Trajectory-based multi-configuration approaches to Bose-Hubbard dynamics

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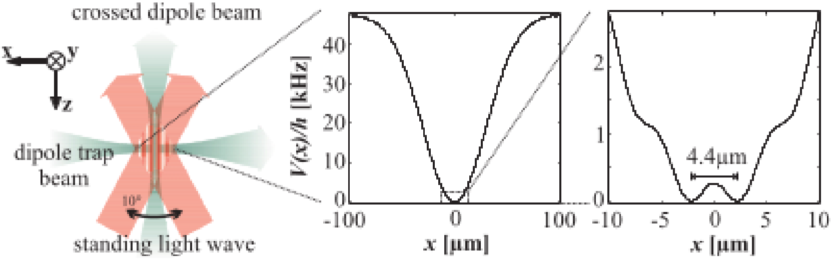
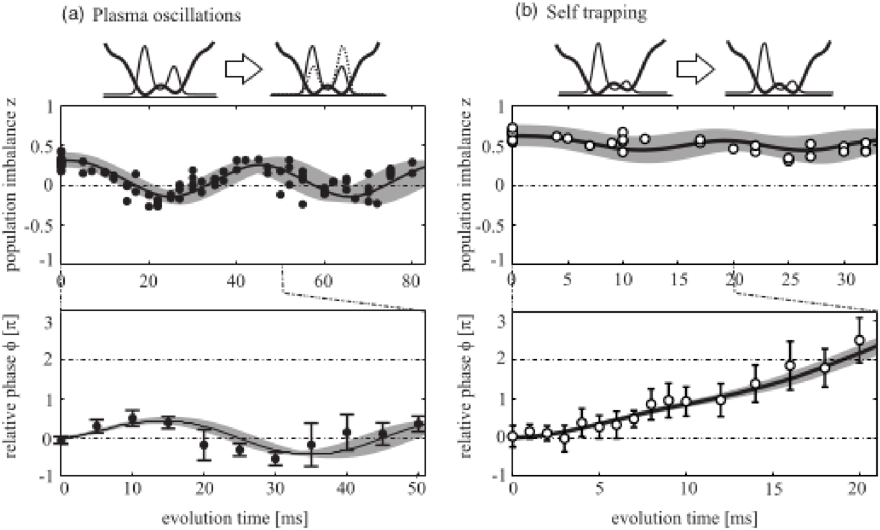
Weakly coupled macroscopic quantum systems

- ac and dc Josephson effects in superconductors
- weakly coupled superfluid Helium baths
- BEC in a double well trap: bosonic Josephson junction (JJ)



R Gati and M K Oberthaler, J. Phys. B: At. Mol. Opt. Phys. **40**, *R61 (2007)*

Bosonic JJ: Dynamics



R. Gati and M. K. Oberthaler, J. Phys. B: At. Mol. Opt. Phys. **40**, *R61 (2007)*

Overview

1. Revivals of Glauber CS in the single well BH case
   - Glauber Coherent states
   - Revival time scale
   - Comparison of methodologies
2. Single particle tunneling in the double well
   - Model and tunneling dynamics
   - Tayloring grids to gain "understanding"
3. Many particle tunneling: Josephson Junction
   - Mean-field Dynamics
   - Beyond Mean Field

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Glauber Coherent States

Gaussians are ubiquitous and

well suited to describe dynamics of harmonic baths and much more...

E. Schrödinger, Die Naturwissenschaften **14**, *664 (1926), . . . ; L. Schulman, Symmetry* **13**, *527 (2021)*

Frozen Gaussians

position representation of fixed width Gaussian

$$\boxed{\Psi(x) = \left(\frac{\gamma}{\pi}\right)^{1/4} \exp\left\{-\frac{\gamma}{2}(x-q)^2 + \frac{i}{\hbar}p(x-q/2)\right\}}$$

$$p, q \in \Re$$

complexified notation, representation free

$$z = \frac{\gamma^{1/2} q + \mathrm{i}\gamma^{-1/2} p}{\sqrt{2}}$$

$$\Psi(x,t) \to |z(t)\rangle = |q_t, p_t\rangle$$

The single well case: revival dynamics

Onsite interaction and confinement of bosonic particles: "Kerr oscillator"

$$\hat{H} = \omega_{\mathrm{e}}\, \hat{a}^\dagger \hat{a} + \frac{U}{2} \hat{a}^\dagger \hat{a}^\dagger \hat{a}\, \hat{a}$$

eigenenergies: *quadratic spectrum* (reordering of interaction term)

$$E_n = \omega_{\mathrm{e}} n + \frac{U}{2} n(n-1)\,, \quad n = 0, 1, 2, \ldots$$

initial Gaussian wavefunction centered at α (mean particle number)

