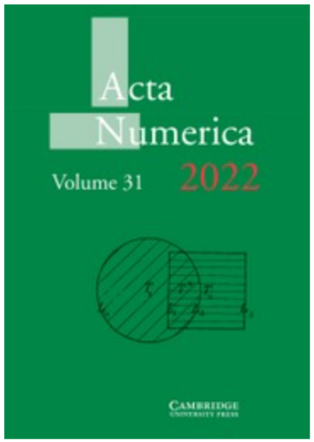

Acta Numerica

Computing quantum dynamics in the semiclassical regime

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Quantum dynamics

Schrödinger equation, state $\psi(t) \in \mathscr{H} = L^2(\mathbb{R}^d)$

$$i\hbar\partial_t\psi(t) = H(t)\psi(t), \quad \psi(0) = \psi_0$$

Heisenberg equation, observable $A(t) \in L(\mathscr{H})$

$$i\hbar\partial_t A(t) = [A(t), H(t)], \quad A(0) = A_0$$

Unitary propagator $U(t,s)$ with $t, s, \in \mathbb{R}$

$$\psi(t) = U(t,0)\psi_0, \quad A(t) = U(t,0)^* A_0 U(t,0)$$

Classical dynamics

Hamiltonian equation, state $z(t) \in \mathbb{R}^{2d}$

$$\dot{z}(t) = J\nabla_z h(t, z(t)), \quad z(0) = z_0$$

Liouville equation, observable $a(t) \in C(\mathbb{R}^{2d})$

$$i\partial_t a(t) = \{a(t), h(t)\}, \quad a(0) = a_0$$

Flow map $\Phi^{t,s}$ with $t, s, \in \mathbb{R}$

$$z(t) = \Phi^{t,0} z_0, \quad a(t) = a_0 \circ \Phi^{t,0}$$

Egorov's theorem (1969)

Robert, Combescure (2nd edition, 2021)[1]

Theorem: Assume that $H(t) = \mathrm{op}(h(t))$ and $A_0 = \mathrm{op}(a_0)$ in Weyl quantization. Then,

$$\boxed{A(t) = \mathrm{op}(a_0 \circ \Phi^{t,0}) + \textstyle\sum_{j \geqslant 2} \hbar^j A_j(t),}$$

where $A_j(t)$, $j \geqslant 2$ depends on $\partial_z^\alpha h(t)$ with $|\alpha| \geqslant 2$.

▷ Exact, if $z \mapsto h(t,z)$ is a polynomial of degree $\leqslant 2$.

[1] detailed proof in Burkhard, Dörich, Hochbruck, Lasser (2024) → 2nd order observable accuracy for variational Gaussians

Truncated Wigner approximation

The Wigner function satisfies

$$\langle \psi(t), A_0 \psi(t) \rangle = \int_{\mathbb{R}^{2d}} a_0(z)\, W_{\psi(t)}(z)\,\mathrm{d}z.$$

