The effects of trap-confinement and interatomic interactions on Josephson oscillations and macroscopic quantum self-trapping for a Bose–Einstein condensate

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Abstract

We theoretically study the effects of trap-confinement and interatomic interactions on Josephson oscillations (JO) and macroscopic quantum self-trapping (MQST) for a Bose–Einstein condensate confined in a trap which has a symmetric double-well potential along z-axis and 2D harmonic potentials along x- and y-axis. We consider three types of model interaction potentials: contact, long-range dipolar and finite-range potentials. Our results show that by changing the aspect ratio between the axial and radial trap sizes, one can induce a transition from JO to MQST for contact interactions with a small scattering length. For long-range dipolar interatomic interactions, we analyze transition from Rabi to Josephson regime and Josephson to MQST regime by changing the aspect ratio of the trap for a particular dipolar orientation. For a finite-range interaction, we study the effects of relatively large scattering length and effective range on JO and MQST. We show that JO and MQST are possible even if scattering length is relatively large, particularly near a narrow Feshbach resonance due to the finite-range effects.

Keywords: Josephson oscillations, macroscopic quantum self-trapping, trap-confinement, interatomic interactions, Bose–Einstein condensate, double well

1. Introduction

Josephson effect (JE), predicted more than half-a-century ago by Josephson [1], represents an unambiguous manifestation of macroscopic quantum effects. The main feature of this effect is that the electrons in cooper pairs can execute perpetual tunneling without any dissipation between two superconductors when the barrier between the superconductors is thin enough (typically the thickness is less than 10 Å) [2]. This happens because the two macroscopic wave-functions of the superconductors on both sides of the barrier overlap in the classically forbidden region inside the barrier. Though the theory of the Josephson junction was originally developed in the context of superconductivity, it can be applied as well to the physical systems with weakly coupled macroscopic wave-functions. JE with ultra-cold atoms was first proposed by Javanainen in 1986 [3]. After the experimental realization of Bose–Einstein condensate (BEC) in 1995 [4], JE with atomic condensate has attracted renewed interests, giving rise to new effects such as macroscopic quantum self-trapping (MQST) which was first predicted by Smerzi and collaborators [5]. MQST has no analogue in a superconducting Josephson junction. In 2001 JE was observed in an array of Bosonic Josephson junctions (BJJ) [6]. Both Josephson oscillation (JO) and MQST were experimentally demonstrated in a single BJJ [7, 8]. Over the years, several experimental and theoretical works [9–11] have demonstrated many effects such

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as external JE [12, 13], internal JE [14, 15], coherent tunneling oscillations of interacting bosons [16, 17], collapse and revival of JO [18], etc. In most of these works, JE has been studied by modeling the atom–atom interaction with the well-known zero-range contact potential which is valid for a small scattering length or for a weakly interacting system. Recently Spagnolini et al [17] have shown a transition from Rabi to plasma regime via tuning the s-wave scattering length from negative to positive value. This happens because the tunability of the scattering length through a magnetic Feshbach resonance [19] or any other means leads to the change in the effective atom–atom interaction which in turn affects the JE and related phenomena. We here assert that, even without altering the scattering length, it would be possible to obtain Josephson to plasma or MQST transition by changing the aspect ratio between the axial and radial trap frequencies. Because, it is well-known [20, 21] that the effective interaction can be drastically modified by appropriately changing the trap-confinement or aspect ratio, leading to confinement-induced resonances [22, 23] even if the corresponding 3D free space interaction strength or the scattering length is small. In a dipolar BEC, by varying the geometry of the trap [24], dipole polarization axis [25] and shape of a dipolar BEC [26] one can change dipole–dipole interaction (DDI) from attractive to repulsive or vice versa. But by changing the aspect ratio of the trap, the transitions from Rabi to Josephson or Josephson to MQST regimes for a particular dipole orientation are not explored so far.