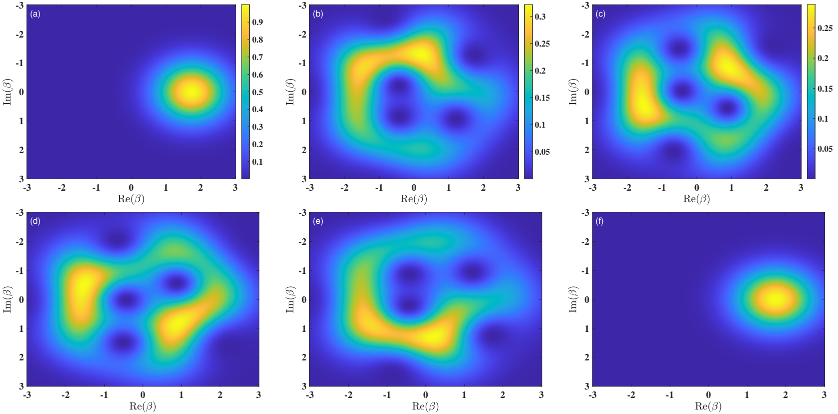
$$c(t) := \langle \alpha | \alpha(t) \rangle = \mathrm{e}^{-|\alpha|^2} \sum_n \frac{|\alpha|^{2n}}{n!} \mathrm{e}^{-\mathrm{i} \frac{U}{2} n(n-1) t}$$

$\boxed{\textit{full revival} \text{ at time } t_r = 2\pi / U}$

M. Greiner et al, Nature **419**, *51 (2002)*

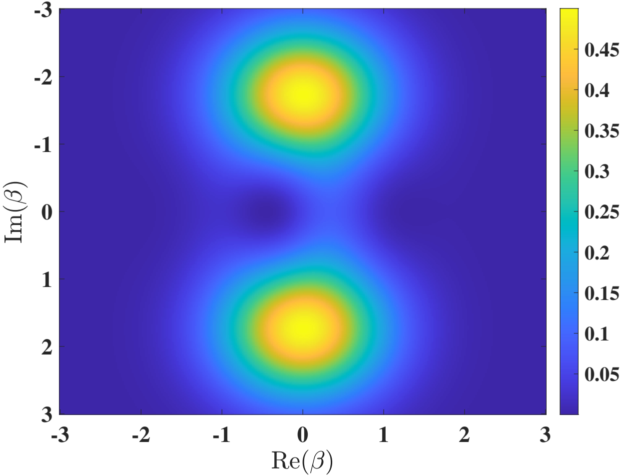
Husimi snapshots: $tU/\pi = 0, 0.4, 0.8, 1.2, 1.6, 2$

$$\Omega(\beta, t) = |\langle\beta|\alpha(t)\rangle|^2$$



M. Greiner et al, Nature **419**, *51 (2002)*, *Y. Qiao, Dissertation, TU Dresden(2024)*

Husimi snapshots: $tU = \pi$



autocorrelation almost zero

Y. Qiao, Dissertation, TU Dresden(2024)

Truncated Wigner Approximation (TWA) (aka LSCIVR)

absolute value of autocorrelation function

$$|c(t)| = \sqrt{\int \frac{\mathrm{d}^2 z_0}{\pi} W(z_0, z_0^*) W(z_t, z_t^*)}$$

$z_t(z_0, z_0^*)$: classical trajectory with initial condition z_0

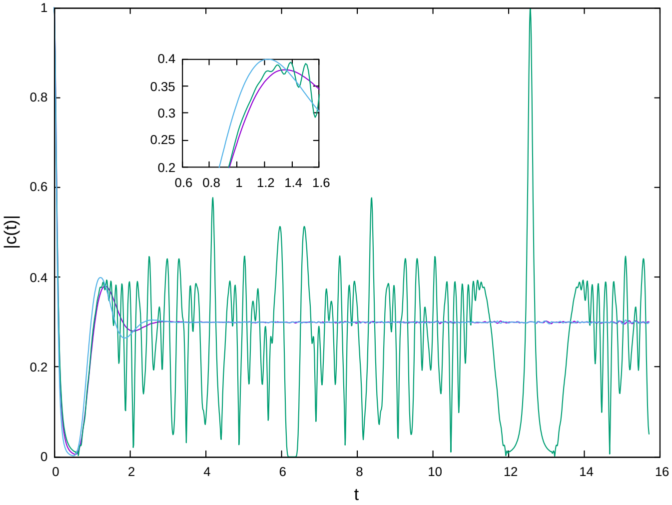
Wigner function of a Gaussian centered around α

$$W(z, z^*) = 2\mathrm{e}^{-2|z-\alpha|^2}$$

$$\boxed{\textit{mean-field (classical) return time } t_c = t_r/\alpha^2}$$

M. Hillary et al, Phys. Rep. **106**, *121 (1984); S. Garashchuk and D. J. Tannor, CPL* **263**, *324 (1996); S. Loho Choudhury and FG, Condens. Matter* **5**, *3 (2020)*

TWA for $U = 0.5$, $\omega_e = 0$, $\alpha = \sqrt{10}$



$t_c = t_r/10$: OK, but no quantum mechanical revival!

