Using mixed many-body particle states to generate exact $\mathcal{PT}$-symmetry in a time-dependent four-well system with gain and loss

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$\mathcal{PT}$ symmetry

For the (non-Hermitian) Hamiltonian $\hat{H}$ of a $\mathcal{PT}$-symmetric systems one has:

$$\left[\hat{H}, \mathcal{PT}\right] = 0$$

Parity operator $\mathcal{P}$ and time reversal operator$\mathcal{T}$:

$$\mathcal{P} : \hat{x} \to -\hat{x},\, \hat{p} \to -\hat{p}$$
$$\mathcal{T} : \hat{x} \to \quad \hat{x},\, \hat{p} \to -\hat{p},\, \mathrm{i} \to -\mathrm{i}$$

Potential V:

$$\operatorname{Re} V(\hat{\boldsymbol{x}}) = \operatorname{Re} V(-\hat{\boldsymbol{x}}), \quad \operatorname{Im} V(\hat{\boldsymbol{x}}) = -\operatorname{Im} V(-\hat{\boldsymbol{x}})$$

$\mathcal{PT}$ symmetry

Probability current density:

$$\boldsymbol{j}(\boldsymbol{x},t) = \frac{\mathrm{i}\hbar}{2m}\left(\psi(\boldsymbol{x},t)\nabla\psi^*(\boldsymbol{x},t) - \psi^*(\boldsymbol{x},t)\nabla\psi(\boldsymbol{x},t)\right)$$

Continuity equation:

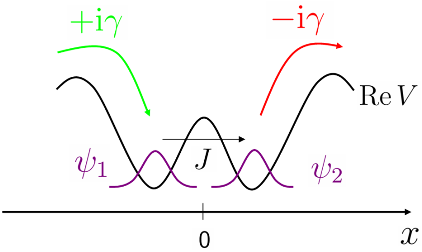
$$\frac{\partial}{\partial t}|\psi(\boldsymbol{x},t)|^2 + \operatorname{div}\boldsymbol{j}(\boldsymbol{x},t) = \frac{2}{\hbar}|\psi(\boldsymbol{x},t)|^2 \operatorname{Im} V(\boldsymbol{x})$$

$\rightarrow$ Positive/negative imaginary parts describe sources/sinks of the probability of presence

$\Rightarrow$ Elegant way of an effective description of open quantum systems with balanced gain and loss

Proposal of a $\mathcal{PT}$-symmetric quantum system

Bose-Einstein condensate in a laser-generated optical double well:



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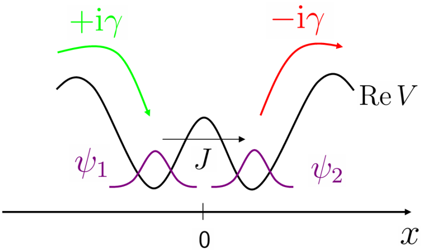


Mean-field description given by Graefe et al. [*J. Phys. A* **45**, 444015 (2012)] using the two-state Gross-Pitaevskii-Gleichung (GPE):

$$\mathrm{i}\frac{\partial}{\partial t}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} = \begin{pmatrix} g|\psi_1|^2+\mathrm{i}\gamma & -J \\ -J & g|\psi_2|^2-\mathrm{i}\gamma\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}$$

Stationary solutions of the two-mode model

$$\mathrm{i}\frac{\partial}{\partial t}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} = \begin{pmatrix} g|\psi_1|^2+\mathrm{i}\gamma & -J \\ -J & g|\psi_2|^2-\mathrm{i}\gamma\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}$$

Stationary solutions $\propto \exp(-\mu t)$ with real μ exist with amplitudes

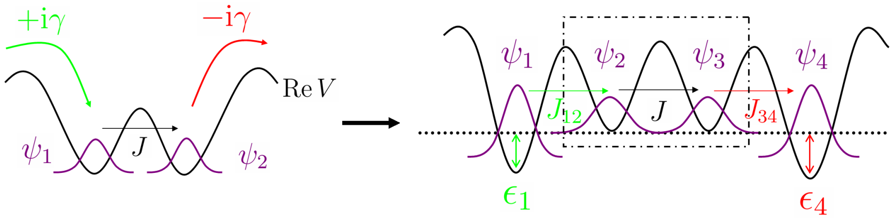
$$\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} = \begin{pmatrix}\sqrt{n}\exp(\mathrm{i}\varphi)\\ \sqrt{n}\exp(-\mathrm{i}\varphi)\end{pmatrix} \qquad \sin(2\varphi) = -\frac{\gamma}{J}\ .$$

occupation number: $n_i(t) = n =$ const.

current density: $\tilde{j}_{12}(t) = -\mathrm{i}(\psi_1^*\psi_2 - \psi_2^*\psi_1) = 2n\gamma/J =$ const.

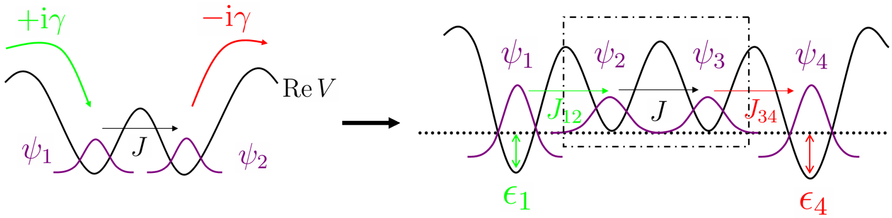
correlation: $c_{12}(t) = (\psi_1^*\psi_2 + \psi_2^*\psi_1) = 2n\sqrt{1-\gamma^2/J^2} =$ const.