Here we investigate the effects of trap-confinement, the effective range and strength of atom–atom interactions on JO and MQST. We find that, by changing the aspect ratio of the trap one can bring about a transition from Josephson to MQST regime and the transition point depends on the strength of interaction. We consider a model finite-range interaction potential of Jost and Kohn [27, 28] for exploring JE and related phenomena in Bose-condensed atoms interacting with a finite-range and relatively large scattering length. Near a Feshbach resonance, JO and MQST may be described considering Jost–Kohn interaction potential. Our results suggest that it may be possible to study JE and MQST near a narrow Feshbach resonance for which the effective range is very large or may even become negative [29–32]. Since a Feshbach resonance occurs due to the existence of a quasi-bound or a quasi-molecular state, such studies will enable one to unravel hitherto unexplored effects of molecular regime on Josephson physics.

The paper is organized in the following way. In section 2, we analyze the method of constructing BJJ under two-mode approximation. In section 3, we present stationary and dynamical solutions of BJJ analytically. In section 4 we present and discuss our results. In the end, we conclude in section 5.

2. BEC in a double-well (DW) potential: BJJ

The time evolution of the condensate wave function \( \psi(r, t) \) in a trap potential \( V_{\text{trap}}(r) \) at \( T = 0 \) K satisfies the Gross–Pitaevskii equation (GPE)

\[
\frac{i\hbar}{\hbar} \frac{\partial \psi(r, t)}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi(r, t) + V_{\text{trap}}(r) \psi(r, t) + \int |\psi(r', t)|^2 \psi(r', t) V_{\text{int}}(|r - r'|) d\mathbf{r}',
\]

(1)

where \( V_{\text{int}}(|r - r'|) \) represent the interatomic interaction between two particles. \( m \) is the mass of an atom. We consider a model trap potential [33] of the form \( V_{\text{trap}}(r) = V(\rho) + V_{\text{int}}(\rho) \), where \( V(\rho) = \frac{1}{2} m \omega_r^2 \rho^2 \) and

\[
V_{\text{int}}(\rho) = \frac{1}{2} \xi^2 (\rho^2 - \eta^2)^2,
\]

which has harmonic oscillations along radial directions (x- and y-axes) and a symmetric DW along z-axis. Here \( \rho^2 = x^2 + y^2 \), \( \omega_r \) is radial frequency, \( z = \pm \eta \) are the two minimum points where the 1D DW potential vanishes and the barrier height is \( V_0 = \frac{1}{2} \xi^2 \eta^4 \). So, the parameter \( \xi^2 \) has the dimension of energy-length\(^{-4} \). If \( V_0 \) is much larger than the ground-state energy of the DW potential, then for a particle in the lowest band of energy, each well can be approximated as a harmonic oscillator having frequency \( \omega_t = \sqrt{2 V_0/\rho} \). We write \( |r| = \sqrt{\rho^2 + z^2} \). In the strong radial confinement regime characterized by \( \omega_r \gg \omega_t \), we assume that all the atoms occupy the ground state of the radial harmonic potential. Then, integrating over the radial harmonic oscillator states, one can obtain an effective 1D Hamiltonian for the system. We solve for single-particle 1D eigen functions and eigenvalues numerically using the method of discrete variable representation. The lowest two energy eigen functions being quasi-degenerate in which atoms can occupy a ground ‘band’ in presence of particle–particle interactions. For symmetric DW, the lowest eigenstate \( \phi_0(z) \) is space-symmetric \( \phi_0(z) = \phi_0(-z) \) and the other quasi-degenerate state \( \phi_n(z) \) is anti-symmetric \( \phi_n(z) = -\phi_n(-z) \).

