The Stability of Atomic and Molecular BECs in a Double-Well Potential

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Abstract. We discuss how the internal Josephson effect between atomic and molecular BECs changes the behavior of atomic Bose-Josephson junctions, especially the stability of $\pi$-states, in which the relative phase between BECs is $\pi$. In this study, we use the four-mode model, and applying the classical analysis, we show that the equally-populated $\pi$-state remains stable in the presence of the atom-molecule Josephson effect. In contrast, the non-equally-populated $\pi$-state exhibits the instability, even for a very small atom-molecule coupling.

1. Introduction
Since its experimental realization, Bose-Einstein condensation (BEC) in dilute atomic gases has been offering opportunities to research macroscopic quantum phenomena. Especially, a single component Bose-Josephson junction (BJJ) has been realized recently. In this experiment, the dynamics of the relative phase and the density of the macroscopic wavefunctions was observed directly[1]. Since BJJ is an isolated system, it has possibilities to exhibit dynamical regimes that are not accessible with superconductor-Josephson junctions[2]. One of such dynamical modes is the $\pi$-state, in which the relative phase between two condensates is equal to $\pi$. Depending on the interaction strength, two kinds of $\pi$-states are known to exist; one is the equally-populated $\pi$-state and the other is the non-equally-populated $\pi$-state[9]. In this letter, we refer to the equally-populated $\pi$-state as P1 and the non-equally-populated $\pi$-state as P2.

The Josephson effect occurs not only between spatial separated BECs but also between internal degrees of freedom. In particular, the Josephson type dynamics between atomic and molecular states has been discussed theoretically[3][4]. On the experimental side, the creation of the coexisting atomic and molecular BECs has been pursued[5][6]. Currently, a mixture of a Rb BEC and a degenerate gas of Rb$_2$ ground-state molecules has been realized using photo-association. The collective oscillation of the population between an atomic state and a molecular state has been observed though not in BEC phase[7][8]. The realization of the atom-molecule Josephson dynamics is forthcoming.

Based on the above backgrounds, we consider the behavior of an atomic and molecular BEC mixture in a double-well potential. In particular, we focus on the stability of $\pi$-states. In the case of a single-component BJJ, $\pi$-states are not always dynamically stable. In general, if there is no equal-energy closed loop around the stationary state in the phase space, a slight perturbation leads the stationary state to dynamical instability. P1 exhibits this type instability in a strong interaction regime[9]. Thus, the shape of equal-energy contour in the phase space determines
the stability of a π-state. Since the atomic and molecular BECs in a double-well potential involve an atom-molecule coupling as a new degree of freedom, the shape of the equal-energy contour is changed and the π-state may become unstable. Our objective is to research how an atom-molecule coupling changes the stability of a π-state.

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

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

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 \( V_{\text{ext}}(\mathbf{r}) \) is the double-well potential. The inter-atomic, the inter-molecule, and the atom-molecule interactions can be approximated in terms of the \( s \)-wave scattering lengths as \( g_i = 4\pi\hbar^2a_{si}/m_i \) \((i = a, b, m_b = 2m_a)\), \( g_{ab} = 6\pi\hbar^2a_{ab}/m_a \). Furthermore, we introduce the four-mode approximation, i.e. we concentrate on condensate modes only, and neglect the effect of the higher modes. Then, the field operators can be approximated as \( \hat{\Psi}_a \approx \Phi_{aL} \hat{a}_L + \Phi_{bL} \hat{a}_R \), \( \hat{\Psi}_b \approx \Phi_{bL} \hat{b}_L + \Phi_{bR} \hat{b}_R \), 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). In addition, we use classical analysis, in which the annihilation operators are replaced by \( \sqrt{N}e^{i\theta} \), where \( N \) and \( \theta \) are the number and phase of the condensate mode. This approximation is justified when the occupation number is macroscopic. Using this procedure, we obtain the classical four-mode Hamiltonian as

\[
H_{cl} = -2J_a \sqrt{N_{aL}N_{aR}} \cos(\theta_{aR} - \theta_{aL}) - 2J_b \sqrt{N_{bL}N_{bR}} \cos(\theta_{bR} - \theta_{bL}) + \Delta(N_{bL} + N_{bR}) + \frac{U_a}{2}(N_{aL}^2 + N_{aR}^2) + \frac{U_b}{2}(N_{bL}^2 + N_{bR}^2) + U_{ab}(N_{aL}N_{bL} + N_{aR}N_{bR}) + 2g[N_{aL}\sqrt{N_{bL}} \cos(2\theta_{aL} - \theta_{bL}) + N_{aR}\sqrt{N_{bR}} \cos(2\theta_{aR} - \theta_{bR})] \tag{2}
\]

Here, the parameters are defined as \( J_i \equiv -\int d\mathbf{r} \Phi_i^\dagger \left[ -\frac{\hbar^2}{2m_i} \nabla^2 + V_{\text{ext}}(\mathbf{r}) \right] \Phi_i \), \( E_i^a \equiv \int d\mathbf{r} \Phi_i^\dagger \left[ -\frac{\hbar^2}{2m_i} \nabla^2 + V_{\text{ext}}(\mathbf{r}) \right] \Phi_i \), \( U_i \equiv g_i \int d\mathbf{r} |\Phi_i|^2, U_{ab} \equiv g_{ab} \int d\mathbf{r} |\Phi_{aL}|^2|\Phi_{bL}|^2, g \equiv \lambda \int d\mathbf{r} \Phi_{aL}^\dagger \Phi_{bL} \Phi_{aL} \Phi_{bL} \), \( \Delta \equiv \delta \int d\mathbf{r} |\Phi_{bL}|^2 + E_{bL} - 2E_{aL}^0 \). Here we have assumed the symmetric double-well potential. Using this classical four-mode Hamiltonian, we study the dynamics of atomic and molecular BECs in a double-well potential with the Hamilton equations such as \( \hbar \dot{N}_{ij} = \frac{\partial E_i}{\partial \theta_j} \), \( \hbar \dot{\theta}_{ij} = -\frac{\partial E_i}{\partial N_{ij}} \) \((i = a, b, j = L, R)\). From the time evolution equations of the particle numbers, we can easily find that the relative phases should be 0 or \( \pi \) in the stationary states.

3. Results
In this section, we consider the stabilities of P1 and P2 under the existence of the atom-molecule coupling. We choose the parameters as follows. The total particle number \( N = 10,000 \). For simplicity, we set \( \Delta = 0 \). As for the tunneling strengths, we set \( J_b/J_a = 0.5 \), since the molecule
is heavier than the atom. As shown in [2][9], P1 is stable in a weak-interaction region only, and P2 exists and is stable in a strong-interaction region. Based on these facts, we study the $\pi$-states with the following parameter sets for inter-atomic and molecular interaction strengths $U_a, U_b$. We investigate P1 with $NU_b/(2J_a) = 10$, which is comparable to the inter-particle interaction strength in the single component experiment[1], and $NU_a/(2J_a) = 1$. Then we investigate P2 with $NU_b/(2J_a) = 15$, which is equal to the inter-particle interaction strength in the single component experiment[1], and $NU_a/(2J_a) = 5$. First, we consider the $g$-dependence of the stationary population of P2 in the case of $NU_{ab}/(2J_a) = 0, -5$. In order to obtain the

![Figure 1](image1.png)

**Figure 1.** The $g$-dependence of the particle numbers of P2. In left picture $U_{ab} = 0$, and in right picture $NU_{ab}/J_a = -5$. In both pictures red green lines represent the atomic particle numbers in the left and right wells. Blue and violet lines correspond to the molecular particle number in the left and right wells respectively.

![Figure 2](image2.png)

**Figure 2.** The time-evolution of the slightly perturbed P2 under the existence of the atom-molecule coupling. (a) The $g$-dependence of the imaginary part of the excitation frequency. the red and blue lines represent $NU_{ab}/(2J_a) = 0$, and $-5$. (b) The time evolution of the inter-atomic relative particle number when $\sqrt{Ng}/J_a = 0.1$,and $U_{ab} = 0$ (c) The Fourier spectrum of (b).

stationary states, we solve the Hamilton equations numerically. In this procedure, we set the atomic relative phase $(\theta_{aR} - \theta_{aL}) = \pi$, the molecular relative phase $(\theta_{bR} - \theta_{bL}) = 0$, and the atom-molecule relative phases $(2\theta_{aL(R)} - \theta_{bL(R)}) = \pi$, respectively. The last condition provide the lower energy for positive $g$, as one can see from Eq.(4). In Fig 1, the particle numbers of all modes are greater than 500, and the classical analysis is applicable. From Fig. 1 (a), if $g = 0$, the molecular particle numbers are equal, but when $g$ is finite, they are influenced by the non-equally populated atoms. Comparing Fig. 1 (a) and Fig. 1 (b), we see that the attractive atom-molecule interaction accelerates the particle localization in one well.

Solving the linearized Hamilton equations, we obtained the three eigen-frequencies, which correspond to the excitation spectra from the stationary states. We investigate the stability
of the system using these spectra. If the excitation frequency $\omega$ has an imaginary part, such stationary state exhibits dynamical instability, i.e., if the stationary state is perturbed slightly, the small-amplitude oscillation exponentially grows in time.

From this linear analysis, we find that P2 can become dynamically unstable in the presence of the atom-molecule coupling, i.e. Im ($\omega$) $\neq$ 0. In fact from Fig. 2 (a), the imaginary part of the excitation spectrum appears for $\sqrt{Ng/J_a} > 0.096$. Fig. 2 (b) shows the time-evolution of $(N_{aL} - N_{aR})/N$. Fig. 2 (c) is the Fourier spectrum of Fig. 2 (b). These figures clearly indicate the dynamical instability. In contrast, P1 is dynamically stable in the presence of the atom-molecule coupling, i.e. Im ($\omega$) = 0. Fig. 3 (a) shows the time-evolution of $N_{aL}/N$. Fig. 3 (b) shows the Fourier spectrum of Fig. 3 (a). These figures indicate that the dynamics of P1 is regarded as the superposition of three normal mode oscillations.

The instability of an atom-molecule mixture is drastically different from that of a single component, as suggested by the comparison of Fig. 2 (c) with Fig. 4. In a single component BJJ, the dynamical degrees of freedom are the relative particle number and the relative phase, so the dimension of the system is two. Because of the uniqueness of the solutions of ordinary differential equations, the trajectories in the phase space cannot intersect with each other. Then, significantly complex trajectories cannot exist even around dynamically unstable points in a 2D systems. However, in higher dimensional systems, the trajectories in the phase space travel around much more freely than 2D dynamical systems. This leads to richer dynamical behaviors.

4. References

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Figure 3. The time-evolution of the slightly perturbed P1 under the existence of the atom-molecule coupling. (a) is $N_{aL}$ when $\sqrt{Ng/J_a} = 0.1$, and $U_{ab} = 0$ (b) the Fourier spectrum of (a)

Figure 4. The Fourier spectrum of the relative phase number oscillation around an unstable equally populated single component $\pi$-state