Herman-Kluk (HK) time-evolution operator

$$\boxed{\mathrm{e}^{-\mathrm{i}\hat{H}t} \approx \int \frac{\mathrm{d}^2 z_0}{\pi} R_t(z_0, z_0^*) \mathrm{e}^{\mathrm{i}S_t(z_0, z_0^*)} \left| z_t(z_0, z_0^*) \right\rangle \left\langle z_0 \right|}$$

in terms of c-numbers: "classical action"

$$S_t(z, z_0^*) = \int_0^t \mathrm{d}t' \, L(z(t'), z^*(t'), t'),$$

classical Lagrangian ($\hat{a} \to z$, $\hat{a}^\dagger \to z^*$)

$$L = \frac{\mathrm{i}}{2} \left[z^*(\partial_t z) - (\partial_t z)^* z \right] - H(z, z^*)$$

total prefactor

$$R_t(z_0, z_0^*) = \mathrm{e}^{\mathrm{i}\theta_t(z_0, z_0^*)} R_t^{\mathrm{HK}}(z_0, z_0^*)$$

phase correction term (only for normal ordering)

$$\theta_t(z_0, z_0^*) = \int_0^t \mathrm{d}t' \frac{1}{2} \mathrm{Tr} \left[\partial_{z^*} \partial_z H|_{z = z_{t'}} \right],$$

M. Herman and E. Kluk, CP **91***, 27 (1984); M. S. Child and D. Shalashilin, JCP* **118***, 2061 (2003)*

Classical ingredients for *normal ordering*

$$H_{\rm ord}(z, z^*) = \omega_e |z|^2 + \frac{U}{2}|z|^4,$$

Complexified classical EOM and its solution

$$\mathrm{i}\partial_t z = \partial_{z^*} H_{\rm ord}(z, z^*) = (\omega_e + U|z|^2)z$$

$$z_t = \mathrm{e}^{-\mathrm{i}(\omega_e + U|z_0|^2)t} z_0 \ ,$$

action

$$S_t(z_0, z_0^*) = \frac{U}{2}|z_0|^4 t$$

HK prefactor

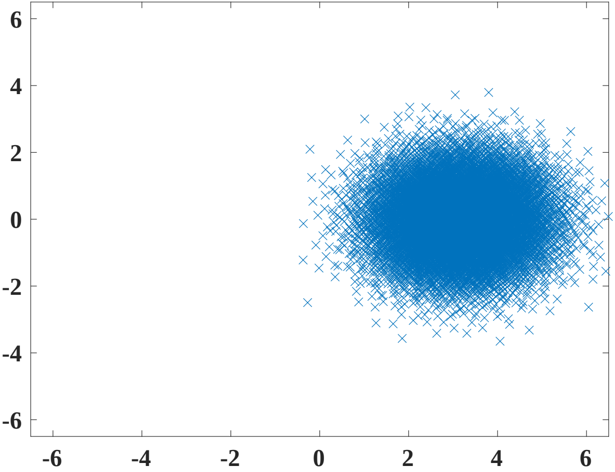
$$R_t^{\rm HK}(z_0, z_0^*) = \sqrt{1 - \mathrm{i}U|z_0|^2 t}\ \mathrm{e}^{-\frac{\mathrm{i}}{2}(\omega_e + U|z_0|^2)t}$$

phase correction term

$$\theta_t(z_0, z_0^*) = \left(\frac{1}{2}\omega_e + U|z_0|^2\right) t$$

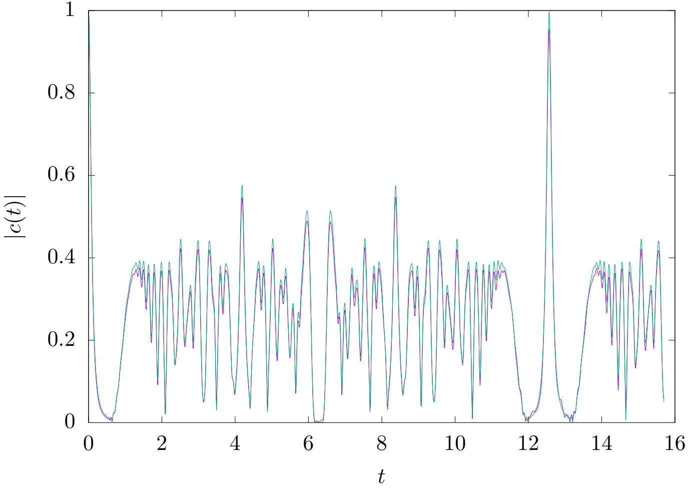
S. Ray et al, J. Phys. A **49**, *168303 (2016)*

