Quantum dynamics of attractive versus repulsive bosonic Josephson junctions: Bose-Hubbard and full-Hamiltonian results

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Abstract

The quantum dynamics of one-dimensional bosonic Josephson junctions with attractive and repulsive interparticle interactions is studied using the Bose-Hubbard model and by numerically-exact computations of the full many-body Hamiltonian. A symmetry present in the Bose-Hubbard Hamiltonian dictates an equivalence between the evolution in time of attractive and repulsive Josephson junctions with attractive and repulsive interactions of equal magnitude. The full many-body Hamiltonian does not possess this symmetry and consequently the dynamics of the attractive and repulsive junctions are different.

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Quantum dynamics of interacting Bose-Einstein condensates is an active and lively research field [1, 2, 3]. Here, one of the basic problems studied is the dynamics of tunneling of interacting Bose-Einstein condensates in double-wells, which in this context are referred to as bosonic Josephson junctions. The dynamics of bosonic Josephson junctions has drawn much attention both theoretically and experimentally, see, e.g., Refs. [4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18] and references therein.

In this work we would like to compare the dynamics of one-dimensional bosonic Josephson junctions with attractive and repulsive interparticle interactions. Explicitly, we will compare systems where the magnitude of attractive and repulsive interactions is alike. We prepare the interacting bosons in one well, and then monitor the evolution of the systems in time. We compute and analyze the respective dynamics both within the two-site Bose-Hubbard model often employed for this problem as well as within the full Hamiltonian of the systems. The main result of this work, shown both analytically and numerically, is that within the Bose-Hubbard model the dynamics of the attractive and repulsive junctions is equivalent. In contrast, the dynamics of attractive and repulsive junctions computed from the full many-body Hamiltonian are different from one another. As a complementary result we provide here for the first time in literature numerically-exact quantum dynamics of an attractive Josephson junction, thus matching our recent calculations on repulsive Josephson junctions [18].

We begin with the two-site Bose-Hubbard Hamiltonian:

\[
\hat{H}(U) = -J \left( \hat{b}_L^\dagger \hat{b}_R + \hat{b}_R^\dagger \hat{b}_L \right) + \frac{U}{2} \left( \hat{b}_L^\dagger \hat{b}_L \hat{b}_R^\dagger \hat{b}_R + \hat{b}_R^\dagger \hat{b}_R \hat{b}_L^\dagger \hat{b}_L \right). \tag{1}
\]

Here and hereafter all quantities are dimensionless. We remind the reader that the Bose-Hubbard Hamiltonian (1) is derived from the full many-body Hamiltonian \( \hat{H} = \int dx \hat{\Psi}^\dagger(x) h(x) \hat{\Psi}(x) + \frac{\lambda_0}{2} \int dx \hat{\Psi}^\dagger(x) \hat{\Psi}^\dagger(x) \hat{\Psi}(x) \hat{\Psi}(x) \), where \( h(x) \) is the one-body Hamiltonian and \( \lambda_0 \) the interparticle interaction strength. Explicitly, by restricting the field operator to a sum of two terms \( \hat{\Psi}(x) = \hat{b}_L \phi_L(x) + \hat{b}_R \phi_R(x) \), where \( \phi_L(x) \) and \( \phi_R(x) \) are the left- and right-localized Wannier functions, substituting into the many-body Hamiltonian \( \hat{H} \), neglecting the off-diagonal interaction terms and eliminating the diagonal one-body terms, one arrives at the Bose-Hubbard Hamiltonian (1). The one-body Hamiltonian reads \( h(x) = \frac{1}{2} \frac{\partial^2}{\partial x^2} + V(x) \), where \( V(x) \) is a symmetric double-well potential. The left- and right-localized Wannier functions are obtained as linear combinations of the ground (gerade) and
first-exited (ungerade) states of \( h(x) \), i.e., \( \phi_L(x) = \frac{\phi_u(x)+\phi_d(x)}{\sqrt{2}} \) and \( \phi_R(x) = \frac{\phi_u(x)-\phi_d(x)}{\sqrt{2}} \), and are real-valued functions. The Bose-Hubbard parameters are given by \( U = \lambda_0 \int_{-\infty}^{\infty} dx \phi^4_L(x) \) and \( J = -\int_{-\infty}^{\infty} dx \phi_L(x) h(x) \phi_R(x) \).