Embedding into a hermitian four-well system



Idea: [Kreibich et al., *Phys. Rev. A* **87**, 051601 (2013)]
Simulate the non-hermitian open two-well system by a time-dependent adjustment of the outer tunneling coefficients $J_{12}(t)$, $J_{34}(t)$ and the energy offsets $\epsilon_1(t)$, $\epsilon_4(t)$

Embedding into a hermitian four-well system



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Simulate the non-hermitian open two-well system by a time-dependent adjustment of the outer tunneling coefficients $J_{12}(t)$, $J_{34}(t)$ and the energy offsets $\epsilon_1(t)$, $\epsilon_4(t)$

Goal: To obtain the behaviour of the open $\mathcal{PT}$-symmetric two-well quantum system by embbeding into the four-well system

Embedding into a hermitian four-well system

$$\mathrm{i}\frac{\partial}{\partial t}\begin{pmatrix}\psi_2\\ \psi_3\end{pmatrix}=\begin{pmatrix}g|\psi_2|^2+\mathrm{i}\gamma & -J\\ -J & g|\psi_3|^2-\mathrm{i}\gamma\end{pmatrix}\begin{pmatrix}\psi_2\\ \psi_3\end{pmatrix}$$

$$\mathrm{i}\frac{\partial}{\partial t}\begin{pmatrix}\psi_1(t)\\ \psi_2(t)\\ \psi_3(t)\\ \psi_4(t)\end{pmatrix}=\mathcal{H}_4\begin{pmatrix}\psi_1(t)\\ \psi_2(t)\\ \psi_3(t)\\ \psi_4(t)\end{pmatrix}$$

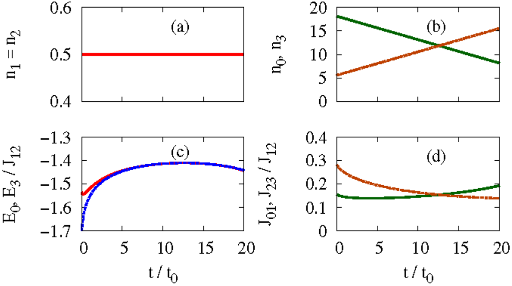
$$\mathcal{H}_4=\begin{pmatrix}g|\psi_1|^2+\varepsilon_1(t) & -J_{12}(t) & 0 & 0\\ -J_{12}(t) & g|\psi_2|^2 & -J & 0\\ 0 & -J & g|\psi_3|^2 & -J_{34}(t)\\ 0 & 0 & -J_{34}(t) & g|\psi_4|^2+\varepsilon_4(t)\end{pmatrix}$$

$$-J_{12}(t)\psi_1(t)=\mathrm{i}\gamma\psi_2(t),\qquad -J_{34}(t)\psi_4(t)=-\mathrm{i}\gamma\psi_3(t)$$

Embedding into a hermitian four-well system

Result [Kreibich et al., *Phys. Rev. A* **87**, 051601 (R) (2013)]

By requiring that the two inner wells behave exactly as in the $\mathcal{PT}$-symmetric two-well system, conditions can be derived which allow for the explicit calculation of the time dependence of the tunneling coefficients $J_{12}(t)$, $J_{34}(t)$ and the energy offsets $\epsilon_1(t)$, $\epsilon_4(t)$.



Embedding into a hermitian four-well system

Result [Kreibich et al., *Phys. Rev. A* **87**, 051601 (R) (2013)]

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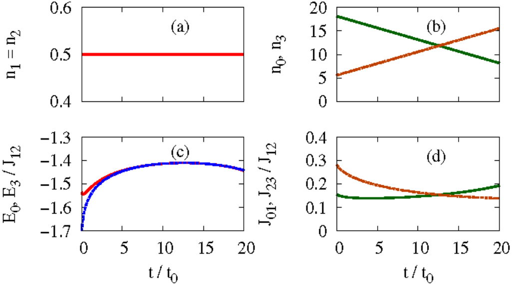


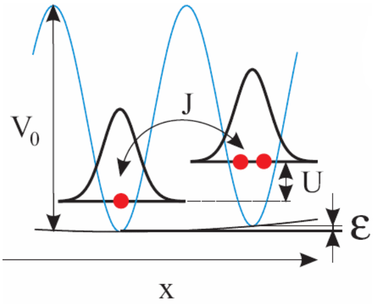
Criticism: Will the behavior survive in a many-body description?