Trajectories initially centered around $\alpha = \sqrt{10}$



5000 trajectories in phase space $q \sim Rez$, $p \sim Imz$

First try to recover full revival, $U = 0.5, \omega_e = 0$

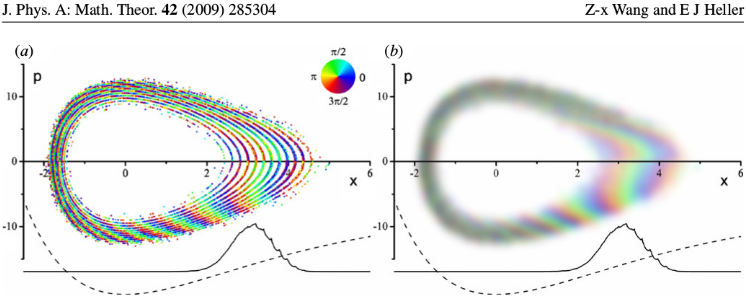


$t_r = 4\pi$: "nice" but not perfect (50000 trajectories)

Revival in Morse oscillator

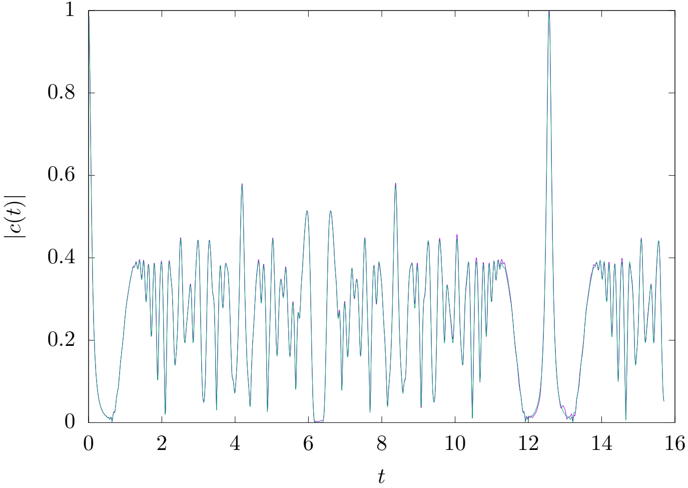
$$\boxed{V(x) = D[1 - \exp(-\lambda x)]^2}$$

quadratic spectrum: $E_n = \omega_e(n + 1/2) - x_e\omega_e(n + 1/2)^2$



subtle "phase effect" responsible for full revival!

Second try for full revival, using symmetric ordering



almost perfect (50000 trajectories)

Coupled Coherent States (CCS) multi-configuration ansatz

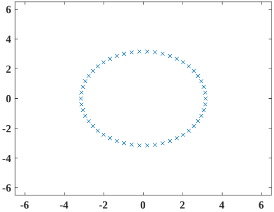
$$\boxed{|\Psi(t)\rangle = \sum_i a_i(t)|z_i(t)\rangle}$$

$\{z_i\}$: classical trajectories, $\{a_i\}$: fully quantum mechanical coefficients

EOM from time-dependent variational principle (TDVP)

3 different types of initial condition “sampling” yield same error measure

- annular grid (on a ring in phase space)

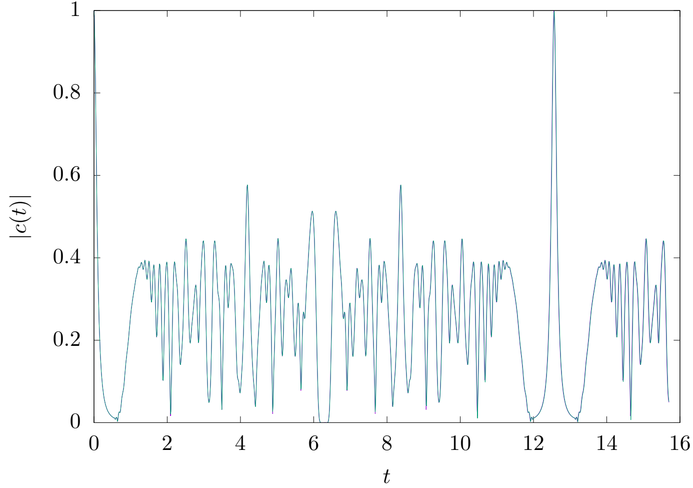


trajectories stay on the ring!