There is an interesting symmetry connecting the Bose-Hubbard Hamiltonian (1) with repulsive \( \hat{H}(U) \) and attractive \( \hat{H}(-U) \) interactions of equal magnitude [19, 20]. Explicitly, defining the unitary operator (transformation)

\[
\hat{R} = \{ \hat{b}_L \rightarrow \hat{b}_L, \hat{b}_R \rightarrow -\hat{b}_R \},
\]

(2)

it is simple to see that [19, 20]

\[
\hat{R} \hat{H}(U) \hat{R} = -\hat{H}(-U).
\]

(3)

What is the impact of the symmetry (2) and the resulting relation (3) on the evolution in time of attractive and repulsive bosonic Josephson junctions?

We consider a system of \( N \) bosons initially prepared as mentioned above in, say, the left well, \( |N,0\rangle = \frac{1}{\sqrt{N!}} \hat{b}^\dagger_L N |vac\rangle \). Its evolution in time is simply given by \( e^{-i\hat{H}(U)t} |N,0\rangle \).

Then, the “survival probability” of finding the bosons in the left well as a function of time is defined as \( p_L(t;U) = \frac{1}{N} \int_{-\infty}^{0} dx \left\langle N,0 \big| e^{+i\hat{H}(U)t} \left[ \hat{\Psi}^\dagger(x) \hat{\Psi}(x) \right] e^{-i\hat{H}(U)t} \big| N,0 \right\rangle \), where the expression \( \left\langle \ldots \right\rangle \) is the system’s density. Plugging into the “survival probability” the expansion of the field operator and after some algebra the final result reads:

\[
p_L(t;U) = \left( 1 - \int_{-\infty}^{0} dx \phi^2_L(x) \right) - \left( 1 - 2 \int_{-\infty}^{0} dx \phi^2_L(x) \right) \cdot \frac{1}{N} \times \left\{ \left\langle N,0 \big| \cos[\hat{H}(U)t] \hat{b}^\dagger_L \hat{b}_L \cos[\hat{H}(U)t] + \sin[\hat{H}(U)t] \hat{b}^\dagger_L \hat{b}_L \sin[\hat{H}(U)t] \big| N,0 \right\rangle \right\} .
\]

(4)

In obtaining the r.h.s. of (4) we made use of the facts that the expectation value of \( \hat{b}^\dagger_L \hat{b}_L \) (hermitian operator) is real, and that \( \int_{-\infty}^{0} dx \phi_L(x) \phi_R(x) = 0 \).

Employing the \( \hat{R} \) symmetry (2) to the \( p_L(t;U) \) matrix element (4) and making use of relation (3), one immediately finds that

\[
p_L(t;-U) = p_L(t;U),
\]

(5)

which concludes our first proof. In other words, the “survival probability” of bosons is identical for attractive and repulsive interactions (of equal magnitude) within the Bose-Hubbard model. We emphasize that the result (5) holds at all times \( t \).
Next, we discuss the impact of the symmetry (2) on the eigenvalues of the reduced one-body density matrix within the two-site Bose-Hubbard model. The eigenvalues of the reduced one-body density matrix of a Bose system determine the extent to which the system is condensed or fragmented [21, 22]. For the two-site Bose-Hubbard problem the reduced one-body density matrix can be written as a two-by-two matrix:

\[
\rho^{(1)}(t; U) = \begin{pmatrix} \rho_{LL}(t; U) & \rho_{LR}(t; U) \\ \rho_{LR}^*(t; U) & \rho_{RR}(t; U) \end{pmatrix},
\]

where \(\rho_{LL}(t; U) = \langle N, 0 | e^{+i\hat{H}(U)t} \hat{b}_L^\dagger \hat{b}_L e^{-i\hat{H}(U)t} | N, 0 \rangle\), and \(\rho_{LR}(t; U)\) and \(\rho_{RR}(t; U)\) are given analogously. Plugging the symmetry (2) into each of the matrix elements of \(\rho^{(1)}(t; U)\) and making use of relation (3), one can straightforwardly express the reduced one-body density matrix for attractive interaction as follows:

\[
\rho^{(1)}(t; -U) = \begin{pmatrix} \rho_{LL}(t; U) & -\rho_{LR}(t; U) \\ -\rho_{LR}^*(t; U) & \rho_{RR}(t; U) \end{pmatrix}.
\]

