# Exact dynamics of two ultra-cold bosons in a one-dimensional double-well potential


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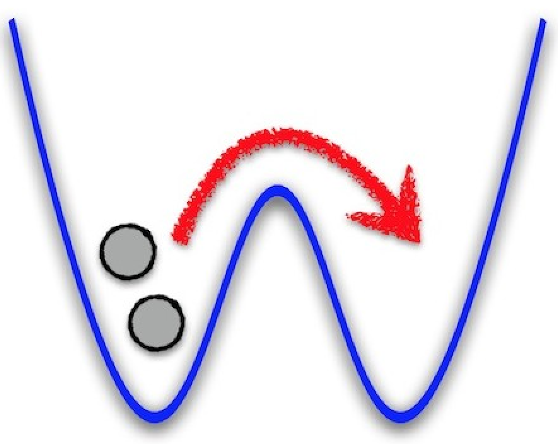


## Abstract


The dynamics of two ultra-cold bosons confined in a one-dimensional double-well potential is studied.

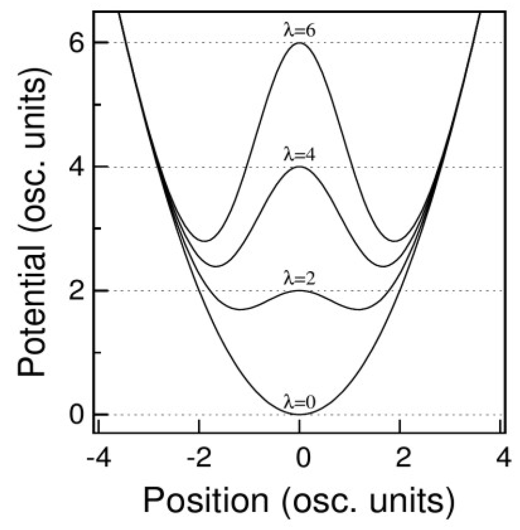
We compare an exact dynamics governed by a full two-body Hamiltonian with the dynamics obtained in a two-mode model approximation.

We show that for sufficiently large interactions the two-mode model breaks down and higher single-particle states have to be taken into account to describe dynamical properties of the system correctly.


## Double-well potential

We consider dynamical properties of two ultra-cold bosons in a double-well potential:

$$V(x) = \hbar\Omega\left[\frac{m\Omega}{2\hbar}x^2 + \lambda\exp\left(-\frac{m\Omega}{2\hbar}x^2\right)\right]$$



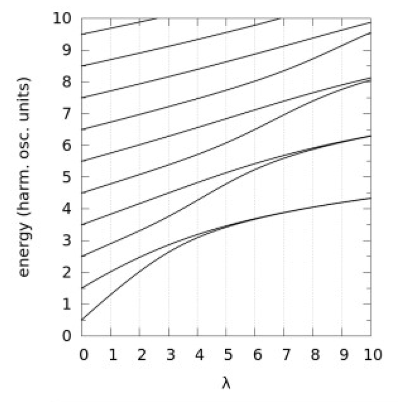

$\lambda$ – dimensionless parameter controlling the height of the potential barrier

## Single-particle basis

Dimensionless Schrödinger equation:

$$\left[-\frac{1}{2}\frac{d^2}{dx^2} + V(x)\right]\varphi_i(x) = \mathcal{E}_i\varphi_i(x)$$

The resulting one-particle eigenenergies $\mathcal{E}_i$, depending on well depth $\lambda$, are shown:

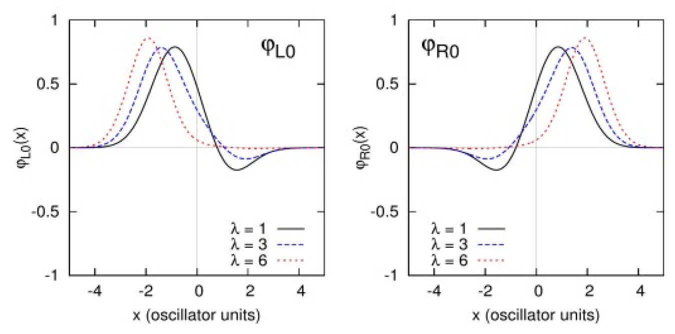



We introduce the „left-right" basis, in which individual wavefunctions have density profiles localized in the left ($L$) or the right ($R$) well:

$$\phi_{Li}(x) = \frac{\varphi_{2i}(x) - \varphi_{2i+1}(x)}{\sqrt{2}}$$

$$\phi_{Ri}(x) = \frac{\varphi_{2i}(x) + \varphi_{2i+1}(x)}{\sqrt{2}}$$

The lowest-energy „left-right" basis wavefunctions are shown below:




## Two-particle Hamiltonian

We assume a short-range pointlike interparticle interaction potential:

$$V_{int} = g\delta(x - x')$$

$x$, $x'$ – boson positions; $g$ – interaction strength

The two-body Hamiltonian can be written in the second-quantized form:

$$\hat{\mathcal{H}} = \int \mathrm{d}x\left[\hat{\Psi}^\dagger(x)H_0\hat{\Psi}(x) + \frac{g}{2}\hat{\Psi}^\dagger(x)\hat{\Psi}^\dagger(x)\hat{\Psi}(x)\hat{\Psi}(x)\right]$$

$\hat{\Psi}(x)$ – field operator annihilating a particle in position $x$. Obeys bosonic commutation relations:

$$\left[\hat{\Psi}(x), \hat{\Psi}^\dagger(x')\right] = \delta(x - x')$$

$$\left[\hat{\Psi}(x), \hat{\Psi}(x')\right] = 0$$

$H_0$ – single-particle Hamiltonian, which has diagonal and off-diagonal elements when expressed in the „left-right" basis:

$$H_0 = \sum_i \mathcal{E}_i|\varphi_i\rangle\langle\varphi_i| = \sum_i E_i(|\phi_{Li}\rangle\langle\phi_{Li}| + |\phi_{Ri}\rangle\langle\phi_{Ri}|) - \sum_i J_i(|\phi_{Ri}\rangle\langle\phi_{Li}| + |\phi_{Li}\rangle\langle\phi_{Ri}|)$$

## Two-boson Hamiltonian in the single-particle basis

We decompose the field operator in the single-particle „left-right" basis: $\hat{\Psi}(x) = \sum_\sigma\sum_i \hat{a}_{\sigma i}\phi_{\sigma i}(x)$ $\quad \sigma \in \{L, R\}$

The resulting form of the Hamiltonian:

$$\hat{\mathcal{H}} = \sum_\sigma\sum_i E_i\hat{a}^\dagger_{\sigma i}\hat{a}_{\sigma i} - \sum_i J_i(\hat{a}^\dagger_{Li}\hat{a}_{Ri} + \hat{a}^\dagger_{Ri}\hat{a}_{Li}) + \frac{1}{2}\sum_{ABCD} U_{ABCD}\hat{a}^\dagger_A\hat{a}^\dagger_B\hat{a}_C\hat{a}_D,$$

where:

$$U_{ABCD} = g\int \mathrm{d}x\,\phi^*_A(x)\phi^*_B(x)\phi_C(x)\phi_D(x) \qquad J_i = \frac{\mathcal{E}_{2i+1} - \mathcal{E}_{2i}}{2}, \qquad E_i = \frac{\mathcal{E}_{2i+1} + \mathcal{E}_{2i}}{2}$$

*A, B, C, D*: special indices that represent index pairs ($\sigma$,$i$). $\sigma$ denotes the well ($L$,$R$); $i$= 0,1,2,… is the excitation index

$E_i$, $J_i$: the diagonal and off-diagonal elements of the single-particle Hamiltonian in the „left-right" basis

$J_i$ are called the tunneling amplitudes

## Two-mode models

Two-mode models resulting from the approximation where only the lowest two states are taken into account in the one-particle basis. This is equivalent to limiting the „left-right" basis to the lowest-energy state for either well: $\hat{\Psi}(x) = \hat{a}_{L0}\phi_{L0}(x) + \hat{a}_{R0}\phi_{R0}(x)$

