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Effective two-mode description of a few ultra-cold bosons in a double-well potential

Jacek Dobrzyniecki *, Tomasz Sowiński

Institute of Physics, Polish Academy of Sciences, Aleja Lotnikow 32/46, PL-02668 Warsaw, Poland

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ABSTRACT

We present a construction of an improved two-mode model for modeling the dynamics of interacting ultra-cold bosons confined in a one-dimensional double well trap. Unlike in the typically used two-mode model based on the lowest single-particle eigenstates of the external potential, the improved model uses a basis of properly chosen effective wave functions originating in the many-body model. Accuracy of the improved model is examined and it is shown that within a certain limit of inter-particle interaction strength, the model recovers an exact evolution of the wells' populations much more closely than the traditional two-mode model.

1. Introduction

Dynamical properties of ultra-cold gases have been enjoying increasing interest since the experimental achievement of the Bose–Einstein condensation in 1995 [1,2]. Modern experimental methods, including advanced trapping techniques and controlling of mutual interactions, enable experimental investigation of many problems which would previously be considered on a theoretical level only. This opens a whole new research field of strongly correlated systems with potential applications in such fields as quantum computing or quantum simulating of condensed matter problems [3–6]. One example of a widely studied problem in the field is the system of a few particles confined in a double-well potential [7–17]. Such systems have been realized experimentally, and used to study the physics of bosonic condensates with a great effect [18–23].

On a theoretical level, the dynamics of bosons in a double-well system is usually studied in a framework of a simplified two-mode model. The model relies on the assumption that all particles occupying a particular well can be described with a single orbital. Thus, the single-particle basis is limited to two modes, chosen as the lowest-energy wave functions localized in the left and the right well, respectively. They are constructed from the ground and the first excited eigenstate of the single-particle Hamiltonian. In consequence, the dynamics of the bosonic system can be calculated almost straightforwardly [24–28]. Although the model is commonly used, its applicability is essentially limited. The fundamental assumption hidden in this approximation is that the on-site interaction energy is much smaller than the excitation energy needed to reach higher energy levels. It means that the model becomes increasingly inadequate when the interaction strength increases. Additionally, the model completely neglects local inter-particle correlations. In a strong-interaction regime, local multi-particle correlations arise in each well and so the particles in a single site can no longer be adequately described [29–32].

For intermediate interactions, some improvement of the two-mode approach can be conceived. In the traditional approach, the shapes of the single-particle wave functions are entirely independent of the interaction strength. By taking into account an influence of inter-particle interactions on the shape of single-particle wave functions, the two-mode description can be improved. Techniques of obtaining improved orbitals through variational and mean-field methods have been studied assuming time-independent [33,34] as well as time-dependent [35–37] orbital wave functions.

In this paper we investigate a different, much simpler method, of obtaining an effective time-independent two-mode basis. In our approach the shapes of the basis wave functions emerge naturally after diagonalization of the single-particle density matrix of properly chosen eigenstates of the many-body Hamiltonian. We describe a construction of such an effective basis for a system of two, three, and four interacting bosons in a one-dimensional double-well potential. Then, we examine an accuracy of the resulting two-mode model by comparing its predictions with those obtained by both the exact model and the traditional two-mode model. It is shown that the effective model indeed allows one to

* Corresponding author.
E-mail address: dobrzyniecki@ifpan.edu.pl (J. Dobrzyniecki).

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extend validity of two-mode approximations to higher interaction strengths.

2. The system under study

We consider a system of N spinless bosons of mass m, confined in a one-dimensional double-well potential $V(x)$ and interacting via short-range interactions. We concentrate on systems of $N = 2$, $N = 3$, and $N = 4$ particles, but generalization to larger Ns, besides numerical complexity, is straightforward. The short-range inter-particle interaction is approximated with a point-like potential $g\delta(x - x')$, where the parameter g, related to the s-wave scattering length, controls the interaction strength [38]. Note that in the one-dimensional case the Dirac δ function is a well-defined self-adjoint Hermitian operator and therefore it does not require any regularization [39]. We focus on repulsive interactions, $g > 0$. Experimentally, a quasi-one-dimensional geometry can be realized by introducing a strong harmonic confinement in two remaining spatial directions. In this way the dynamics in these directions is frozen and particles occupy single ground-states. Consequently, the system becomes effectively one-dimensional.

The many-body Hamiltonian of the system, expressed in the second quantization formalism, has the form:

$$\hat{\mathcal{H}} = \int \mathrm{d}x\, \hat{\Psi}^\dagger(x)\mathcal{H}_0\hat{\Psi}(x) + \frac{g}{2}\int \mathrm{d}x\, \hat{\Psi}^\dagger(x)\hat{\Psi}^\dagger(x)\hat{\Psi}(x)\hat{\Psi}(x). \tag{1}$$

Here $\hat{\Psi}(x)$ is a bosonic field operator that annihilates a particle at position x. The operator fulfills the bosonic commutation relations, $\left[\hat{\Psi}(x), \hat{\Psi}^\dagger(x')\right] = \delta(x-x')$ and $\left[\hat{\Psi}(x), \hat{\Psi}(x')\right] = 0$. The single-particle part of the Hamiltonian has a form

$$\mathcal{H}_0 = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x). \tag{2}$$

We model an external double-well potential $V(x)$ as a combination of a harmonic oscillator potential with frequency Ω, and a Gaussian barrier which separates the central region into two wells:

$$V(x) = \hbar\Omega\left[\frac{m\Omega}{2\hbar}x^2 + \lambda\exp\left(-\frac{m\Omega}{2\hbar}x^2\right)\right]. \tag{3}$$

The height of the barrier is directly related to the dimensionless parameter λ. In further discussion, we use natural harmonic oscillator units, *i.e.*, energy is measured in $\hbar\Omega$ and length in $\sqrt{\hbar/m\Omega}$.