Obviously, the matrices (6) and (7) have the same characteristic equation, and hence the same eigenvalues. We have thus shown that, within the Bose-Hubbard model, the eigenvalues of the reduced one-body density matrix do not depend on the sign of interparticle interaction, which constitutes our second proof. Again, this result holds for any time \(t\). In particular, the Bose-Hubbard model attributes identical condensation and fragmentation levels to attractive and repulsive systems.

To illustrate the above findings we plot in Figs. 1 and 2 the “survival probability” and occupation numbers, respectively, as a function of time for a repulsive and attractive Bose-Hubbard dynamics with the ratio of parameters \(|U|/J| = 0.226\). These parameters draw from a double-well potential \(V(x)\) formed by connecting two harmonic potentials \(V_{\pm}(x) = \frac{1}{2}(x \pm 2)^2\) with a cubic spline in the region \(|x| \leq 0.5\), and for \(|\lambda_0| = 0.0129\). The number of bosons is \(N = 20\). The Rabi oscillation period is \(t_{Rabi} = \pi/J = 140.66\). As expected, based on Eq. (5) and Eqs. (6,7), the Bose-Hubbard dynamics for attractive and repulsive junctions are identical.

We now move on to the dynamics computed with the full many-body Hamiltonian \(\hat{H}\). Recently, we have reported on the numerically-exact solution of a one-dimensional repulsive bosonic Josephson junction, which has allowed us to unveil novel phenomena associated with the quick loss of the junction’s coherence [18]. We use here the same method to
compute the time evolution of the system with the full many-body Hamiltonian $\hat{H}$. We solve the time-dependent many-boson Schrödinger equation by using the multiconfigurational time-dependent Hartree for bosons (MCTDHB) method [23] (also see [24, 25]), in which a novel mapping of the many-boson configuration space in combination with a parallel implementation of MCTDHB are exploited [26]. This allows us to report, among others, on the first numerically-exact results in literature of a bosonic Josephson junction for attractive interaction, thus matching our recent calculations on repulsive bosonic Josephson junctions [18]. The results of the computations with the full many-body Hamiltonian are collected in Figs. 1 and 2. It is clearly seen that the dynamics of the attractive and repulsive junctions are distinct from each other, and that each is different from the Bose-Hubbard dynamics.

Let us analyze these findings. We first note, in the context of the above analytical results on the Bose-Hubbard dynamics, that the full Hamiltonian $\hat{H}$ does not possesses the symmetry (2) connecting the dynamics of attractive and repulsive systems. This is because $\hat{H}$ contains off-diagonal interaction terms as well as all other terms neglected in the Bose-Hubbard Hamiltonian (1). From this “mathematical” discussion alone, we do not expect the dynamics of attractive and repulsive junctions to be equivalent as found above for the Bose-Hubbard dynamics. What do we expect on physical grounds? Intuitively, we know that attractive bosons like to be together, whereas repulsive bosons lean to separate from one another. These tendencies are exactly what we see in Fig. 1. The full-Hamiltonian’s “survival probability” is larger (smaller) for attractive (repulsive) interaction than the Bose-Hubbard “survival probability”, at least up to $t/t_{\text{Rabi}} = 1.5$. In other words, the Bose-Hubbard “survival probability” underestimates the “survival probability” for attractive and overestimates it for repulsive interaction for short and intermediate times. For longer times, as seen in Fig. 1 the dynamics becomes more complex and anticipating the differences between the exact and the Bose-Hubbard dynamics cannot rest on the above-mentioned physical intuition alone. Finally, Fig. 2 presents a complementary picture of the dynamics of occupation numbers. It has been shown in [18] that the Bose-Hubbard dynamics underestimates fragmentation and overestimates coherence of repulsive bosonic Josephson junctions. We may analogously anticipate that the reverse happens with attractive interactions, which indeed is the physical picture unveiled in Fig. 2.

Let us conclude. We have shown, both analytically and numerically, that a symmetry present in the two-site Bose-Hubbard Hamiltonian dictates an equivalence between the evo-
olution in time of attractive and repulsive bosonic Josephson junctions. The full many-body Hamiltonian does not possess this symmetry and consequently the dynamics of the attractive and repulsive junctions are distinct. The Bose-Hubbard dynamics underestimates the “survival probability” and overestimates fragmentation of attractive one-dimensional bosonic Josephson junctions and the reverse is true for repulsive junctions. Note that the parameters used here are within the range of expected validity of the Bose-Hubbard model for Josephson junctions \[4\]. The clear deviations from the numerically-exact results show that criteria for the validity of the Bose-Hubbard model which have been derived for static junctions cannot be transferred for dynamically evolving junctions (also see \[18\]). The present investigation of attractive versus repulsive junctions sheds additional light on the restrictions of the Bose-Hubbard model to describe dynamics.

As an outlook, we mention that an analogous symmetry to (2) can be found for the multi-site Bose-Hubbard model. Consider the multi-site one-dimensional Bose-Hubbard model: 

$$\hat{H}_{BH}(U) = -J \sum_j \hat{b}_j \hat{b}_{j+1} + \frac{U}{2} \sum_j \hat{b}_j \hat{b}_j \hat{b}_j \hat{b}_j.$$ 

Then, 

$$\hat{R}_{BH} \hat{H}_{BH}(U) \hat{R}_{BH} = -\hat{H}_{BH}(-U)$$ 

where  

$$\hat{R}_{BH} = \{ \hat{b}_{2j} \rightarrow \hat{b}_{2j}, \hat{b}_{2j-1} \rightarrow -\hat{b}_{2j-1} \}.$$ 

The extension to the Bose-Hubbard model of orthorhombic lattices in higher dimensions is straightforward. It would be interesting to search for the consequences of this symmetry in the dynamics of attractive and repulsive bosons in a lattice.

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FIG. 1: (Color online) Bose-Hubbard versus full-Hamiltonian, numerically-exact dynamics of attractive and repulsive Josephson junctions. Shown is the “survival probability” as a function of time, $p_L(t)$, computed with the full many-body Hamiltonian for attractive [solid gray (green) line] and repulsive [solid black (blue) line] interaction. The Bose-Hubbard result [dashed (magenta) line] is for both attractive and repulsive interactions. The parameters used are $N = 20$, $|U| = 0.226$, $|\lambda_0| = 0.0129$, and $t_{Rabi} = 140.66$. The inset shows the ratio $p_L^(-)/p_L^+$ of attractive to repulsive “survival probabilities” as a function of time. The black–solid line is the full-Hamiltonian results which exhibit a complex dynamics, whereas the dashed–magenta line is the Bose-Hubbard result, showing no dynamics at all. All quantities are dimensionless.
FIG. 2: (Color online) Bose-Hubbard versus full-Hamiltonian, numerically-exact dynamics of attractive and repulsive Josephson junctions. Shown are the occupation numbers of the reduced one-body density matrix as a function of time, $n^{(1)}_i(t)$, computed with the full many-body Hamiltonian for attractive [solid gray (green) line] and repulsive [solid black (blue) line] interaction. The Bose-Hubbard result [dashed (magenta) line] is for both attractive and repulsive interactions. The two-site Bose-Hubbard dynamics has two occupation numbers only. The full-Hamiltonian dynamics has many occupation numbers. It is seen that the occupation numbers $n^{(1)}_{i>2}(t)$ are essentially zero. The parameters used are the same as in Fig. 1. All quantities are dimensionless.