The two-mode Hamiltonian:

$$\hat{\mathcal{H}}_{\mathtt{2Mode}} = -J(\hat{a}^\dagger_{L0}\hat{a}_{R0} + \hat{a}^\dagger_{R0}\hat{a}_{L0}) + \frac{U}{2}\left(\hat{a}^{\dagger 2}_{L0}\hat{a}^2_{L0} + \hat{a}^{\dagger 2}_{R0}\hat{a}^2_{R0}\right) + V\hat{a}^\dagger_{L0}\hat{a}_{L0}\hat{a}^\dagger_{R0}\hat{a}_{R0} + T\left(\hat{a}^\dagger_{L0}\,\hat{n}_0\,\hat{a}_{R0} + \hat{a}^\dagger_{R0}\,\hat{n}_0\,\hat{a}_{L0}\right) + \frac{V}{4}\left(\hat{a}^{\dagger 2}_{L0}\hat{a}^2_{R0} + \hat{a}^{\dagger 2}_{R0}\hat{a}^2_{L0}\right)$$

$$\hat{n}_{\sigma i} = \hat{a}^\dagger_{\sigma i}\hat{a}_{\sigma i} \qquad \hat{n}_i = \hat{n}_{Li} + \hat{n}_{Ri}$$

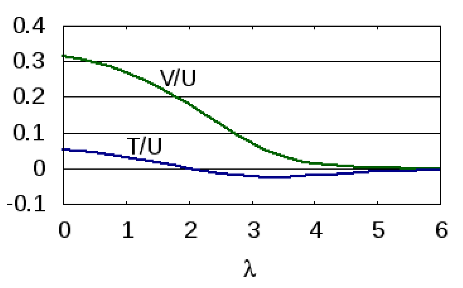
Here J = $J_0$ and the interaction parameters are:

$$U = g\int dx[\phi_{L0}(x)]^4 = g\int dx[\phi_{R0}(x)]^4$$

$$V = 2g\int dx[\phi_{L0}(x)\phi_{R0}(x)]^2$$

$$T = g\int dx\phi_{L0}(x)[\phi_{R0}(x)]^3$$

Further approximation – neglect V and T. This is valid in the deep well limit, as V and T are small compared to U:




Then we get the Bose-Hubbard-like Hamiltonian:

$$\hat{\mathcal{H}}_{\mathrm{R}} = -J(\hat{a}^\dagger_{L0}\hat{a}_{R0} + \hat{a}^\dagger_{R0}\hat{a}_{L0}) + \frac{U}{2}\left(\hat{a}^{\dagger 2}_{L0}\hat{a}^2_{L0} + \hat{a}^{\dagger 2}_{R0}\hat{a}^2_{R0}\right)$$

The dynamics is dependent only on the U/J ratio

## The initial state and its evolution

Initial state: two bosons located in the left well: $|\mathtt{ini}\rangle = \frac{1}{\sqrt{2}}\hat{a}^{\dagger 2}_{L0}|\mathtt{vac}\rangle$

Time evolution of the state is obtained straightforwardly: $|\psi(t)\rangle = \sum_i \alpha_i e^{-i\epsilon_i t}|i\rangle$

where $|i\rangle$ are the eigenstates of the two-particle Hamiltonian, $\epsilon_i$ are their corresponding eigenenergies, and $\alpha_i = \langle i|\mathtt{ini}\rangle$

