IMPERIAL

A Coherent State Semi-Classical Propagator

Capturing Quantum Breakdown, Revival and Tunnelling

Elana Todd-Miller, Eva-Maria Graefe

Semi-classical Quantum Mechanics: Classical dynamics can approximate quantum systems in the limit of large quantum numbers i.e. when the classical action is large compared to Planck's constant $\hbar$ - leads to a continuum of energy levels and probability distributions becoming δ−functions. Often these methods are employed in theoretical chemistry to study atomic and molecular dynamics in many particle systems [1, 2] for their potential to significantly reduce computation time for complex quantum systems. Further these methods allow us to examine quantum phenomena such as chaos, breakdown, revival, and tunnelling. Understanding the transition between these realms remains a fundamental challenge and motivates the development of semi-classical methods which connect probabilistic quantum dynamics to deterministic classical phase space evolution.

Coherent states: Minimum uncertainty states which originated from Schrödinger's study of the quantum harmonic oscillator and have been generalised to arbitrary Lie groups [3]. They are considered the 'most classical' quantum states and by tracking how their centres evolve in phase space, we may connect quantum behaviour to classical trajectories and provide a bridge between micro- and macroscopic regimes.

Abstract: We propose a semi-classical coherent state propagator and its extension to capture the highly quantum behaviour of a Bose-Hubbard (BH) dimer. Using a single coherent state time dependent variational principle (SCS-TDVP), we derive equations of motion for the centre and phase of the time evolved state. With these we construct an integral propagator that accurately captures breakdown and revival. We extend this with a time-slicing method to capture tunnelling effects of the full BH dimer, near and far from the semi-classical limit.

COHERENT STATES AND $SU(2)$

$SU(2)$ Lie group is generated by any three $\{\hat J_x, \hat J_y, \hat J_z\}$ satisfying

$$[\hat J_i, \hat J_j] = \mathrm{i}\epsilon_{ijk}\hat J_k$$

- Topologically identical to a 3D sphere
- An $n = 2j+1$ irreducible representation of $SU(2)$ can represent a spin j system
- Then $\hat J_i$ are $n \times n$ complex matrices which rotate states
- $\hat J_z|j,m\rangle = m|j,m\rangle, \quad m \in \{-j, -j+1 \ldots j-1, j\}$ [3]

Spin coherent states

$$|\zeta\rangle := (1+|\zeta|^2)^{-j} e^{\zeta \hat J_+}|j,j\rangle$$

$$\zeta = e^{\mathrm{i}\phi}\tan\frac{\theta}{2}$$

- Stereographic projection of complex plane onto unit sphere
- In the limit $j \to \infty$ coincides with Fock CS [1]
- Form a non-orthogonal, over-complete basis

Resolution of Identity

$$\hat I = \frac{2j+1}{4\pi}\int |\theta,\phi\rangle\langle\theta,\phi| d\Omega$$

EQUATIONS OF MOTION

TDVP with Single Coherent State

$$\mathrm{i}\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat H|\psi(t)\rangle$$

$$\psi(t)\rangle = c(t)|\zeta(t)\rangle$$

$$|\psi(0)\rangle = c_0|\zeta_0\rangle$$

Dirac-Frenkel Variational Principle

$$\mathrm{i}\langle\delta\psi|\dot\psi\rangle = \langle\delta\psi|\hat H|\psi\rangle$$

Mutually independent variations $\delta c, \delta\zeta, \delta\zeta^* \Rightarrow$ equate coefficients

$$\mathrm{i}\hbar\dot\zeta = \frac{(1+|\zeta|^2)^2}{2j}\frac{\partial\langle\hat H\rangle}{\partial\zeta^*} \quad \mathrm{i}\hbar\dot c = c\left[\langle\hat H\rangle + \mathrm{i}\hbar\frac{j}{1+|\zeta|^2}(\zeta^*\dot\zeta - \zeta\dot\zeta^*)\right]$$

Reparametrising with $z = \cos\theta$ and defining $H = \frac{\langle\hat H\rangle}{j}$:

$$\dot\phi = \frac{1}{\hbar}\frac{H}{\partial z} \quad \dot z = -\frac{1}{\hbar}\frac{\partial H}{\partial\phi}$$

$$\mathrm{i}\hbar\dot c = cj\left[H + (1-z)\frac{\partial H}{\partial z}\right]$$