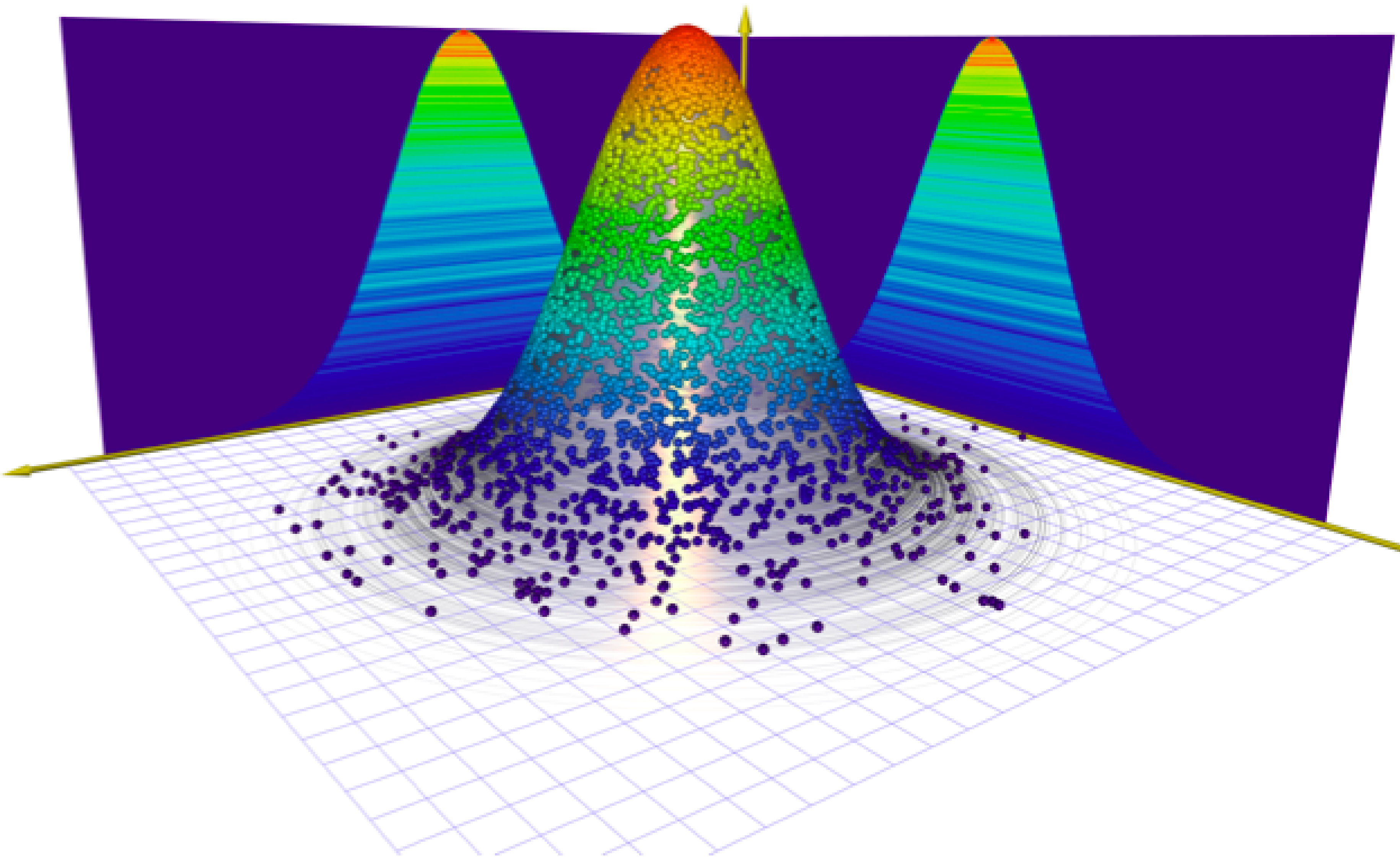
Egorov's theorem, $A(t) = \mathrm{op}(a_0 \circ \Phi^{t,0}) + \mathscr{O}(\hbar^2)$, implies

$$\boxed{W_{\psi(t)} = W_{\psi_0} \circ \Phi^{0,t} + \mathscr{O}(\hbar^2)}$$

in the weak sense.

Also known as:

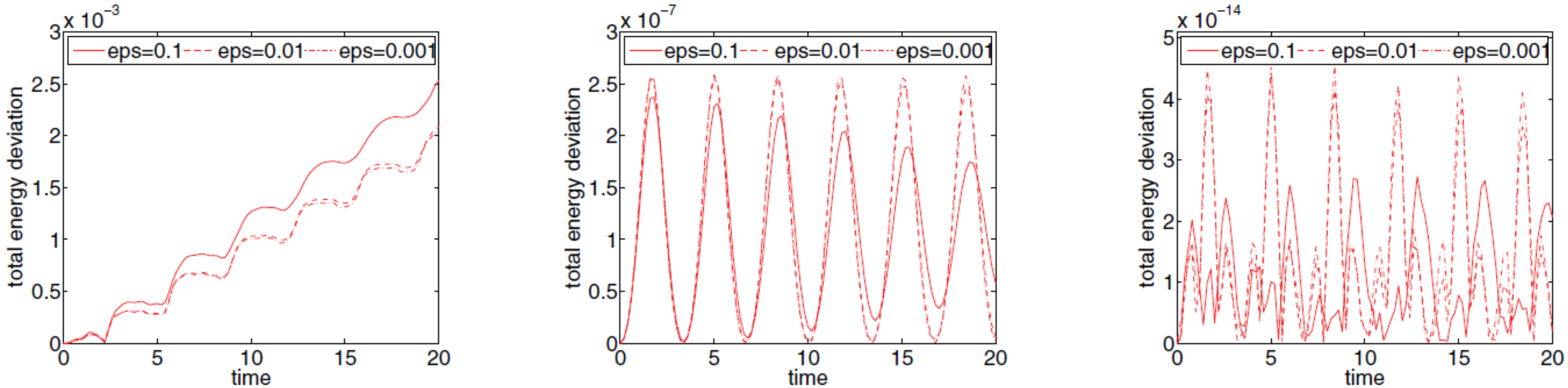
1. Linearized semi-classical initial value representation (Miller 1974)
2. Wigner phase space method (Heller 1976)
3. Statistical quasi-classical method (Lee, Scully 1980)



Truncated Wigner algorithm

1. Choose samples $z_1, \dots, z_N$ according to W_{ψ_0}.
2. Symplectically[2] propagate $z_1(t), \dots, z_N(t)$.
3. Sum to obtain

$$\langle \psi(t), A_0 \psi(t) \rangle \;\approx\; \int_{\mathbb{R}^{2d}} a_0(\Phi^{t,0}(z))\, W_{\psi_0}(z)\, \mathrm{d}z \;\approx\; \sum_{n=1}^{N} a_0\left(z_n(t)\right).$$