Many-body description

Bose-Hubbard model (BHM)

Bose-Einstein condensates in optical lattices can be described by the Bose-Hubbard-Model:

$$\hat{H}_{\mathrm{BH}} = -\sum_{\langle m,m'\rangle} J_{mm'}\hat{a}_m^\dagger \hat{a}_{m'} + \frac{1}{2}\sum_m U_m \hat{n}_m(\hat{n}_m - 1) + \sum_m \epsilon_m \hat{n}_m$$



Jaksch et al.,
Phys. Rev. Lett. **81**, 3108 (1998)

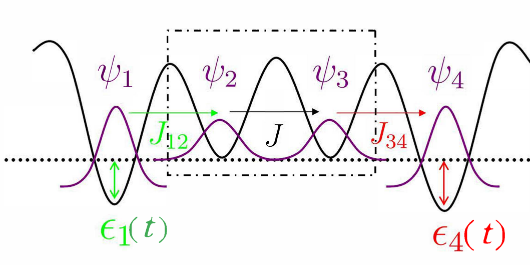
U: strength of the contact interaction, ϵ: on-site energies

Many-body description

Time-dependent Bose-Hubbard model

The four-well condensate will be described by a *time-dependent* Bose-Hubbard-Model:

$$\hat{H}_{\mathrm{BH}}(t) = -\sum_{\langle m,m'\rangle} J_{mm'}(t)\hat{a}^\dagger_m \hat{a}_{m'} + \frac{1}{2}\sum_m U_m \hat{n}_m(\hat{n}_m - 1) + \sum_m \epsilon_m(t)\hat{n}_m$$



Bogoliubov back reaction (BBR) method

Dynamics in the BBR approximation

von Neumann equation for the full density matrix:

$$\mathrm{i}\frac{\partial}{\partial t}\langle\hat{\rho}\rangle = \left\langle\left[\hat{\rho},\hat{H}\right]\right\rangle$$

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Reduced density matrices $\sigma_{kl} = \langle\hat{a}_k^\dagger\hat{a}_l\rangle$, $\sigma_{klmn} = \langle\hat{a}_k^\dagger\hat{a}_l\hat{a}_m^\dagger\hat{a}_n\rangle$, etc.

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BBGKY hierarchy (Bogoliubov–Born–Green–Kirkwood–Yvon):

$$\mathrm{i}\frac{\partial}{\partial t}\langle\hat{\sigma}_{kl}\rangle = f\left(\langle\hat{\sigma}_{kl}\rangle, \langle\hat{\sigma}_{klmn}\rangle\right)$$

$$\mathrm{i}\frac{\partial}{\partial t}\langle\hat{\sigma}_{klmn}\rangle = f\left(\langle\hat{\sigma}_{kl}\rangle, \langle\hat{\sigma}_{klmn}\rangle, \langle\hat{\sigma}_{klmnrs}\rangle\right)$$

$$\ldots = \ldots$$

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Approximation (back reaction):

$$\hat{\sigma}_{klmnrs} = \hat{\sigma}_{kl}\hat{\sigma}_{mnrs} + \hat{\sigma}_{rs}\hat{\sigma}_{klmn} + \hat{\sigma}_{mn}\hat{\sigma}_{klrs} - 2\hat{\sigma}_{kl}\hat{\sigma}_{mn}\hat{\sigma}_{rs}$$

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$\rightarrow 4^2 + 4^4 = 16 + 256 = 272$ time-dependent coupled differential eqns

Reduced many-body density matrices in MF

- In the mean-field description the single-particle density matrix is simply given by $\sigma_{kl}(t) = \psi_k^*(t)\psi_l(t)$

  occupation number of well k: $n_k(t) = \sigma_{kk}(t)$

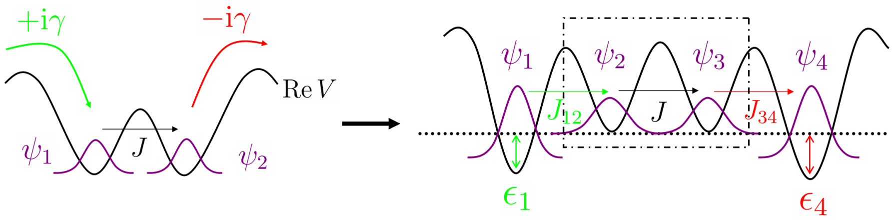
  current from well k to well l: $j_{kl} = J_{kl}\tilde{j}_{kl}$, with

  $\tilde{j}_{kl} = -\mathrm{i}(\psi_k^*\psi_l - \psi_l^*\psi_k) = -\mathrm{i}(\sigma_{kl} - \sigma_{lk}) = 2\,\mathrm{Im}(\sigma_{kl})$

  correlation: $c_{kl} = (\psi_k^*\psi_l + \psi_l^*\psi_k) = 2\,\mathrm{Re}(\sigma_{kl})$

Time dependences of the control parameters

Requirements



$$\mathrm{i}\frac{\partial}{\partial t}\boldsymbol{\psi} = \begin{pmatrix} g|\psi_1|^2 + \mathrm{i}\gamma & -J \\ -J & g|\psi_2|^2 - \mathrm{i}\gamma \end{pmatrix} \boldsymbol{\psi} \qquad \mathrm{i}\frac{\partial}{\partial t}\sigma_{kl} = f\left(\sigma_{kl}, \sigma_{klmn}\right)$$

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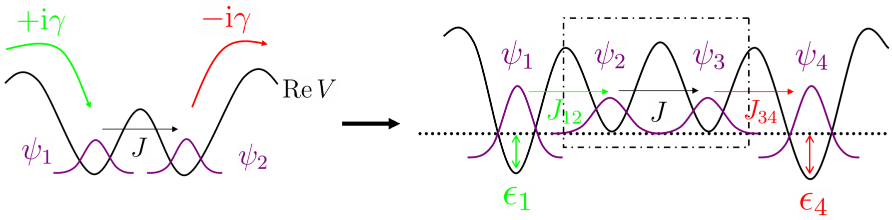