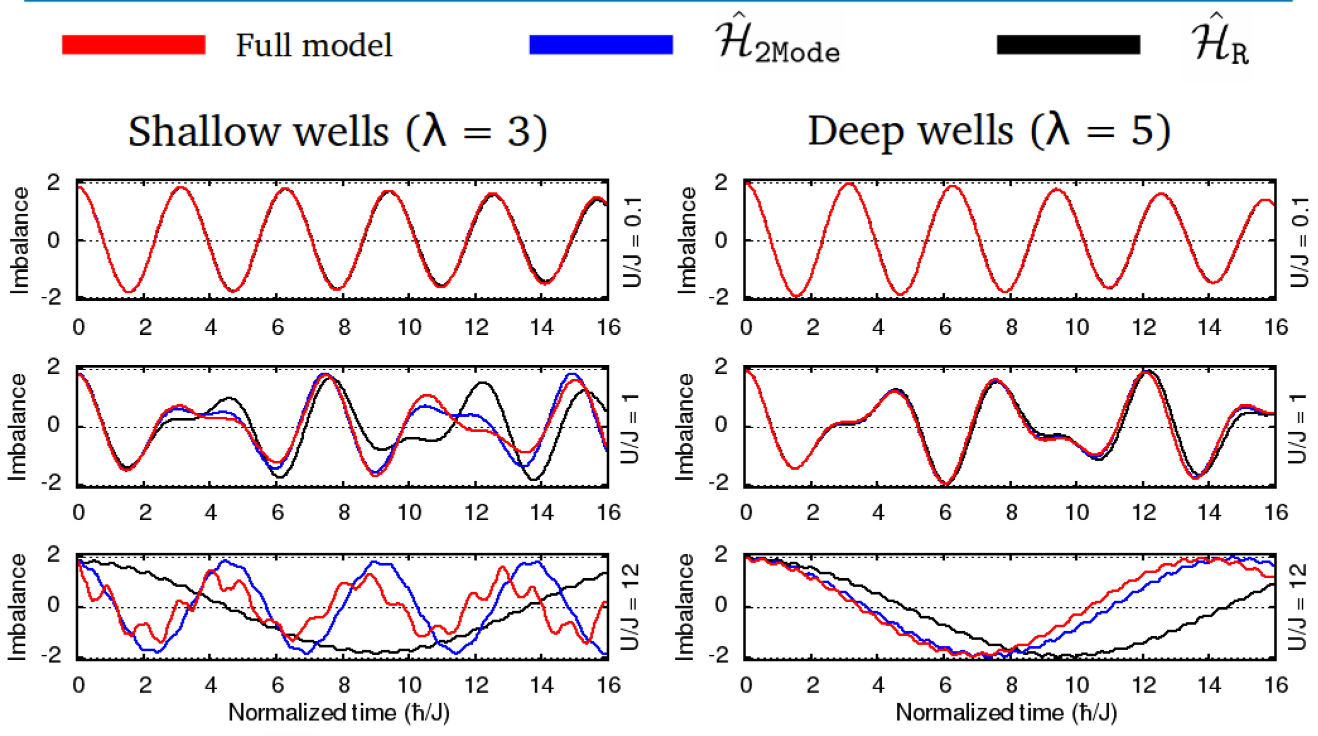
Properties of the state of the system can be characterized through well populations.

Right well population: $\hat{N}_R = \int_0^\infty \mathrm{d}x\,\Psi^\dagger(x)\Psi(x)$

Left well population: $\hat{N}_L = \int_{-\infty}^0 \mathrm{d}x\,\Psi^\dagger(x)\Psi(x)$

Population imbalance: $I(t) = \langle\psi(t)|\hat{N}_L - \hat{N}_R|\psi(t)\rangle$

## Evolution of the population imbalance *I(t)*




The $\hat{\mathcal{H}}_{\mathrm{R}}$ model fails for shallow wells and strong interactions.

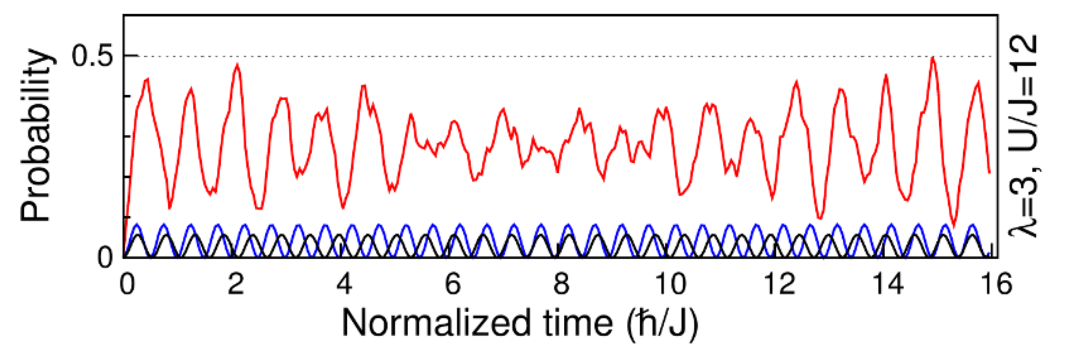
However, the $\hat{\mathcal{H}}_{\mathtt{2Mode}}$ model at first glance seems to reproduce the exact dynamics properly

## The interparticle correlations

The inaccuracy of the two-mode model becomes evident when interparticle correlations are considered.

Evolution of the probability of finding two bosons in opposite wells:

$$\mathcal{P}(t) = \sum_{ij}\langle\psi(t)|\hat{n}_{Lj}\hat{n}_{Ri}|\psi(t)\rangle$$




Two-mode models ignore tunneling via excited states, giving false results.