- in $j \to \infty$ limit these become classical EOM
- Note the similarity to Hamilton's classical EOM
- Exact for linear potentials

BOSE-HUBBARD DIMER

$$\hat H_{BH} = 2\varepsilon\hat J_z + 2\nu\hat J_x + \frac{2\kappa}{j}\hat J_z^2$$

Expectation value in spin coherent states:

$$\langle\hat H_{BH}\rangle = 2\varepsilon z + 2\nu\cos\phi(1-z^2)^{1/2} + 2\kappa(1-\frac{1}{2j})z^2$$

Equations of motion:

$$\dot\phi = 2\varepsilon - 2\nu z\cos\phi(1-z^2)^{-1/2} + 4\kappa(1-1/2j)z$$

$$\dot z = 2\varepsilon(1-z^2)^{1/2}\sin\phi$$

$$\dot c = -2\mathrm{i}cj\left[\varepsilon + \nu\cos\phi(1-z^2)^{1/2}(1+z)^{-1} - \kappa(1-1/2j)(z^2-2z)\right]$$

REFERENCES

[1] Heller, E. J. (1981), 'Frozen Gaussians: A very simple semiclassical approximation', Journal of Chemical Physics 75(6), 2923–2931

[2] Qiao, Y. and Grossmann, F. (2023), 'Revealing quantum effects in bosonic josephson junctions: a multi-configuration atomic coherent state approach', Frontiers in Physics 11, 1221614

[3] Zhang, W.-M., Gilmore, R. et al. (1990), 'Coherent states: Theory and some applications', Reviews of Modern Physics 62(4), 867

[4] Ray, S., Ostmann, P., Simon, L., Grossmann, F. and Strunz, W. T. (2016), 'Dynamics of interacting bosons using the herman–kluk semiclassical initial value representation', Journal of Physics A: Mathematical and Theoretical 49(16), 165303

[5] Huber, D. and Heller, E. J. (1988), 'Hybrid mechanics: A combination of classical and quantum mechanics', The Journal of chemical physics 89(8), 4752–4760

[6] E. M. Graefe, H. J. Korsch, and A. E. Niederle, Phys. Rev. A 82 (2010) 013629

COHERENT STATE SEMI-CLASSICAL PROPAGATOR (CS-SCP)

$$\hat U^{SC}(t) := \frac{2j+1}{4\pi}\int_0^{2\pi}\int_{-1}^{1} c(t;\phi_0,z_0)|\zeta(t;\phi_0,z_0)\rangle\langle\phi_0,z_0| dz_0 d\phi_0$$

- Utilising resolution of identity for CS
- Approximating $\hat U(t)|\phi_0,z_0\rangle$ using the classical equations of motion i.e. with $H = \lim_{j\to\infty}\langle\hat H\rangle/j$
- Exact in linear case