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Requirements: $$J_{12}(t) \overset{!}{=} \frac{\gamma\,\mathrm{Re}(\sigma_{22}(t))}{\mathrm{Im}(\sigma_{12}(t))}, \qquad J_{34}(t) \overset{!}{=} \frac{\gamma\,\mathrm{Re}(\sigma_{33}(t))}{\mathrm{Im}(\sigma_{34}(t))}$$

$$-J_{12}(t)\sigma_{13}(t) + J_{34}(t)\sigma_{24}(t) \overset{!}{=} 0$$

Time dependences of the control parameters

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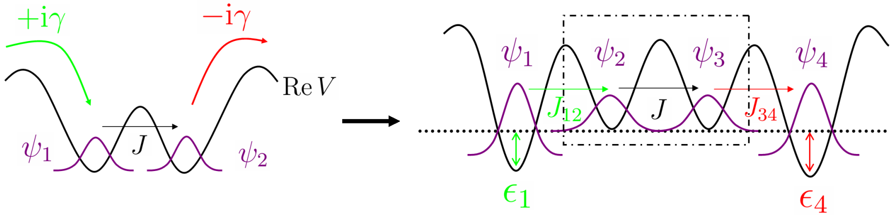

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$$-J_{12}(t)\sigma_{13}(t) + J_{34}(t)\sigma_{24}(t) \stackrel{!}{=} 0$$

$\rightarrow$ Tunnel rates follow directly from the comparison of the dynamics.

Time dependences of the control parameters

Time dependence of the on-site energies

Requirement: $$-J_{12}(t)\sigma_{13}(t) + J_{34}(t)\sigma_{24}(t) \stackrel{!}{=} 0$$

Time dependences of the control parameters

Time dependence of the on-site energies

Requirement: $-J_{12}(t)\sigma_{13}(t) + J_{34}(t)\sigma_{24}(t) \overset{!}{=} 0$

Fulfill requirement for all t:

$$\frac{\partial}{\partial t}\left(-J_{12}(t)\sigma_{13}(t) + J_{34}(t)\sigma_{24}(t)\right) \overset{!}{=} 0$$

Time dependences of the control parameters

Time dependence of the on-site energies

Requirement: $-J_{12}(t)\sigma_{13}(t) + J_{34}(t)\sigma_{24}(t) \stackrel{!}{=} 0$

Fulfill requirement for all t:

$$\frac{\partial}{\partial t}\left(-J_{12}(t)\sigma_{13}(t) + J_{34}(t)\sigma_{24}(t)\right) \stackrel{!}{=} 0$$

$\Rightarrow$ System of equations of the form:

$$\alpha_r(t)\epsilon_1(t) + \beta_r(t)\epsilon_4(t) = \Omega_r(t)$$
$$\alpha_i(t)\epsilon_1(t) + \beta_i(t)\epsilon_4(t) = \Omega_i(t)$$

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Solutions:

$$\epsilon_1(t) = \frac{\beta_i(t)\Omega_r(t) - \beta_r(t)\Omega_i(t)}{\alpha_r(t)\beta_i(t) - \beta_r(t)\alpha_i(t)}, \qquad \epsilon_4(t) = -\frac{(\alpha_i(t)\Omega_r(t) - \alpha_r(t)\Omega_i(t))}{\alpha_r(t)\beta_i(t) - \beta_r(t)\alpha_i(t)}$$

Abbreviations in ϵ_1 und ϵ_4

$$X_{kl} = 2\,\mathrm{Re}\,(Z_{kl})\,, \qquad Y_{kl} = 2\,\mathrm{Im}\,(Z_{kl})$$

$$\alpha_r = \frac{1}{2} J_{12} \left(\frac{c_{12} c_{13}}{\tilde{j}_{12}} + \tilde{j}_{13} \right), \qquad \beta_r = \frac{1}{2} J_{34} \left(\frac{c_{34} c_{24}}{\tilde{j}_{34}} + \tilde{j}_{24} \right)$$

$$\alpha_i = \frac{1}{2} J_{12} \left(\frac{c_{12} \tilde{j}_{13}}{\tilde{j}_{12}} - c_{13} \right), \qquad \beta_i = \frac{1}{2} J_{34} \left(\frac{c_{34} \tilde{j}_{24}}{\tilde{j}_{34}} - c_{24} \right),$$

$$\begin{aligned} \Omega_r = {} & \frac{1}{2} J_{12} \left(\frac{Y_{22} c_{13}}{2n_2} + \frac{X_{12} c_{13}}{\tilde{j}_{12}} + \frac{X_{22} \tilde{j}_{13}}{2n_2} + Y_{13} \right) \\ & - \frac{1}{2} J_{34} \left(\frac{Y_{33} c_{24}}{2n_3} + \frac{X_{34} c_{24}}{\tilde{j}_{34}} + \frac{X_{33} \tilde{j}_{24}}{2n_3} + Y_{24} \right), \end{aligned}$$

$$\begin{aligned} \Omega_i = {} & \frac{1}{2} J_{12} \left(-\frac{X_{22} c_{13}}{2n_2} + \frac{Y_{22} \tilde{j}_{13}}{2n_2} + \frac{X_{12} \tilde{j}_{13}}{\tilde{j}_{12}} - X_{13} \right) \\ & - \frac{1}{2} J_{34} \left(-\frac{X_{33} c_{24}}{2n_3} + \frac{Y_{33} \tilde{j}_{24}}{2n_3} + \frac{X_{34} \tilde{j}_{24}}{\tilde{j}_{34}} - X_{24} \right) \end{aligned}$$