(a) ode45 (b) Störmer-Verlet (c) SPRK4

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[2] Lasser, Röblitz, 2010

Position densities

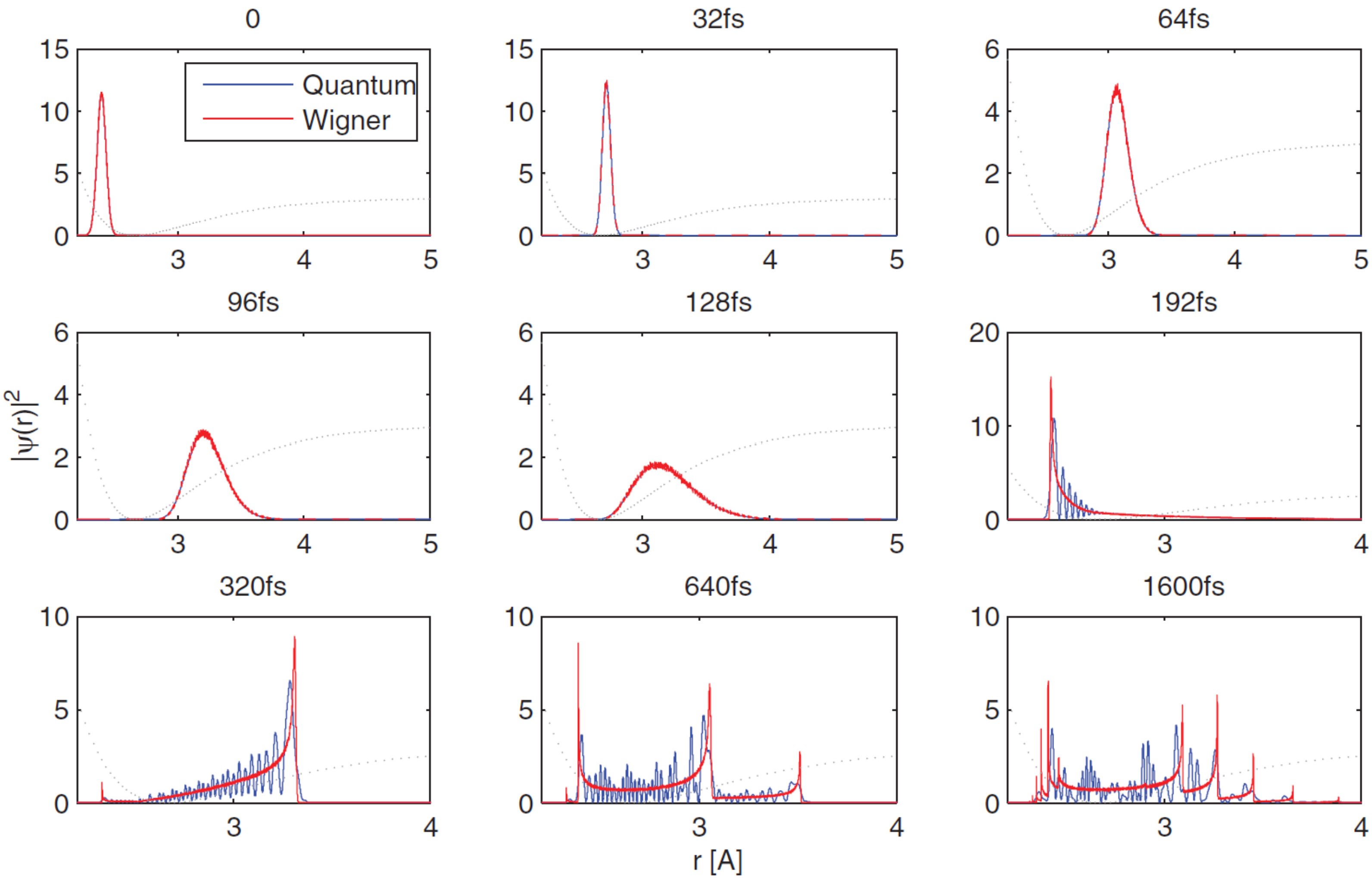
$$
\begin{aligned}
|\psi(t,q)|^2 &= (2\pi)^{-d} \int_{\mathbb{R}^{2d}} \mathrm{e}^{-i\eta\cdot(x-q)} |\psi(t,x)|^2 \,\mathrm{d}(x,\eta) \\
&= \int_{\mathbb{R}^d} \langle \psi(t), \mathrm{op}(b_{\eta,q})\psi(t)\rangle \,\mathrm{d}\eta \\
&= \int_{\mathbb{R}^d} \int_{\mathbb{R}^{2d}} W_{\psi(t)}(x,\xi) b_{\eta,q}(x) \,\mathrm{d}(x,\xi,\eta) \\
&\approx \int_{\mathbb{R}^d} \int_{\mathbb{R}^{2d}} W_{\psi_0}(x,\xi)(b_{\eta,q}\circ\Phi^{t,0})(x,\xi) \,\mathrm{d}(x,\xi,\eta)
\end{aligned}
$$

with $b_{\eta,q}(x) = (2\pi)^{-d}\mathrm{e}^{-i\eta\cdot(x-q)}$.

▷ One additional integral is needed.