To reduce the 3D GPE in 1D form, we assume that in the radial direction the BEC is confined in ground state \( \psi_0(r) = \exp(-r^2/2\lambda) / \sqrt{\pi \lambda} \) of the transverse trap and the condensed wave function \( \psi(r, t) = \psi_{1D}(z, t) \psi_0(r) \), where \( \lambda = \frac{\omega_t}{\omega_r} \) is the aspect ratio of the trap. Here we have used \( a_c = \frac{\hbar}{\sqrt{m \omega_c}} \) as the unit of length and \( \hbar \omega_c \) as the unit of energy, and also in our subsequent discussions we will use these units if not otherwise specified. The 1D form of the GPE becomes

\[
\frac{i\hbar}{\hbar} \frac{\partial \psi_{1D}(z, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} \psi_{1D}(z, t) + V_{\text{int}}(z) \psi_{1D}(z, t) + \int |\psi_{1D}(z', t)|^2 \psi_{1D}(z, t) V_{\text{int}}(|z - z'|) dz',
\]

(2)

where the interaction potential defined as

\[
V_{\text{int}}(|z - z'|) = \frac{4}{\lambda^2} \int V_{\text{int}}(|r - r'|) e^{-2\lambda^2 \rho^2 \rho' d\rho d\rho'}. \]

(3)
Under tight-binding approximation, one can form two mode basis states $\phi_i(z) = \frac{\phi(z) + \phi(z)}{\sqrt{2}}$, $\phi_i(z) = \frac{\phi(z) - \phi(z)}{\sqrt{2}}$. The validity of this two-mode approximation for BEC rests on the fulfillment of the two conditions: (i) the temperature is much below $\hbar \omega_i$ (and so also much below $\hbar \omega_j$) (ii) both the interaction energy per particle and the chemical potential must be much below $\hbar \omega_i$. Let us consider $\phi_i(z)$ as the left-well localized state and $\phi_j(z)$ as the right-well localized state. To better understand the dynamical oscillations of two weakly linked BEC's, the time-dependent condensed wave-function $\psi_{1D}(z, t)$ can be written as a linear combination of two wave-functions which are localized in either site of the DW under two-mode approximation

$$\psi_{1D}(z, t) = \psi_1(t)\phi_1(z) + \psi_2(t)\phi_2(z).$$

The interesting relevant axial dynamics is determined by the wave-function $\psi_{1D}(z, t)$. Let us consider the time-dependent amplitudes $\psi_1(t) = \sqrt{N_1(t)}\exp[i\theta_1(t)]$ and $\psi_2(t) = \sqrt{N_2(t)}\exp[i\theta_2(t)]$, $N_i(z)$ is the number of atoms and $\theta_1(t)$ the phase in the well left(right). The normalization of the total wave function $\psi_{1D}(z, t)$ is fixed by the total atom number $N = N_1 + N_2$ and in order to fulfill the condition for a weak link, we have $\int \phi_1(z)\phi_2(z)dz \ll 1$.

Substituting the two-mode condensed wave-function $\psi_{1D}(z, t)$ in the time-dependent GPE and integrating over the spatial coordinates, we get

$$i\hbar \frac{\partial \psi_1(t)}{\partial t} = [E_1 + U_1|\psi_1(t)|^2 + U_2|\psi_2(t)|^2 \]
$$
$$+ K|\psi_2(t)|^2] \psi_1(t) + [-J + 2I|\psi_1(t)|^2 + I|\psi_2(t)|^2] \psi_2(t) + K\psi_2^2(t)\psi_1^2(t) + I\psi_1^2(t)\psi_2^2(t) \]

\(\frac{i}{\hbar} \frac{\partial \psi_2(t)}{\partial t} = [E_2 + U_2|\psi_2(t)|^2 + U_1|\psi_1(t)|^2 \]
$$
$$+ K|\psi_1(t)|^2] \psi_2(t) + [-J + 2I|\psi_1(t)|^2 + I|\psi_2(t)|^2] \psi_1(t) + I\psi_1^2(t)\psi_2^2(t) + K\psi_1^2(t)\psi_2^2(t) \]