Time dependences of the control parameters

Time dependence of the on-site energies

Requirement: $-J_{12}(t)\sigma_{13}(t) + J_{34}(t)\sigma_{24}(t) \stackrel{!}{=} 0$

Fulfill requirement for all t:

$$\frac{\partial}{\partial t}\left(-J_{12}(t)\sigma_{13}(t) + J_{34}(t)\sigma_{24}(t)\right) \stackrel{!}{=} 0$$

$\Rightarrow$ System of equations of the form:

$$\alpha_r(t)\epsilon_1(t) + \beta_r(t)\epsilon_4(t) = \Omega_r(t)$$
$$\alpha_i(t)\epsilon_1(t) + \beta_i(t)\epsilon_4(t) = \Omega_i(t)$$

Solutions:

$$\epsilon_1(t) = \frac{\beta_i(t)\Omega_r(t) - \beta_r(t)\Omega_i(t)}{\alpha_r(t)\beta_i(t) - \beta_r(t)\alpha_i(t)}, \qquad \epsilon_4(t) = -\frac{(\alpha_i(t)\Omega_r(t) - \alpha_r(t)\Omega_i(t))}{\alpha_r(t)\beta_i(t) - \beta_r(t)\alpha_i(t)}$$

$\Rightarrow$ Dynamics of any initial state of the many-body system can be simulated.

Determining suitable inital states

Constraints

So far:

Determining suitable inital states

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1. $-J_{12}(0)\,\mathrm{Re}(\sigma_{13}(0)) + J_{34}(0)\,\mathrm{Re}(\sigma_{24}(0)) \stackrel{!}{=} 0$ from comparison

Determining suitable inital states

Constraints

So far:

1. $-J_{12}(0)\,\mathrm{Re}(\sigma_{13}(0)) + J_{34}(0)\,\mathrm{Re}(\sigma_{24}(0)) \overset{!}{=} 0$ from comparison
2. $-J_{12}(0)\,\mathrm{Im}(\sigma_{13}(0)) + J_{34}(0)\,\mathrm{Im}(\sigma_{24}(0)) \overset{!}{=} 0$ from comparison

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$\mathcal{PT}$-symmetric states of the open two-well condensate yield three real-valued constraints for the elements of the single-particle density matrix:

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3. $\mathrm{Re}\,\sigma_{22}(0) \overset{!}{=} \mathrm{Re}\,\sigma_{33}(0)$ initial occupation

Determining suitable inital states

Constraints

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$\mathcal{PT}$-symmetric states of the open two-well condensate yield three real-valued constraints for the elements of the single-particle density matrix:

3. $\mathrm{Re}\,\sigma_{22}(0) \stackrel{!}{=} \mathrm{Re}\,\sigma_{33}(0)$ initial occupation
4. $\mathrm{Im}\,\sigma_{23}(0) \stackrel{!}{=} \sqrt{\mathrm{Re}\,\sigma_{22}(0)\,\mathrm{Re}\,\sigma_{33}(0)}\;\frac{\gamma}{J}$ current

Determining suitable inital states

Constraints

So far:

1. $-J_{12}(0)\,\mathrm{Re}(\sigma_{13}(0)) + J_{34}(0)\,\mathrm{Re}(\sigma_{24}(0)) \overset{!}{=} 0$ from comparison
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3. $\mathrm{Re}\,\sigma_{22}(0) \overset{!}{=} \mathrm{Re}\,\sigma_{33}(0)$ initial occupation
4. $\mathrm{Im}\,\sigma_{23}(0) \overset{!}{=} \sqrt{\mathrm{Re}\,\sigma_{22}(0)\,\mathrm{Re}\,\sigma_{33}(0)}\,\frac{\gamma}{J}$ current
5. $\mathrm{Re}\,\sigma_{23}(0) \overset{!}{=} \sqrt{\mathrm{Re}\,\sigma_{22}(0)\,\mathrm{Re}\,\sigma_{33}(0)}\sqrt{1-\frac{\gamma^2}{J^2}}$ correlation

Determining suitable initial states

Pure initial states

Pure initial many-body particle state (MF):

$$|\psi, N_{ges}\rangle = \sum_{\substack{n_1,n_2,n_3,n_4 \\ n_1+n_2+n_3+n_4=N_{\text{ges}}}} \underbrace{\sqrt{\frac{N_{\text{ges}}!}{n_1!n_2!n_3!n_4!}}\psi_1^{n_1}\psi_2^{n_2}\psi_3^{n_3}\psi_4^{n_4}}_{=c_{n_1,n_2,n_3,n_4}} |n_1,...,n_4\rangle$$

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$$\begin{pmatrix} \psi_1(0) \\ \psi_2(0) \\ \psi_3(0) \\ \psi_4(0) \end{pmatrix} = \begin{pmatrix} -\mathrm{i}\sqrt{n_1(0)}\exp(\mathrm{i}\varphi) \\ \sqrt{n(0)}\exp(\mathrm{i}\varphi) \\ \sqrt{n(0)}\exp(-\mathrm{i}\varphi) \\ \mathrm{i}\sqrt{n_4(0)}\exp(-\mathrm{i}\varphi) \end{pmatrix} \qquad \sin(2\varphi) = -\frac{\gamma}{J}\ .$$