HOW DOES IT PERFORM ON INTERACTION TERM

Locally Kerr Type Hamiltonian

$$\hat h = \frac{2\kappa}{j}\hat J_z^2$$

True Propagator Matrix Elements

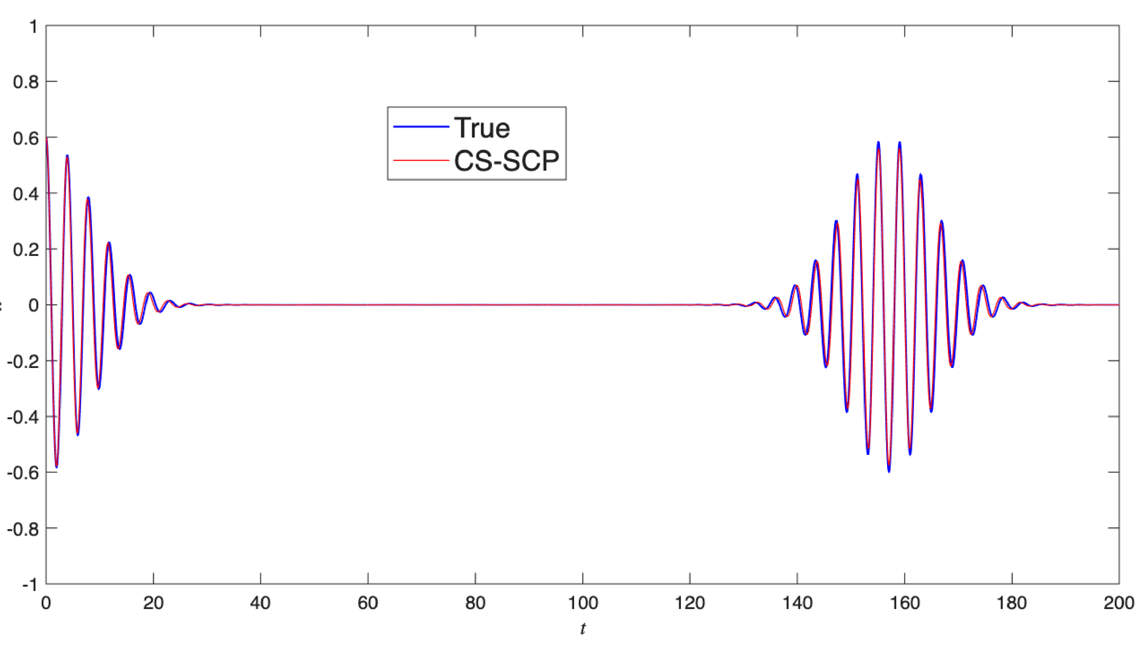
$$U^{True}_{n,m}(t) = \delta_{nm}e^{-2\kappa\mathrm{i}tm^2/j}$$

CS-SCP Matrix Elements

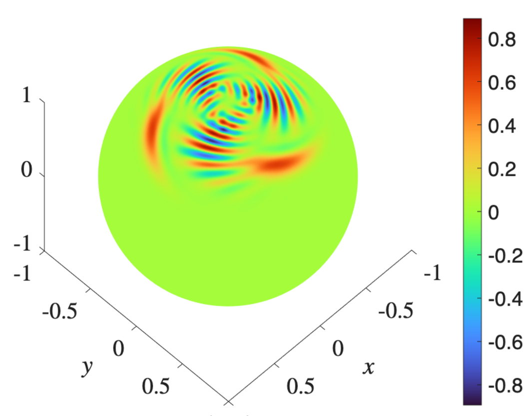
$$U^{SC}_{n,m} = \delta_{nm}e^{-2\kappa\mathrm{i}tm^2/j}g_m(2t\kappa)$$

$$g_m(A) = \frac{2j+1}{2^{2j+1}}\binom{2j}{j+m}\int_{-1}^{1}(1+p_0)^{j+m}(1-p_0)^{j-m}e^{\mathrm{i}Aj(p_0-\frac{m}{j})^2}dp_0$$

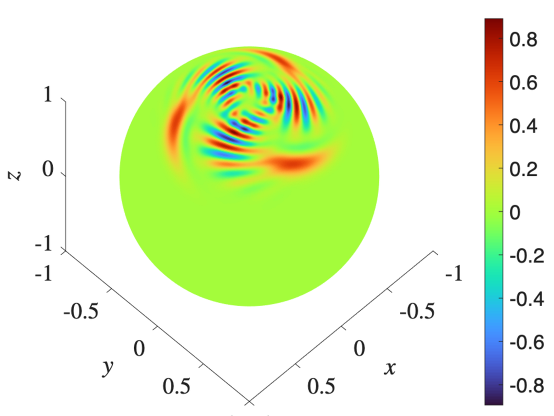
Breakdown & Revival



True Wigner $t = 50$



SC-SCP Wigner $t = 50$



LARGE j SADDLE POINT APPROXIMATION

$$g_m(A) = \frac{2j+1}{2^{2j+1}}\binom{2j}{j+m}\int_{-1}^{1}e^{j\Phi(z_0)}dz_0$$

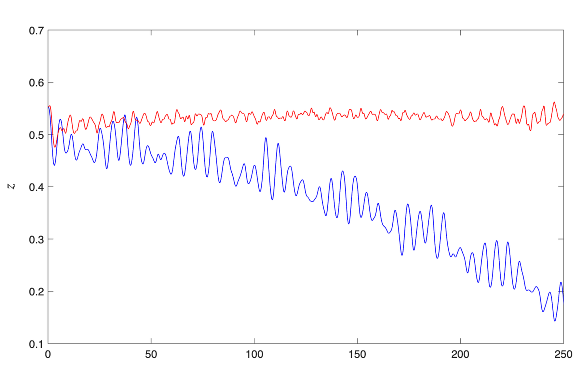
$$\Phi(z_0) = (1+\frac{m}{j})\ln(1+z_0) + (1-\frac{m}{j})\ln(1-z_0) + \mathrm{i}A(z_0-\frac{m}{j})^2$$