- doubly dense von Neumann rectangular grid
- random grid (Sobol or Halton) according to Gaussian distribution

D. Shalashilin and M. Child, JCP **113***, 10028 (2000)*

CCS method (using normal ordering)

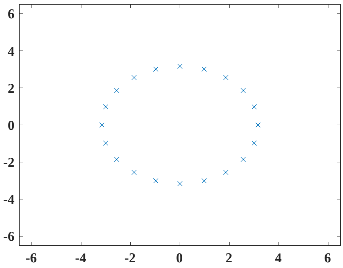


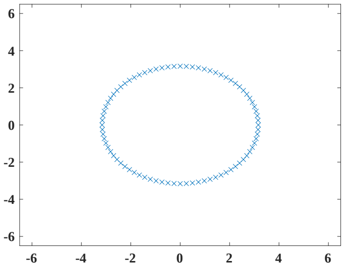
even better than HK (30 trajectories on a ring) but similar clock time

Variational Coherent States (VCS) method

- also $\{z_i(t)\}$ ▸ fully variational
- similar agreement with full quantum as CCS
- even 20 trajectories are leading to converged results
- coefficients as well as CS parameters are all coupled
- interesting "behavior" of trajectories

M. Werther, S.Loho Choudhury and FG, IRPC **40**, *81 (2021)*





Overview

Model and tunneling dynamics

Hamiltonian for a double well potential with barrier height D

$$\hat{H}(\hat{p}, \hat{q}) = \frac{\hat{p}^2}{2} + V(\hat{q}),$$

$$V(q) = -\frac{1}{4}q^2 + \frac{1}{64D}q^4 + D$$

CCS autocorrelation

$$c(t) = \langle\alpha|\Psi(t)\rangle = \sum_{i=1}^{M} a_i \langle\alpha|z_i(t)\rangle$$

tunneling splitting for $D = 1$

$$\Delta := E_2 - E_1 \approx 2.392 \times 10^{-2},$$

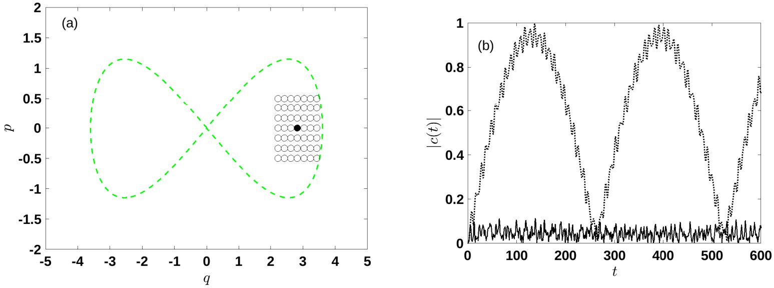
tunneling period for $D = 1$

$$T_t := 2\pi/\Delta \approx 262,$$

FG et al, Z. Phys. B **84***, 315 (1991)*

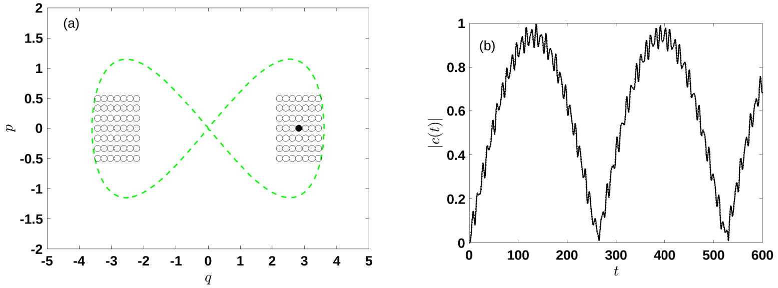
Dense grid below barrier ($M = 49$): CCS versus SOFFT

initial state centered at $q = \sqrt{8D}$ inside separatrix:



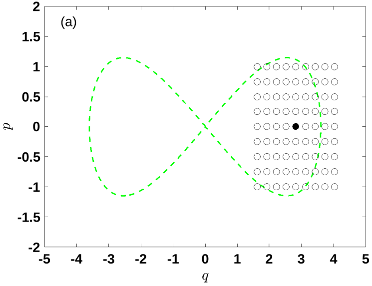
no tunneling!