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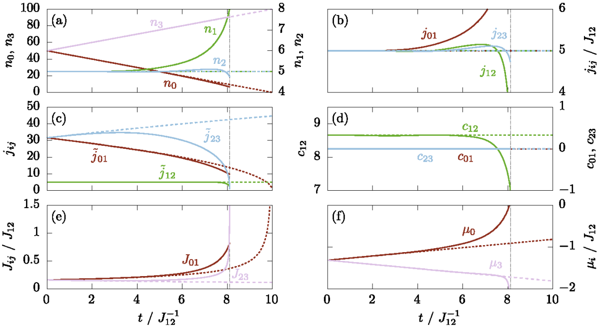
Result [Dizdarevic et al., *Phys. Rev. A* **77**, 013623 (2018)]: No quasi-stationary behavior can be found in the two inner wells:



Determining suitable initial states

Perturbing pure initial states

Pure many-body particle state (MF):

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Perturbation by random numbers with Gaussian distribution z_{n_1,n_2,n_3,n_4}:

$$|\boldsymbol{\psi}, N_{ges}\rangle = \sum_{\substack{n_1,n_2,n_3,n_4 \\ n_1+n_2+n_3+n_4=N_{\text{ges}}}} z_{n_1,n_2,n_3,n_4} c_{n_1,n_2,n_3,n_4} |n_1, n_2, n_3, n_4\rangle$$

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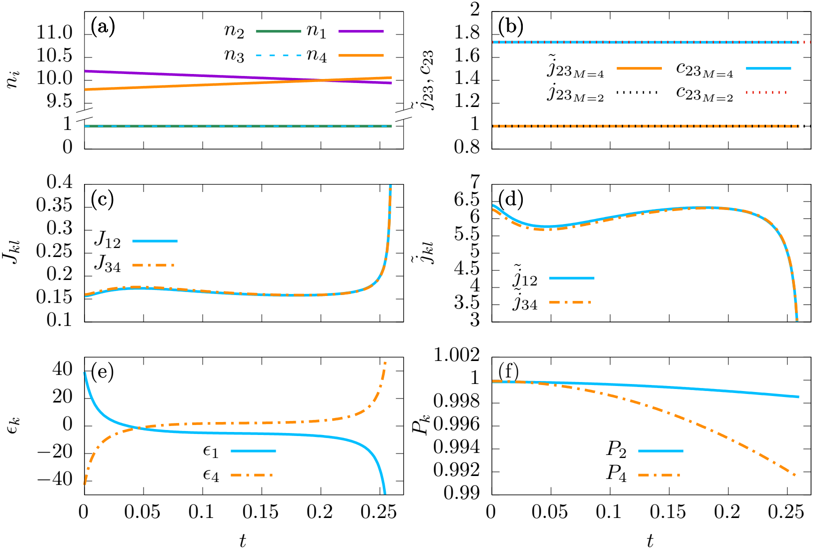
$\Rightarrow$ expectation values $\sigma_{kl} = \langle\psi|\hat{a}_k^\dagger\hat{a}_l|\psi\rangle$, $\sigma_{klmn} = \langle\psi|\hat{a}_k^\dagger\hat{a}_l\hat{a}_m^\dagger\hat{a}_n|\psi\rangle$ yield the initial values for determining the dynamics with the required symmetry

Numerical results

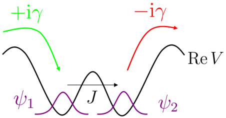
Dynamics of the first-order moments

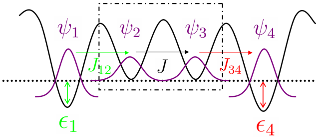


Tina Mathea et al., arXiv:1802.01323v2

Summary

- Goal: Reproduce the dynamics of the $\mathcal{PT}$-symmetric BEC in the two inner wells in a many-body description





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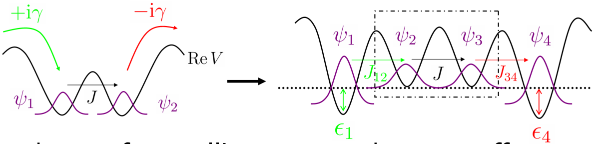

- Time dependence of tunnelling rates and energy offsets:

$$J_{12}(t) = \frac{\gamma\,\mathrm{Re}(\sigma_{22})}{\mathrm{Im}(\sigma_{12})}, \qquad \epsilon_1(t) = \frac{\beta_i\Omega_r - \beta_r\Omega_i}{\alpha_r\beta_i - \beta_r\alpha_i},$$

$$J_{34}(t) = \frac{\gamma\,\mathrm{Re}(\sigma_{33})}{\mathrm{Im}(\sigma_{34})}, \qquad \epsilon_4(t) = -\frac{(\alpha_i\Omega_r - \alpha_r\Omega_i)}{\alpha_r\beta_i - \beta_r\alpha_i}$$

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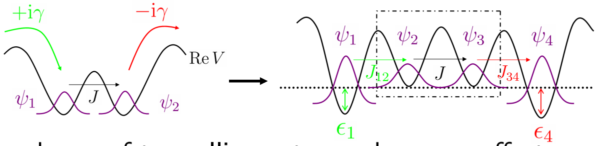

