Effective two-mode description of the dynamics of interacting bosons confined in a double-well trap

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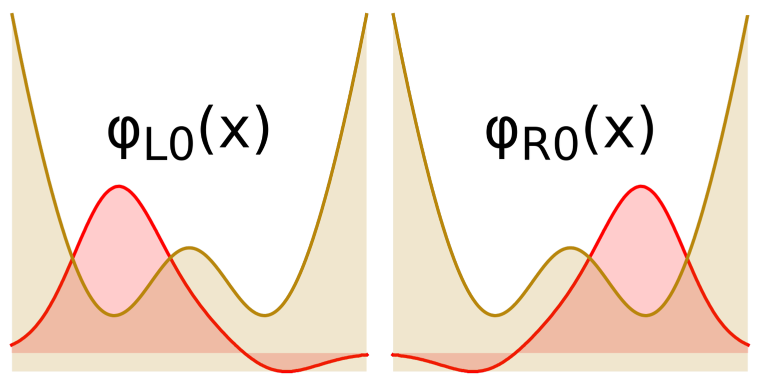
Abstract

The two-mode model is a simple approximation, useful for studying the dynamics of a few bodies in a double potential well. However, the model rapidly becomes inaccurate as the interparticle interaction strength grows. Here we discuss the methods of extending its applicability. We describe two different approaches. In the first method, we describe the system in terms of a specific basis of effective wave functions, uniquely tailored to the problem under study. The basis modes are directly derived from the many-body Hamiltonian. The shapes of the resulting basis wave functions take into account the interaction-induced modifications of the natural orbitals. This effective model gives accurate predictions over a wider range of interactions than the traditional model. The second method involves extending the many-body Hamiltonian with effective three-body interaction terms. These terms effectively account for various corrections that arise from virtual transitions to excited energy states. Two such terms, an on-site three-body interaction and an interaction-induced single-particle tunneling, are sufficient to recover the exact dynamics with excellent accuracy.

The double well

Hamiltonian of the N-boson system:

$$H=\sum_{i=1}^{N}\left[-\frac{1}{2}\frac{\partial^2}{\partial x_i^2}+V(x_i)+g\sum_{j=i+1}^{N}\delta(x_i-x_j)\right]$$



L/R basis: A convenient single-particle basis, with states localized in the left/right well: $\varphi_{Li}(x)$, $\varphi_{Ri}(x)$ (i = excitation index)

Hamiltonian in the 2nd quantized form:

$$\hat{\mathcal{H}}=\sum_{\sigma}^{\{L,R\}}\sum_i E_i\hat{a}^\dagger_{\sigma i}\hat{a}_{\sigma i}-\sum_i J_i(\hat{a}^\dagger_{Li}\hat{a}_{Ri}+\hat{a}^\dagger_{Ri}\hat{a}_{Li})+\frac{1}{2}\sum_{IJKL}U_{IJKL}\hat{a}^\dagger_I\hat{a}^\dagger_J\hat{a}_K\hat{a}_L$$

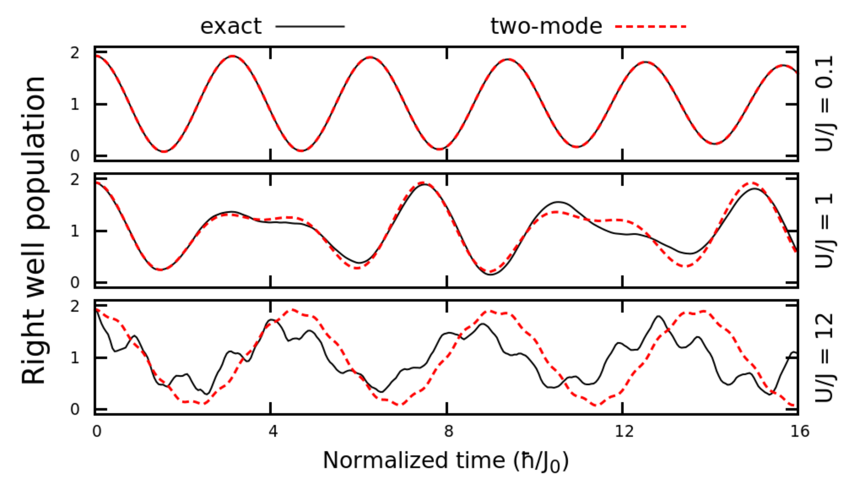
Interaction terms U_{IJKL} ~ interaction strength g

Two-mode approximation: The single-particle basis is cut down to the two lowest L/R states, i.e. φ_{L0}, φ_{R0}