EOM + overlap identity + Stirling's formula $\to$

$$U^{SC-Kerr}_{n,m}(t:\text{large } j) = \delta_{nm}e^{-2\kappa\mathrm{i}tm^2/j}\left[1-2\kappa\mathrm{i}t(1-\frac{m^2}{j^2})\right]^{-1/2}$$

- Norm decay when non-linearity present
- Moral issue: Hermitian systems preserve norm
- **However**, not uncommon for semiclassical propagators [4] and propagator produces a states with near identical expectation and Wigner values

CS-SCP FOR BOSE-HUBBARD DIMER



- Captures breakdown and revival
- Accuracy improving with spin size
- Unable to tunnel; extension required

TIME-SLICING

$$\hat U^{TS}(t) = \lim_{M\to\infty}\prod_{m=1}^{M}\hat U^{SC}(\frac{t}{M})$$

- Split $[0,t]$ into M intervals of width δt
- Evolve up to time δt using CS-SCP
- Take this to be he new initial state, reset time to zero, repeat

CS-SCP near exact for the interaction term over short times e.g. δt small enough, motivating this approach. Similar methods have been done in flat space [5]

Caveat: generates a scaling in the non-linear coefficient

$\to$ Can predict for interaction term

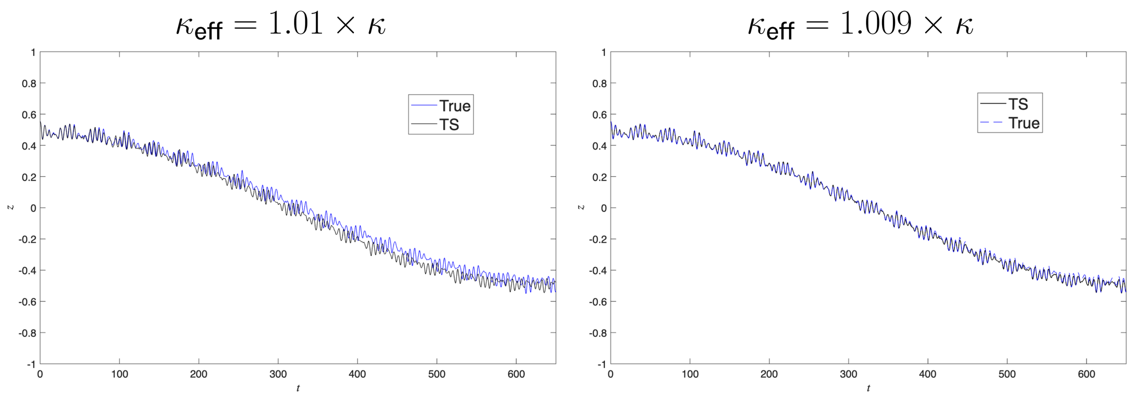
$$\hat U^{TS}_{n,n'}(t) = \delta_{nn'}e^{-2\kappa\mathrm{i}\,(1+\frac{1}{2j})n^2/j}e^{2\kappa\mathrm{i}t/2}$$

- 2^{nd} exponential term is constant $\Rightarrow$ dynamics unaffected
- In limit of $j \to \infty$, TSP under $\kappa_{\text{eff}} = \kappa(1+1/2j)$ yields same dynamics as true propagator under κ!