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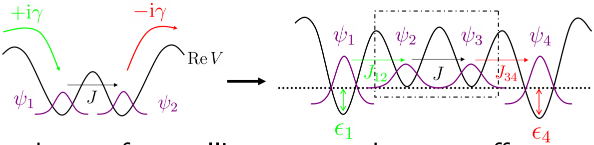

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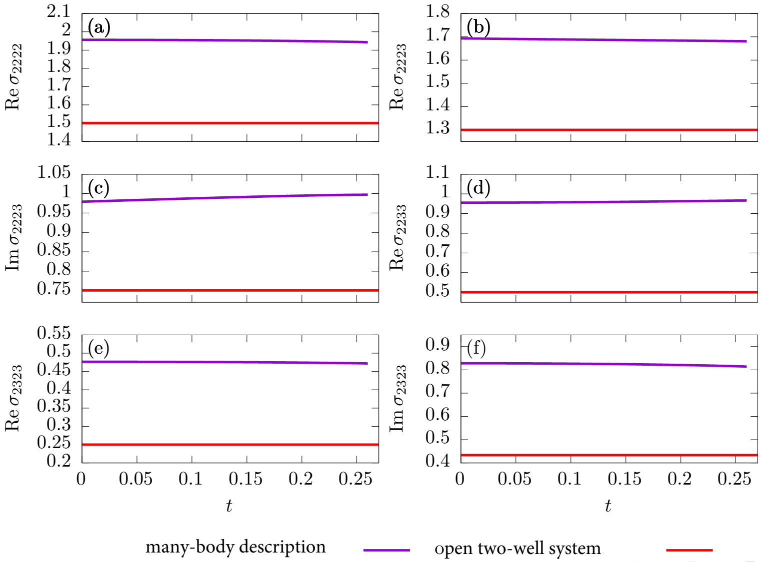
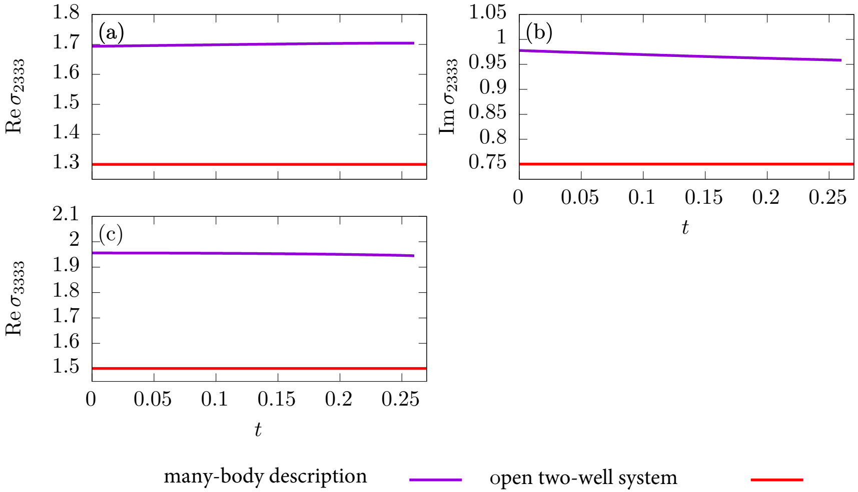
Behaviour of the $\mathcal{PT}$-symmetric BEC in the two inner wells can be described in the first order of the many-body description hierarchy

Dynamics of the second-order moments



Dynamics of the second-order moments



Many-body description

BBR approximation

$$\hat{H}_{\mathrm{BH}} = -\sum_{\langle m,m'\rangle} J_{mm'}\hat{\sigma}_{mm'} + \frac{1}{2}\sum_m U_m \hat{\sigma}_{mmmm} + \sum_m \epsilon_m \hat{\sigma}_{mm}$$

Elements of the density matrices :

$$\langle\hat{\sigma}_{kl}\rangle = \langle\psi|\hat{a}_k^\dagger \hat{a}_l|\psi\rangle$$

$$\langle\hat{\sigma}_{klmn}\rangle = \langle\psi|\hat{a}_k^\dagger \hat{a}_l \hat{a}_m^\dagger \hat{a}_n|\psi\rangle$$

Reduced current density:

$$\tilde{j}_{kl} = 2\,\mathrm{Im}\left(\sigma_{kl}\right)$$

Current :

$$j_{kl} = J_{kl}\tilde{j}_{kl}$$

Correlations:

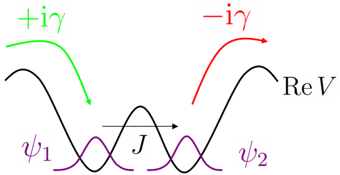
$$c_{kl} = 2\,\mathrm{Re}\left(\sigma_{kl}\right)$$