Diatomic iodine

Keller, Lasser, 2014



Gaussians

$$\psi(x) \sim \exp\left(\frac{i}{\hbar}\left(\tfrac{1}{2}(x-q_0)^\top C(x-q_0) + p_0^\top(x-q_0)\right)\right)$$

with $q_0, p_0 \in \mathbb{R}^d$ and $C = C^\top \in \mathbb{C}^{d\times d}$, $\mathrm{Im}\, C > 0$

$$W_\psi(z) \sim \exp\left(-\frac{1}{\hbar}(z-z_0)^\top G(z-z_0)\right)$$

with $z_0 = (q_0, p_0) \in \mathbb{R}^{2d}$ and $G = G^\top \in \mathbb{R}^{2d\times 2d}$ symplectic

$\triangleright$ simple Monte Carlo sampling by drawing from a normal distribution

Hermite–Laguerre connection ($d = 1$)

The kth Hermite function

$$\varphi_k(x) \sim \left(A^\dagger\right)^k \mathrm{e}^{-\frac{1}{2}x^2}, \quad x \in \mathbb{R},$$

generated by the raising operator

$$A^\dagger = \frac{1}{\sqrt{2}}(\hat{q} - i\hat{p})$$

has the Wigner function[3]

$$W_{\varphi_k}(z) \sim L_k(2|z|^2)\mathrm{e}^{-|z|^2}, \quad z \in \mathbb{R}^2.$$

▷ The integrals $\int_{\mathbb{R}} a(z) W_{\psi_k}(z) \mathrm{d}z$ have a Gaussian weight.

[3] Groenewold, 1946

Hagedorn–Laguerre connection

The kth Hagedorn function, $k \in \mathbb{N}^d$,

$$\varphi_k(x) \sim \left(A^\dagger\right)^k \varphi_0(x), \quad x \in \mathbb{R}^d,$$

is generated by the raising operator

$$A^\dagger = \frac{i}{\sqrt{2\hbar}}\left(P^*(\hat{q} - q_0) - Q^*(\hat{p} - p_0)\right),$$

where $Q, P \in \mathbb{C}^{d\times d}$ satisfy a symplecticity condition. It has the Wigner function[4]

$$W_{\varphi_k}(x,\xi) \sim \mathrm{e}^{-|z|^2/\hbar} \prod_{j=1}^{d} L_{k_j}(\tfrac{2}{\hbar}|z_j|^2), \quad (x,\xi) \in \mathbb{R}^{2d}$$

with $z = P^\top(x - q_0) - Q^\top(\xi - p_0)$.

[4] Lasser, Troppmann, 2014

Spectrogram expansions

If $\varphi, \psi \in L^2(\mathbb{R}^d)$ are normalised, then $W_\varphi * W_\psi$ is a probability distribution on $\mathbb{R}^{2d}$.

The Husimi function $\mathscr{H}_\psi = W_{\varphi_0} * W_\psi$ is a probability distribution with $\mathscr{H}_{\psi(t)} = \mathscr{H}_{\psi_0} \circ \Phi^{0,t} + \mathscr{O}(\hbar)$.

The Husimi correction $\mathscr{H}_\psi^c = \mathscr{H}_\psi - \frac{\hbar}{4}\Delta\mathscr{H}_\psi$ satisfies[5]

1. second order Egorov theorem: $\mathscr{H}^c_{\psi(t)} = \mathscr{H}^c_{\psi_0} \circ \Phi^{0,t} + \mathscr{O}(\hbar^2)$,
2. linear combination of spectrograms: $\mathscr{H}^c_\psi = \left(1 + \frac{d}{2}\right)\mathscr{H}_\psi - \frac{1}{2}\sum_{j=1}^d W_{\varphi_j} * W_\psi$.

[5]Keller, Lasser, Ohsawa 2016; Keller, 2019

Conclusion

Truncated Wigner approximation

1. is $\mathscr{O}(\hbar^2)$,
2. combines with Monte-Carlo quadrature and (parallel) classical trajectories.

The Hagedorn–Laguerre connection brings normal distributions.

Correcting the Husimi function by a spectrogram expansion gives an $\mathscr{O}(\hbar^2)$ Egorov description with positive sampling.

▷ Upcoming analysis of the discrete truncated Wigner approximation for large spin systems by Oliver Schwarze (TUM)

Thank you