The resulting two-mode Hamiltonian:

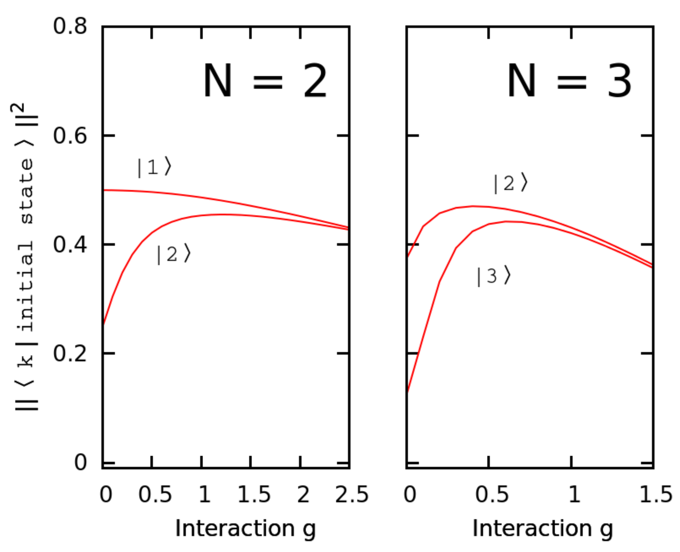
$$\hat{\mathcal{H}}_{\text{2Mode}}=-J(\hat{a}^\dagger_{L0}\hat{a}_{R0}+\hat{a}^\dagger_{R0}\hat{a}_{L0})+\frac{U}{2}(\hat{a}^{\dagger 2}_{L0}\hat{a}^2_{L0}+\hat{a}^{\dagger 2}_{R0}\hat{a}^2_{R0})+V\hat{a}^\dagger_{L0}\hat{a}_{L0}\hat{a}^\dagger_{R0}\hat{a}_{R0}+\sum_{\sigma}^{\{L,R\}}T(\hat{a}^\dagger_{L0}\hat{a}^\dagger_{\sigma 0}\hat{a}_{\sigma 0}\hat{a}_{R0}+\hat{a}^\dagger_{R0}\hat{a}^\dagger_{\sigma 0}\hat{a}_{\sigma 0}\hat{a}_{L0})+\frac{V}{4}(\hat{a}^{\dagger 2}_{L0}\hat{a}^2_{R0}+\hat{a}^{\dagger 2}_{R0}\hat{a}^2_{L0})$$

Limitations of the model: The underlying assumption is that the interaction energy is insufficient to bridge the gap between ground and excited states; thus the two-mode model fails for strong interactions



The effective-mode approach

Motivation: For *N* bosons initially localized in one well, within a certain range of *g* the initial state is dominated by at most two Hamiltonian eigenstates (|N> and |N-1>); recreating them suffices to approximately recover the time-evolved state



$$\rho^{(k)}(x,x')=\frac{1}{N}\langle k|\hat{\Psi}^\dagger(x)\hat{\Psi}(x')|k\rangle$$

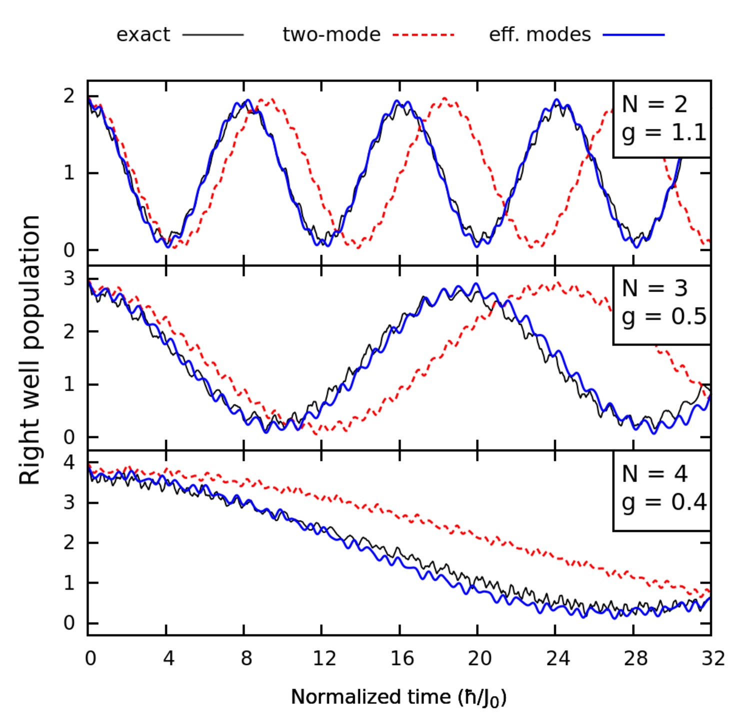
$$\rho^{(N)}(x,x')\approx\psi_0^*(x)\psi_0(x')$$

Finding effective modes: We calculate the one-body reduced density matrices for the individual eigenstates |N>, |N-1>.