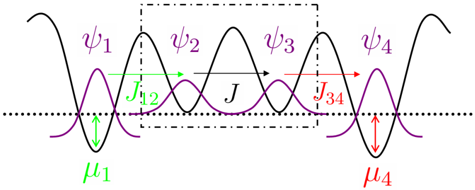
Differential equations of the BBR method

$$
\begin{aligned}
\mathrm{i}\frac{\partial}{\partial t}\sigma_{kl} =& J_{k-1,k}\sigma_{k-1,l} + J_{k+1,k}\sigma_{k+1,l} - J_{l,l-1}\sigma_{k,l-1} - J_{l,l+1}\sigma_{k,l+1} \\
& - U_k\left(\sigma_{kkkl} - \sigma_{kl}\right) + U_l\left(\sigma_{klll} - \sigma_{kl}\right) - \left(\epsilon_k - \epsilon_l\right)\sigma_{kl} \\
=& Z_{kl} - \left(\epsilon_k - \epsilon_l\right)\sigma_{kl}
\end{aligned}
$$

$$
\begin{aligned}
\mathrm{i}\frac{\partial}{\partial t}\sigma_{klmn} =& J_{k-1,k}\sigma_{k-1,lmn} + J_{k+1,k}\sigma_{k+1,lmn} - J_{l,l-1}\sigma_{k,l-1,mn} \\
& - J_{l,l+1}\sigma_{k,l+1,mn} + J_{m-1,m}\sigma_{kl,m-1,m} + J_{m+1,m}\sigma_{kl,m+1,n} \\
& - J_{n,n-1}\sigma_{klm,n-1} - J_{n,n+1}\sigma_{klm,n+1} \\
& - U_k\left(\sigma_{kkklmn} - \sigma_{klmn}\right) + U_l\left(\sigma_{klllmn} - \sigma_{klmn}\right) \\
& - U_m\left(\sigma_{klmmmn} - \sigma_{klmn}\right) + U_n\left(\sigma_{klmnnn} - \sigma_{klmn}\right) \\
& - \left(\epsilon_k - \epsilon_l + \epsilon_m - \epsilon_n\right)\sigma_{klmn}
\end{aligned}
$$

Derivation of the tunneling rates





$$\mathrm{i}\frac{\partial}{\partial t}\boldsymbol{\psi} = \begin{pmatrix} g|\psi_1|^2 + \mathrm{i}\gamma & -J \\ -J & g|\psi_2|^2 - \mathrm{i}\gamma \end{pmatrix} \boldsymbol{\psi} \qquad \mathrm{i}\frac{\partial}{\partial t}\langle\hat{\sigma}_{kl}\rangle = f\left(\langle\hat{\sigma}_{kl}\rangle, \langle\hat{\sigma}_{klmn}\rangle\right)$$

Compare the dynamics, for example:

$$\dot{\sigma}_{22} = 2\gamma\sigma_{22} - 2J_{23}\,\mathrm{Im}\left(\sigma_{23}\right) \qquad \dot{\sigma}_{22} = 2J_{12}\,\mathrm{Im}\left(\sigma_{12}\right) - 2J_{23}\,\mathrm{Im}\left(\sigma_{23}\right)$$

$\Rightarrow$ Yields directly expressions for the tunneling rates:

$$J_{12} \overset{!}{=} \frac{\gamma\,\mathrm{Re}(\sigma_{22})}{\mathrm{Im}(\sigma_{12})}, \qquad J_{34} \overset{!}{=} \frac{\gamma\,\mathrm{Re}(\sigma_{33})}{\mathrm{Im}(\sigma_{34})}$$

Pure initial state

Pure initial state is represented by:

$$\sigma_{kl} = \psi_k^* \psi_l$$

$\Rightarrow$ The determinant of the system of equations for ϵ_1 und ϵ_4 vanishes:

$$\alpha_r \beta_i - \beta_r \alpha_i = 0$$

$\Rightarrow$ There remains an equation of the form

$$A\epsilon_1 + B\epsilon_4 = C$$

$\Rightarrow$ Additional degree of freedom $F(t)$, possible choice of solutions: :

$$\epsilon_1 = \frac{-F(t) + \frac{1}{2}\Omega_r}{\alpha_r}$$
$$\epsilon_4 = \frac{F(t) + \frac{1}{2}\Omega_r}{\beta_r}$$

Pure initial state

For a many-particle state one has:

$$\hat{a}_k^\dagger |\boldsymbol{\psi}, N_{\text{ges}}\rangle = \sqrt{N_{\text{ges}}}\psi_k |\boldsymbol{\psi}, N_{\text{ges}} - 1\rangle$$

This implies initial values of the single-particle and two-particle density matrices of a pure state:

$$\sigma_{kl} = \langle \boldsymbol{\psi}, N_{\text{ges}} | \hat{a}_k^\dagger \hat{a}_l | \boldsymbol{\psi}, N_{\text{ges}} \rangle = N_{\text{ges}} \psi_k^* \psi_l,$$

$$\begin{aligned}
\sigma_{klmn} &= \langle \boldsymbol{\psi}, N_{\text{ges}} | \hat{a}_k^\dagger \hat{a}_l \hat{a}_m^\dagger \hat{a}_n | \boldsymbol{\psi}, N_{\text{ges}} \rangle \\
&= \langle \boldsymbol{\psi}, N_{\text{ges}} | \hat{a}_k^\dagger \left(\hat{a}_m^\dagger \hat{a}_l + \delta_{lm} \right) \hat{a}_n | \boldsymbol{\psi}, N_{\text{ges}} \rangle \\
&= N_{\text{ges}} \left(N_{\text{ges}} - 1 \right) \psi_k^* \psi_l \psi_m^* \psi_n + N_{\text{ges}} \delta_{lm} \psi_k^* \psi_n .
\end{aligned}$$