APPLICATION TO BOSE-HUBBARD DIMER

$$j = 50, \nu = 1, \kappa = 0.6, \phi_0 = 0, z_0 = \sqrt{0.3}$$

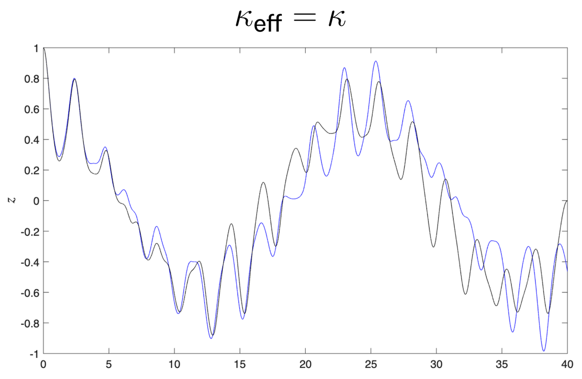
$\kappa_{\text{eff}} = 1.01 \times \kappa$ $\qquad$ $\kappa_{\text{eff}} = 1.009 \times \kappa$



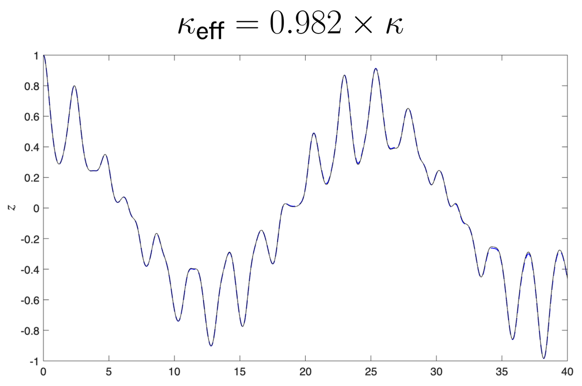
- Small changes in scaling factor can lead to large change in evolution
- But wouldn't expect approximation to be this good for long times
- Nearing predicted scaling factor as $j \uparrow$

$$j = 2.5, \nu = 1, \kappa = 0.6, \phi_0 = 0, z_0 = \sqrt{0.3}$$

$\kappa_{\text{eff}} = \kappa$



$\kappa_{\text{eff}} = 0.982 \times \kappa$

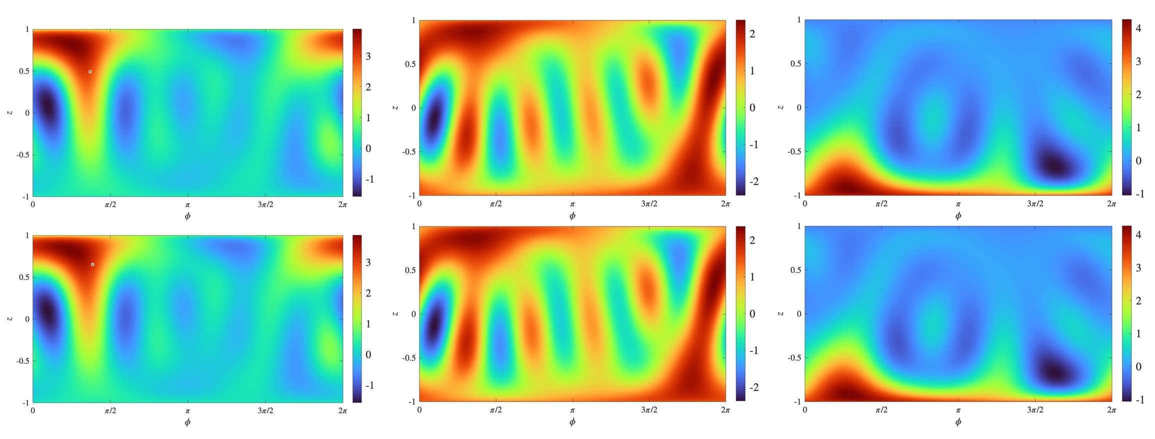


For low spin the scaling factor is found through numerical testing

A good approximation even far from semi-classical limit!

$\to$ not expected from semi-classical methods

True vs TS $t = 2$ $\qquad$ True vs TS $t = 6$ $\qquad$ True vs TS $t = 13$



CONCLUSION & NEXT STEPS

Results: we developed an approximation for the true quantum propagator based on classical trajectories. Utilising $SU(2)$ coherent states, this method captures the breakdown and revival phenomena of the $\hat J_z^2$ operator and, by extending it with time-slicing, we are able to replicate quantum tunnelling away from the semi-classical limit - an uncommon capability.

Further research topics:

- Uncover the source of the non-linear coefficient scaling
- Translating these methods to a non-Hermitian context
- Extension to $SU(M)$ for M boson sites

QR code for Wigner function videos: