Quantum Dynamics of Atom-molecule BECs in a Double-Well Potential

A. Motohashi · T. Nikuni

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Abstract We investigate the dynamics of two-component Bose-Josephson junction composed of atom-molecule BECs. Within the semiclassical approximation, the multi-degree of freedom of this system permits chaotic dynamics, which does not occur in single-component Bose-Josephson junctions. By investigating the level statistics of the energy spectra using the exact diagonalization method, we evaluate whether the dynamics of the system is periodic or non-periodic within the semiclassical approximation. Additionally, we compare the semiclassical and full-quantum dynamics.

1 Introduction

Since its experimental realization, Bose-Einstein condensation in dilute atomic gases has been offering opportunities to research macroscopic quantum phenomena. Especially, one of the most fascinating macroscopic quantum phenomena is the Josephson effect between two Bose-Einstein condensations (BECs) trapped in a double-well potential, which is called the Bose-Josephson Junction (BJJ). BJJ has been realized experimentally, which allowed direct observation of the dynamics of macroscopic wave-functions directly. Though in BJJ the spatial coherence of BECs is focussed, the Josephson effect occurs not only between spatial separated BECs but also between internal degrees of freedom in a single BEC. In particular, the Josephson-like effects between atomic and molecular states have been discussed theoretically. In this paper, we consider atom-molecule BECs in a double-well potential. In this two component BJJ, the internal atom-molecule tunneling has significant influence on the ground state property and dynamics. As shown later, this internal tunneling induces the localized ground states. As for the dynamics, the multi-degree of freedom of this system permits chaotic dynamics, by adding the atom-molecule tunneling as a new degree of freedom.

First, we explain the semiclassical dynamics of BJJ. In a single component BJJ, the dynamical degrees of freedom are the relative particle number and the relative...
2 Model and approximations

In this section, we explain our model and approximations. The second-quantized Hamiltonian for Bose atoms and molecules can be written as

$$\hat{H} = \sum_{i=a,b} \int dx \left[ \frac{\hbar^2}{2m_i} \nabla i \hat{\psi}_i + V_{\text{ext}}(r)\hat{\psi}_i + \frac{\hbar^2}{2} \sum_{i=a,b} \int dx \hat{\psi}_i \nabla i \hat{\psi}_i \right] + \frac{\hbar^2}{2} \sum_{i=a,b} \int dx \hat{\psi}_i \nabla i \hat{\psi}_i + g_{ab} \int dx \hat{\psi}_a \hat{\psi}_b \hat{\psi}_a - \lambda \int dx \left( \hat{\psi}_a \hat{\psi}_a \hat{\psi}_a + \hat{\psi}_b \hat{\psi}_b \hat{\psi}_b \right) + \delta \int dx \hat{\psi}_b \hat{\psi}_b, \tag{1}$$

where $\hat{\psi}_a$ and $\hat{\psi}_b$ represent field operators for Bose atoms and molecules respectively, $\lambda$ is the coupling strength between atomic and molecular states, $\delta$ is the energy difference between atoms and molecules, and $V_{\text{ext}}(r)$ is the double-well potential. The interatomic, the inter-molecule, and the atom-molecule interactions can be approximated in terms of the s-wave scattering lengths as $g_i = 4\pi \hbar^2 a_{si}/m_i$, $g_{ab} = 6\pi \hbar^2 a_{sab}/m_a(i = a, b, m_b = 2m_a)$. Here, $m_a$ is the mass of a Bose atom. Furthermore, we introduce the four-mode approximation, which concentrates on condensate modes only, and neglect the effect of the particles occupying other modes. Then, field operators can be approximated as $\hat{\psi}_a \simeq \Phi_{aL} \hat{a}_L + \Phi_{aR} \hat{a}_R$, $\hat{\psi}_b \simeq \Phi_{bL} \hat{b}_L + \Phi_{bR} \hat{b}_R$, where $\Phi_{aL}, \Phi_{aR}(\Phi_{bL}, \Phi_{bR})$ are the wavefunctions of the atomic(molecular) condensate modes in the left well and the right well respectively. $\hat{a}_L, \hat{a}_R(\hat{b}_L, \hat{b}_R)$ are annihilation operators for the atomic(molecular) condensate modes in the left well and the right well respectively. Applying these approximations to Eq.(1), we obtain the quantum four-mode Hamiltonian (four-mode model).

$$\hat{H} = -J_a \left( a_{RL} a_R + a_{LR} a_L \right) - J_b \left( b_{RL} b_R + b_{LR} b_L \right) + \Delta \left( b_{LR} b_L + b_{RL} b_R \right)$$

$$+ \frac{U_a}{2} \left( a_{RL} a_{RL} a_R a_L + a_{LR} a_{LR} a_R a_L \right) + \frac{U_b}{2} \left( b_{RL} b_{RL} b_R b_L + b_{LR} b_{LR} b_R b_L \right)$$

$$+ U_{ab} \left( a_{RL} a_{LR} b_L b_R + a_{LR} a_{RL} b_R b_L \right)$$

$$- g \left( b_{LR} a_{RL} a_R + b_{RL} a_{LR} a_R + b_{LR} a_{LR} a_R + b_{RL} a_{RL} a_R \right). \tag{2}$$

Here, the parameters are defined as follows:

$$J_i \equiv - \int dr |\phi_{iL}|^2 \left[ \frac{\hbar^2}{2m_i} \nabla^2 + V_{\text{ext}}(r) \right] \phi_{iR}, \tag{3}$$
where $i = a$ represents atomic BEC modes, $i = b$ represents molecular BEC modes, and $L, R$ express the left well and right well respectively. Also, we use the notation as $z_a = (a^\dagger_L a_L - a^\dagger_R a_R)/N$ as needed.

3 Results

First, we investigate the effect of the atom-molecule tunneling on the ground state. Next, we will show the relation between the level statistics and the periodicity of dynamics. We choose the parameters as follows. The ratio $\lambda = N U_a/(2 J_a)$ is estimated as 15 in the single-component experiment, and the atomic interaction strength normalized by the atomic tunneling strength can be obtained as $U_a/J_a \simeq 3 \times 10^{-2}$. We use this value for the atomic interaction strength. We suppose that the molecular interaction strength is the same as the atomic one and that the shape of condensate wavefunctions of atoms and molecules are also the same. Under this condition $U_h = U_a/2$ from Eq. (5). In this study we set the total particle number as $N = 20$. We next consider the atom-molecule interaction. The experiment\cite{2} indicates that the atom-molecule interaction of $^{87}\text{Rb}$ is attractive, and thus we choose as $U_{ab}/J_a \simeq -2.3 \times 10^{-2}$. Finally, we set $\Delta/J_a = -1$.

3.1 Phase transition of the ground state

Within the semiclassical approximation, the particle localization transition in the ground state is induced by the atom-molecule internal tunneling. The ground state at $\sqrt{N g/J_a} < 2.55$ is symmetric, which has equal particle populations in each well. At $\sqrt{N g/J_a} \simeq 2.55$, the ground state become degenerate. For $\sqrt{N g/J_a} > 2.55$, the ground state obtains non-equal particle population. Here, we investigate this transition within a full-quantum treatment. By the exact diagonalization of the four-mode Hamiltonian\cite{4}, we obtain the eigenstates and energy eigenvalues.

The $g$-dependence of $\langle |z_a| \rangle$ is presented in Fig. 1. $\langle |z_a| \rangle$ increases rapidly at $\sqrt{N g/J_a} \simeq 3.5$. From Fig. 2 we see that the fluctuations of $|z_a|$ is maximum at this point. Furthermore, the ground state become degenerate for $\sqrt{N g/J_a} \geq 3.5$, as shown below. The $g$-dependence of excitation energies is shown in Fig. 3. Increasing the atom-molecule tunneling $g$, the first excitation energy goes to zero at $\sqrt{N g/J_a} \simeq 3.5$. For larger $g$, the ground state and some low lying energy levels become degenerate. These facts indicate that a phase transition to the localized ground state occurs at $\sqrt{N g/J_a} \simeq 3.5$. Finally, we comment on the system-size dependence of the results. We find that the results for

\[
E^0_i \equiv \int dr \Phi^*_iL \left[ -\frac{\hbar^2}{2m_i} \nabla^2 + V_{ext}(r) \right] \Phi_iL = \int dr \Phi^*_iR \left[ -\frac{\hbar^2}{2m_i} \nabla^2 + V_{ext}(r) \right] \Phi_iR, \tag{4}
\]

\[
U_i \equiv g_i \int dr |\Phi_iL|^4 = g_i \int dr |\Phi_iR|^4, \tag{5}
\]

\[
U_{ab} \equiv g_{ab} \int dr |\Phi_{aL}|^2|\Phi_{bR}|^2 = g_{ab} \int dr |\Phi_{aL}|^2|\Phi_{bL}|^2, \tag{6}
\]

\[
g \equiv \lambda \int dr \Phi^*_{bL}\Phi_{aL}\Phi_{aL} = \lambda \int dr \Phi^*_{bR}\Phi_{aR}\Phi_{aR}, \tag{7}
\]

\[
\Delta \equiv \delta \int dr |\Phi_{bL}|^2 + E^0_b - 2E^0_a = \delta \int dr |\Phi_{bR}|^2 + E^0_b - 2E^0_a, \tag{8}
\]
Fig. 1 (color online) The $g$-dependence of $\langle |z_a| \rangle$. $\langle |z_a| \rangle$ are qualitatively the same for different values of $N$. The size dependence appears more prominently in fluctuations; as shown in Fig. 2, the peaks of $\langle |z_a| \rangle$ at the critical point are sharpened for larger $N$. This indicates the occurrence of the quantum phase transition in the thermodynamic limit.

3.2 Level statistics and dynamics

Within a semiclassical approximation, we found the existence of non-periodic dynamics. This motivates us to investigate the full-quantum counterpart.

In this section, we investigate the effect of the atom-molecule tunneling on the periodicity of dynamics. The semiclassical dynamics is periodic in the small and large $\sqrt{Ng/J_a}$ region, however, non-periodic in the intermediate region. Considering this by full-quantum treatment, we show how the level spacing distributions change by varying the strength of the atom-molecule tunneling. From level spacing distribution, one can decide whether the dynamics of the system is periodic or non-periodic.
When a system exhibits regular motions in a semiclassical approximation, level spacing distribution shows Poisson-type distribution $P(S) = e^{-S}$ except some cases where $S$ is the level spacing normalized by mean level spacing. On the other hand, when the semiclassical dynamics of the system is chaotic, level spacing distribution is Wigner-type distribution $P(S) = (\pi/2) S \exp(-\pi S^2/4)$. In this section, we compare the level spacing distribution of the four-mode Hamiltonian (2) with Wigner and Poisson distribution in order to investigate the periodicity of semiclassical dynamics. In addition, we show that the time evolutions in a semiclassical approximation and a full-quantum treatment are different in a chaotic regime. Before the analysis, we need to classify the energy spectra according to the symmetry of the system. Since the double-well potential has the left-right symmetry, we should investigate the odd and even parity spectra separately.

From Fig. 4 the level spacing distribution in the small $g$ regime is very close to Poisson distribution. In this regime, Fig. 5 shows that the time evolutions in a semiclassical approximation resemble the full-quantum dynamics, and both exhibit regular motions. Furthermore, the level spacing distribution is Poisson-like in the larger $g$ region (see Fig. 6). The time evolutions of $N_{aL} \equiv \langle a^L_L a_L \rangle$ exhibit regular motion in both semiclassical and full-quantum treatments, as shown in Fig. 7. In contrast to Fig. 5 we see a remarkable difference between the semiclassical and full-quantum dynamics. This is due to the particle localization in one well, which decreases the particle number in another well and enhances quantum fluctuations. In $\sqrt{Ng}/J_a \gg 1$ and $\sqrt{Ng}/J_a \ll 1$ regions, internal or interwell tunneling are dominant, and thus the multi-degree of freedom of this system does not have strong influence. In contrast, as shown in Fig. 8 the almost all energy spectra obey Wigner distribution in the intermediate coupling region. Fig. 9 shows that the semiclassical dynamics is chaotic and quite different from the full-quantum time evolution. It is shown that the quantum fluctuations induce dynamical localization. The similar behavior was found in a kicked rotor.

4 Conclusions

In this paper, we showed the particle localization in ground states as shown in Fig. 1. Furthermore, we investigated how the internal tunneling deform the level spacing...
distribution and dynamics. Increasing the internal tunneling, the dynamics change to be non-periodic. Further increasing the internal tunneling, periodic time evolution emerges again. In addition, we showed that semiclassical and full-quantum dynamics is quite different in chaotic region; dynamical localization occurs within full-quantum treatment.

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