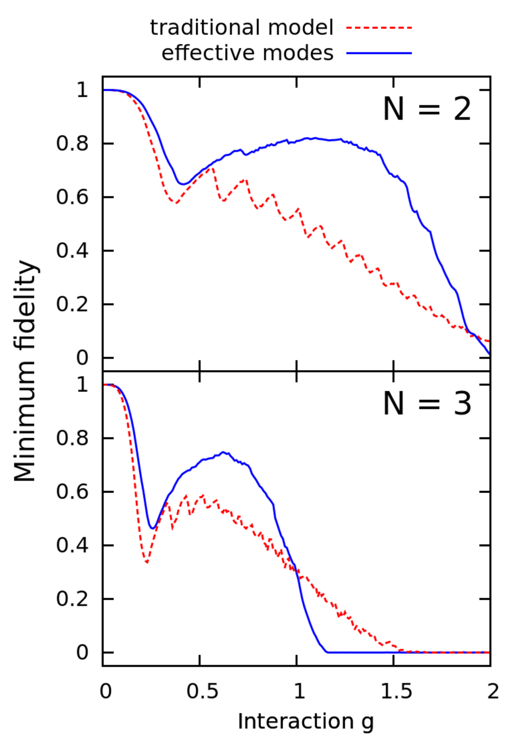
Analyzing their spectra, we find that one or two single-particle states suffice to closely recover |N> and |N-1>. From these we can derive our new basis states, $\phi_A(x)$, $\phi_B(x)$

$$\phi_A(x)=\psi_0(x)=\sum_i[\lambda_{Li}\varphi_{Li}(x)+\lambda_{Ri}\varphi_{Ri}(x)]$$

$$\phi_B(x)=\sum_i(-1)^i[\lambda_{Ri}\varphi_{Li}(x)-\lambda_{Li}\varphi_{Ri}(x)]$$