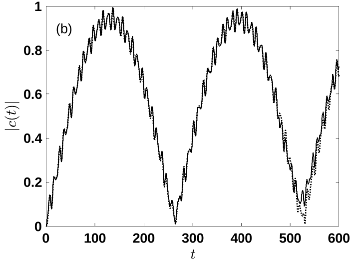
Copied grid ($M = 98$): CCS versus SOFFT



perfect agreement with split operator FFT

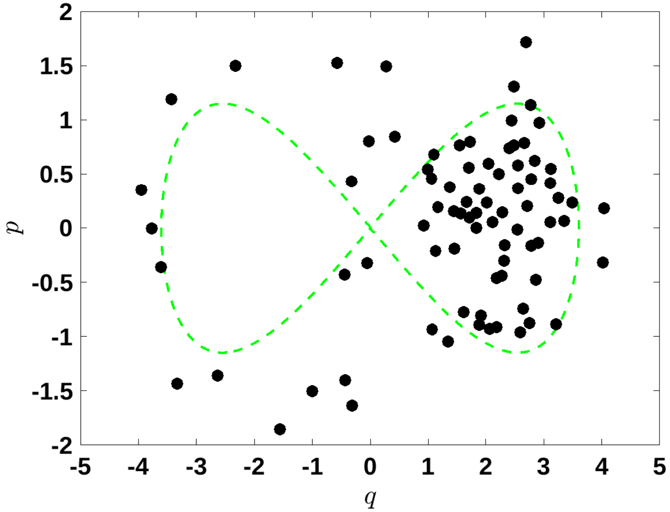
Less dense grid ($M = 81$) with trajectories over the barrier





almost perfect agreement with split operator FFT

High energy trajectories do the job: $t = 131$



FG, IOP Conf. Ser. (2024), submitted

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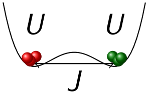
Mean-field Dynamics

Bosonic JJ: restriction to two lowest eigenstates of double well

$$\boxed{\hat{H} = -J(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1) + \frac{U}{2}\sum_{j=1}^{2} \hat{a}_j^{\dagger 2} \hat{a}_j^2,}$$



Site populations

$$\hat{n}_j = \hat{a}_j^\dagger \hat{a}_j, \quad j = 1, 2$$

Expectation value $n_j = \langle \alpha_j | \hat{n}_j | \alpha_j \rangle$

$$\hat{a}_j |\alpha_j(t)\rangle = \alpha_j(t)|\alpha_j(t)\rangle = \sqrt{n_j(t)}\mathrm{e}^{\mathrm{i}\phi_j(t)}|\alpha_j(t)\rangle$$

Mean-field Dynamics

Population imbalance: $z = (n_1 - n_2)/S$
example:

$$n_1 = 3/2, \quad n_2 = 1/2 \rightarrow z(0) = 1/2$$

phase difference: $\phi = \phi_1 - \phi_2$
MF Ansatz for the solution of the TDSE

$$|\Psi(t)\rangle = \frac{1}{\sqrt{S!}} \left(\sqrt{\frac{1+z(t)}{2}} \hat{a}_1^\dagger + \sqrt{\frac{1-z(t)}{2}} e^{-\mathrm{i}\phi(t)} \hat{a}_2^\dagger \right)^S |0,0\rangle$$

in terms of a *single* SU(2) GCS (atomic coherent state) with two real time-dependent parameters, $z(t), \phi(t)$!

Mean-field Dynamics

TDVP $\Rightarrow$EOM for z (population imbalance) and ϕ (phase difference)

$$
\begin{aligned}
\dot{z} &= 2J\sqrt{1-z^2}\sin\phi := f_1 \\
\dot{\phi} &= -2J\frac{z}{\sqrt{1-z^2}}\cos\phi - U(S-1)z := f_2
\end{aligned}
$$

-highly non-linear, non-rigid pendulum type
-Strength parameter

$$\boxed{\Lambda = U(S-1)/(2J)}$$

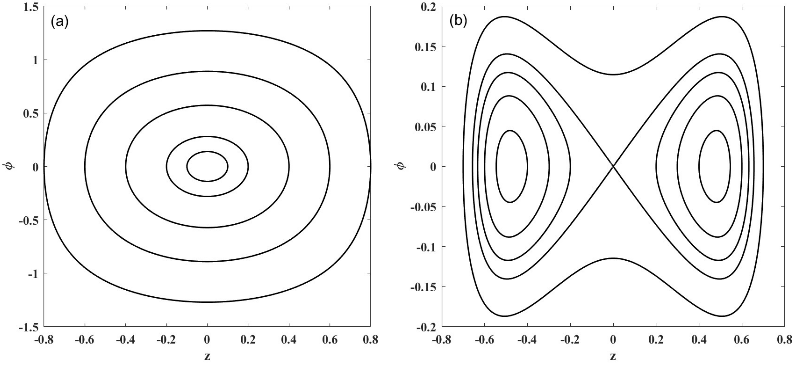
"Josephson regime": $1 < |\Lambda| < S^2$
-Eigenvalues of Jacobi matrix imaginary for $\Lambda > -1$
$\Rightarrow$*Spontaneous Symmetry Breaking* for $\Lambda < -1$
-$E = \frac{US}{4}(S-1)z^2 - JS\sqrt{1-z^2}\cos\phi$ is a constant of motion
$\Rightarrow$*Macroscopic Quantum Self Trapping* for $E(z(0),\phi(0)) > E(0,\pi) = JS$