The spectrum of $\mathcal{H}_0$ can be found numerically via an exact diagonalization on a dense grid in position representation, giving a set of eigenfunctions $\Phi_i(x)$ and their corresponding eigenenergies $\mathcal{E}_i$ [30]. Following the harmonic oscillator convention, we number the individual states beginning from $i = 0$. For $\lambda = 0$, obviously the well-known harmonic oscillator spectrum is recovered.

In the analysis of double-well problems, it is usual to adopt a basis of single-particle wave functions $\{\varphi_{Li}(x), \varphi_{Ri}(x)\}$, where the individual states are localized respectively in the left or the right well. These states are constructed as combinations of the odd and even eigenstates of the Hamiltonian:

$$\begin{aligned}\varphi_{Ri}(x) &= \frac{1}{\sqrt{2}}(\Phi_{2i}(x) + \Phi_{2i+1}(x)),\\ \varphi_{Li}(x) &= \frac{1}{\sqrt{2}}(\Phi_{2i}(x) - \Phi_{2i+1}(x)).\end{aligned} \tag{4}$$

Although states $\{\varphi_{\sigma i}(x)\}$ are not eigenstates of the single-particle Hamiltonian $\mathcal{H}_0$, they form an orthonormal basis. In this basis the Hamiltonian $\mathcal{H}_0$ has both, diagonal (average energies) and off-diagonal (tunnelings) elements:

$$\int \varphi^*_{\sigma i}(x)\mathcal{H}_0\varphi_{\sigma' j}(x)\mathrm{d}x = \delta_{ij}\left[\delta_{\sigma\sigma'}E_i - (1-\delta_{\sigma\sigma'})J_i\right], \tag{5}$$

where

$$E_i = \frac{\mathcal{E}_{2i+1} + \mathcal{E}_{2i}}{2},\ J_i = \frac{\mathcal{E}_{2i+1} - \mathcal{E}_{2i}}{2}. \tag{6}$$

The field operator $\hat{\Psi}(x)$ can be decomposed as

$$\hat{\Psi}(x) = \sum_i \left[\varphi_{Li}(x)\hat{a}_{Li} + \varphi_{Ri}(x)\hat{a}_{Ri}\right], \tag{7}$$

where $\hat{a}_{\sigma i}$ annihilates a boson in state $\varphi_{\sigma i}(x)$. For numerical purposes the summation index i in the decomposition (7) is limited to some cutoff number i_{max}. In the case of the system under study, we have verified that $i_{max} = 15$ is sufficient, as the final results do not change significantly for larger i_{max}. Therefore in further discussion, we will treat the Hamiltonian with $i_{max} = 15$ as equivalent to the full many-body Hamiltonian (1). By substituting (7) into (1), the Hamiltonian can be written as:

$$\begin{aligned}\hat{\mathcal{H}} = &\sum_i \left[E_i(\hat{a}^\dagger_{Li}\hat{a}_{Li} + \hat{a}^\dagger_{Ri}\hat{a}_{Ri}) - J_i(\hat{a}^\dagger_{Li}\hat{a}_{Ri} + \hat{a}^\dagger_{Ri}\hat{a}_{Li})\right]\\ &+ \frac{1}{2}\sum_{IJKL} U_{IJKL}\hat{a}^\dagger_I\hat{a}^\dagger_J\hat{a}_K\hat{a}_L,\end{aligned} \tag{8}$$

where the indices I, J, K, L represent double-indices (σ, i) identifying single-particle states $\varphi_{\sigma i}(x)$. The interaction terms U_{IJKL} can be calculated as:

$$U_{IJKL} = g\int_{-\infty}^{\infty} \varphi^*_I(x)\varphi^*_J(x)\varphi_K(x)\varphi_L(x)\mathrm{d}x. \tag{9}$$

The spectrum of the Hamiltonian (8) can be calculated numerically. To do so, we express the Hamiltonian in a matrix form in the N-particle Fock basis and diagonalize it. Then all properties of the system at any moment can be determined.

Here, our aim is to predict the time evolution of the interacting system of bosons being initially located in the lowest single-particle state of the chosen well. Namely we assume that initially the many-body state of the system is

$$|\mathtt{ini}\rangle = \frac{1}{\sqrt{N}}\left(\hat{a}^\dagger_{R0}\right)^N|\mathtt{vac}\rangle. \tag{10}$$

It means that the state of the system at any later moment t can then be calculated straightforwardly as

$$|\mathbf{\Psi}(t)\rangle = \sum_k \exp\left(\frac{-i\epsilon_k t}{\hbar}\right)\langle \mathtt{k}|\mathtt{ini}\rangle|\mathtt{k}\rangle, \tag{11}$$

where $|\mathtt{k}\rangle$ and ϵ_k are the eigenstates and their corresponding eigenenergies of (8), respectively. It is important to note that $|\mathtt{k}\rangle$ and ϵ_k depend directly on interaction strength g. However, to simplify the notation we do not write out this dependence explicitly.

3. Two-mode approximation

A two-mode model is a natural approximation of any double-well system. Routinely, it involves choosing $i_{max} = 0$ in the decomposition (7), i.e., the single-particle state basis is limited to the two lowest energy states, $\varphi_{L0}(x)$ and $\varphi_{R0}(x)$. Then the field operator $\hat{\Psi}(x)$ can be approximated by

$$\hat{\Psi}(x) \approx \varphi_{L0}(x)\hat{a}_{L0} + \varphi_{R0}(x)\hat{a}_{R0}. \tag{12}$$

By substituting (12) into the Hamiltonian (1), the two-mode many-body Hamiltonian is obtained, and similarly to the full-mode