Results compared to the traditional model



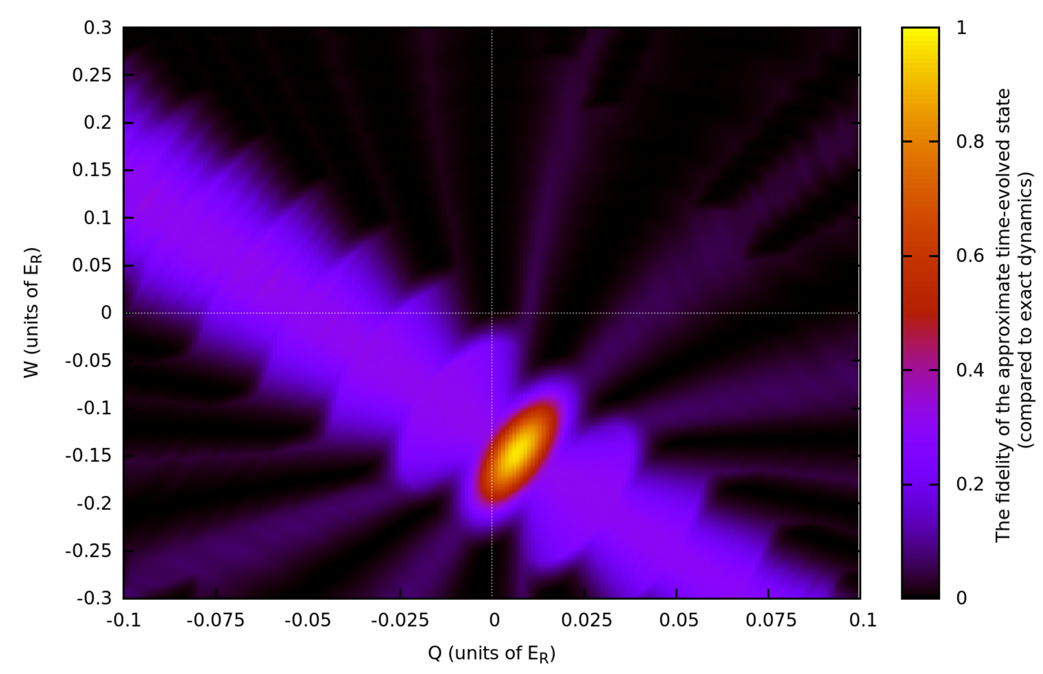
The effective interactions approach

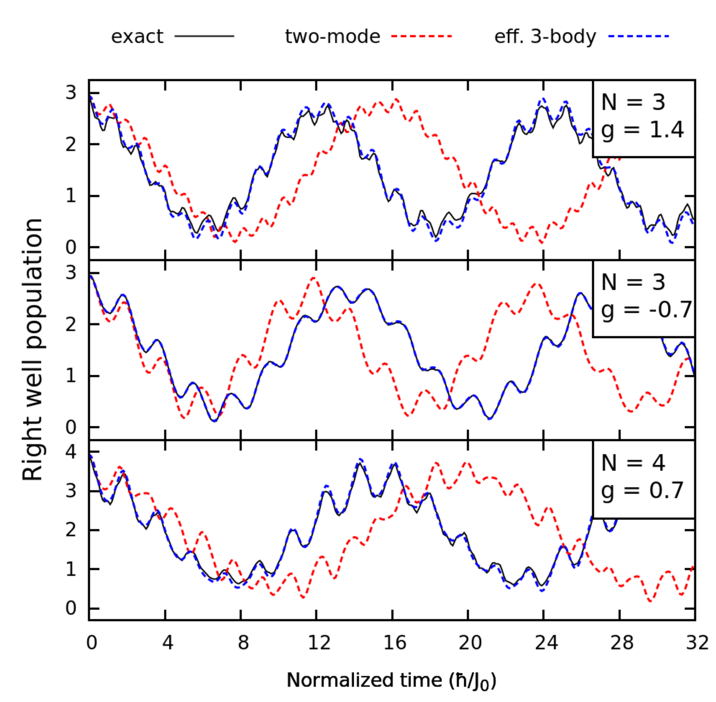
Motivation: The effect of higher modes can be taken into account via effective corrections to Hamiltonian terms. When the number of particles is larger than 2, it turns out that three-body interaction terms can effectively encompass all the required corrections

The effective Hamiltonian:

$$\hat{\mathcal{H}}_{\text{Eff}}=\hat{\mathcal{H}}_{\text{2Mode}}+\frac{W}{6}[\hat{n}_{L0}(\hat{n}_{L0}-1)(\hat{n}_{L0}-2)+\hat{n}_{R0}(\hat{n}_{R0}-1)(\hat{n}_{R0}-2)]+\frac{Q}{2}[(\hat{a}^{\dagger 3}_{L0}\hat{a}^2_{L0}\hat{a}_{R0}+\hat{a}^{\dagger 3}_{R0}\hat{a}^2_{R0}\hat{a}_{L0})+h.c.]$$

Identifying the optimal values of W,Q: Shown here is the accuracy of the approximate model (fidelity of the state) for different values of W and Q





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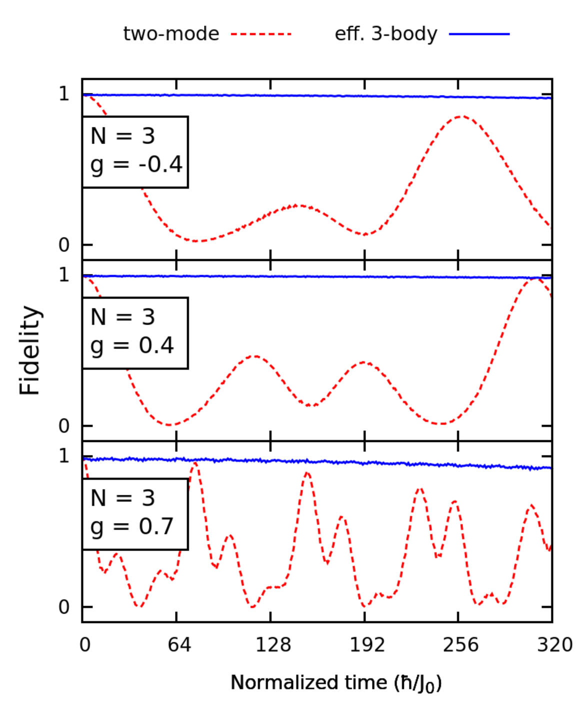

Summary

- We improve the standard two-mode model for describing double-well dynamics, while staying within a two-mode framework.
- The proposed methods include:
  - finding improved basis modes, tailored to the system in question;
  - extending the Hamiltonian with effective three-body interactions.

More details:

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