S. Wimberger et al., PRA **103**, *023326 (2021)*

Phase space trajectories

From one elliptic to one hyperbolic and two elliptic fixed points

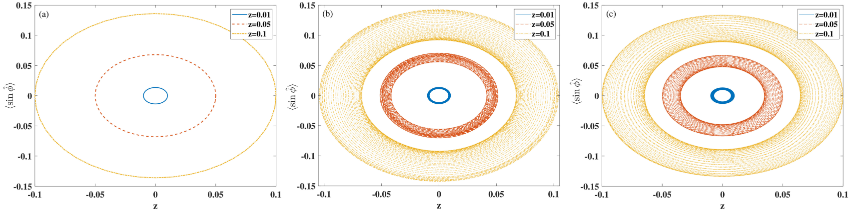
$U/J = 0.1$ $\qquad$ $U/J = -0.12$



Y. Qiao and F.G., Frontiers in Physics (2023)

Beyond mean field: plasma oscillations I

small initial population imbalance, $S = 20$, $U/J = 0.1$

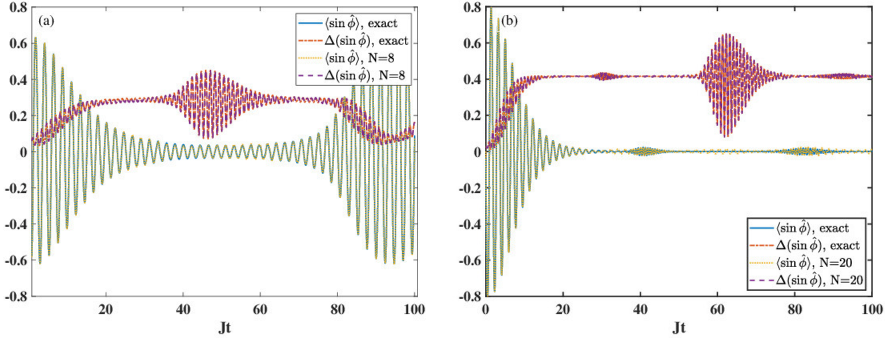


- exact results: expansion of $|\Psi\rangle$ in terms of the S (time-independent) Fock states
- spiraling dynamics of expectation values is unconvered by adding only **one single** additional variational trajectory
  $|\Psi(t)\rangle = \sum_{k=1}^{2} A_k(t)|S, \xi_k(t)\rangle$
- multi-configuration with mean-field trajectories (Herman-Kluk propagator) needs 10^4 trajectories

Y. Qiao and F.G., Frontiers in Physics (2023)

Beyond mean field: plasma oscillations II

large initial population imbalance $z = 0.5$, (a) $S = 20$ (b) $S = 50$



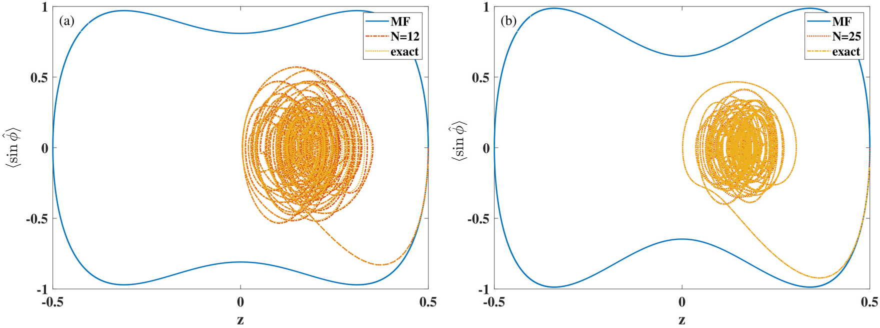
larger multiplicity $N = 8, 20$ is needed

Y. Qiao and F.G., Frontiers in Physics (2023)

Beyond mean field: MQST

Early onset of MQST compared to mean-field prediction:
$z(0) = 0.5, \phi(0) = 0 \Rightarrow \Lambda_{\mathrm{MF}} \approx 15$

(a) $S = 20, \Lambda = 14.4$, (b) $S = 50, \Lambda = 13.0$:



"early onset" predicted correctly by multi-configuration ansatz!

Y. Qiao and F.G., Frontiers in Physics (2023)

Conclusions and Outlook

- Bose-Hubbard/Kerr dynamics:
  - standard *Glauber* CS as time-dependent basis functions
  - multi-configuration results: possibly better scaling than Fock-space calculation for many sites: $(M+S-1)!/S!(M-1)!$
- Tunneling in the double well
  - Discriminating trajectories
- Quantum effects in Josephson Junctions
  - Collapse and revival oscillations
  - Early onset of MQST

  uncovered with surprisingly few *variational* trajectories
- *Boson sampling: exact dynamics*
  Y. Qiao, J. Huh and FG, SciPost Phys. **15**, *007 (2023)*
- *Prediction of new physics in larger systems*

Thanks:

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- S. Ray (Syddansk Universitet)
- A. R. Kolovsky (Siberian Federal University, Krasnoyarsk)
- Gabriel Lando (IBS, South Korea)

IMPRS QDC @ MPI-PKS

for your attention

Wigner function

Back

Quantum optical notation

$$W(\alpha,\alpha^*) = \frac{1}{\pi}\int \mathrm{d}^2\eta\, \exp(-\eta\alpha^* + \eta^*\alpha)\chi(\eta,\eta^*) \tag{1}$$

with

$$\chi(\eta,\eta^*) = \mathrm{Tr}\left[\hat{\rho}\exp(-\eta\hat{a}^\dagger + \eta^*\hat{a})\right] \tag{2}$$

Original formulation for wavefunctions

$$W(x,p) = \int \mathrm{d}y\,\psi^*(x-y/2)\psi(x+y/2)\mathrm{e}^{-\mathrm{i}yp} \tag{3}$$

Result for Gaussian wavefunction centered around α_0

$$W(\alpha,\alpha^*) = 2\mathrm{e}^{-2|\alpha-\alpha_0|^2} \tag{4}$$

C. W. Gardiner and P. Zoller, Quantum Noise, Springer (2004)

CCS equations of motion

Back

Ansatz

$$|\Psi(t)\rangle = \sum_{l=1}^{M} a_l(t)|z_l(t)\rangle \tag{5}$$

TDVP $\langle\delta\Psi|\mathrm{i}\partial_t - \hat{H}|\Psi\rangle = 0$ yields

$$\mathrm{i}\sum_{l=1}^{M}\langle z_k(t)|z_l(t)\rangle \dot{a}_l(t) = \sum_{l=1}^{M}\tilde{H}_{kl}(t)a_l(t), \tag{6}$$

with

$$\tilde{H}_{kl}(t) = \langle z_k(t)|z_l(t)\rangle\Bigg[H_{\mathrm{ord}} - \frac{1}{2}\left(z_l(t)\frac{\partial H_{\mathrm{ord}}}{\partial z_l} - \frac{\partial H_{\mathrm{ord}}}{\partial z_l^*}z_l^*(t)\right) - z_k^*(t)\frac{\partial H_{\mathrm{ord}}}{\partial z_l^*}\Bigg]. \tag{7}$$

VCS equations of motion

Back

TDVP leads to:

$$\mathrm{i}\sum_{l=1}^{M}\langle z_k|z_l\rangle\left[X_l + a_l z_k^* \dot{z}_l\right] = \langle z_k|\hat{H}|\Psi\rangle, \tag{8}$$

$$\mathrm{i}a_k^*\sum_{l=1}^{M}\langle z_k|z_l\rangle\left[z_l X_l + a_l(1+z_k^* z_l)\dot{z}_l\right] = a_k^*\langle z_k|\hat{a}\hat{H}|\Psi\rangle \tag{9}$$

with

$$X_k := \dot{a}_k + a_k\left[-\frac{1}{2}\left(z_k\dot{z}_k^* + \dot{z}_k z_k^*\right)\right] \tag{10}$$

M. Werther and FG, PRB **101**, *174315 (2020)*

Jacobi matrix

◂ Back

Reminder: f_1, f_2 RHSs of EOM
$z^* = 0, \phi^* = 0$:

$$\mathbf{J} = \begin{pmatrix} \left.\frac{\partial f_1}{\partial z}\right|_{z^*,\phi^*} & \left.\frac{\partial f_1}{\partial \phi}\right|_{z^*,\phi^*} \\ \left.\frac{\partial f_2}{\partial z}\right|_{z^*,\phi^*} & \left.\frac{\partial f_2}{\partial \phi}\right|_{z^*,\phi^*} \end{pmatrix} = \begin{pmatrix} 0 & 2J \\ -2J - (S-1)U & 0 \end{pmatrix} \tag{11}$$

eigenvalues:

$$\lambda_\pm = \pm\sqrt{2}J\sqrt{-2 + \frac{U}{J} - \frac{US}{J}}. \tag{12}$$

S. Wimberger, Nonlinear Dynamics and Quantum Chaos: An Introduction, Springer (2022)