Similarly we get

where

\[ J = \int \frac{\hbar^2}{2m}(\nabla \phi_i \nabla \phi_j + \phi_i V_{\text{int}}(z)\phi_j) \]
$$
$$E_{1,2} = \int \frac{\hbar^2}{2m}|\nabla \psi_{i,1}^2 + |\psi_{i,1}^2| V_{\text{int}}(z) \]

with

$$U_{ij} = \int \int|\phi_i(z)|^2|\phi_j(z')|^2 V_{\text{int}}(|z - z'|)dzdz',$$

where $i = \pm, j = \mp$.

$$K = \int \int \phi_i^*(z)\phi_j^*(z')\phi_i(z)\phi_j(z) V_{\text{int}}(|z - z'|)dzdz',$$

$$I = \int \int |\phi_i(z)|^2|\phi_j(z')|^2 V_{\text{int}}(|z - z'|)dzdz'.$$

Here we have four possible interaction parameters, namely, the on-site interaction $U_i = U_{ij} = U_{ji}$ when $i = j$, the intersite interaction $U_i = U_{ij} = U_{ji}$ when $i \neq j$, partial exchange interaction $I$ and exchange interaction $K$. $U_i, K, I$ are vanishingly small for a contact interaction, but they are finite for a long-range dipolar and finite-range interaction potential. Note that, all these interaction parameters are obtained as the matrix element of $V_{\text{int}}$ between the product of two single-particle wave-functions of a two-particle non-interacting system in the trap. However, for strong interaction or resonant interactions, one may require to use the wave-functions of an interacting pair of particles to calculate the interaction matrix elements of the model. We will come back to this issue later in section 4.3.

To characterize the Josephson dynamics, we define the population imbalance $w(t) = \frac{\rho_i(t) - \rho_j(t)}{\rho_i(t) + \rho_j(t)}$ and phase difference $\theta(t) = \theta_j(t) - \theta_i(t)$. The system of equations governing the dynamics of the population imbalance $w(t)$, and phase difference $\theta(t)$ reads as

$$w(t) = -\sqrt{1 - w^2(t)} \sin[\theta(t)] + \tilde{M}(1 - w^2(t))\sin[2\theta(t)],$$

$$\dot{\theta}(t) = Mw(t) + \frac{w(t)}{\sqrt{1 - w^2(t)}}\cos[\theta(t)]$$
$$+ \tilde{M}w(t)(1 - \cos[2\theta(t)]),$$

where, we have rescaled to a dimensionless time $t(2J - 2N_1)/\hbar \rightarrow t$ and $M = \frac{N(\rho_i(t) - \rho_j(t)}{\rho_i(t) + \rho_j(t)], \tilde{M} = \frac{NK}{(2J - 2N_1)}$. The dimensionless parameters $M$ and $\tilde{M}$ determines different dynamical regimes of the BEC atomic tunneling. If we neglect all interaction terms except the on-site interaction, then the equations (7) and (8) reduce to the form of BJ with contact interaction [10]. In that case, if we change the sign of $U$ from repulsive to attractive, then to maintain symmetry between equations (7) and (8) we have to change the phase $\theta \rightarrow -\theta$. So the dynamics of BJ remains same in attractive interactions with a phase shift of $\pi$. But in the case of long-range and finite-range interactions, if we change the dimensionless interaction parameters from positive to negative value we cannot recover the symmetry again with any change of phase shift. This is because of the interaction term $\tilde{M}$. Thus the dynamics of the system with a long- or finite-range interaction is completely different when we go to the repulsive to attractive interaction. The two-mode Hamiltonian can be written in the form

$$H = (M + \tilde{M}) \frac{w^2}{2} + \sqrt{1 - w^2} \cos \theta + \tilde{M}(1 - w^2)\cos 2\theta.$$

In the following we will restrict the discussion of the Josephson dynamics to the case of a symmetric DW potential with $E_1 = E_2$ and equations of motion can be written in Hamiltonian form

$$\dot{w} = -\frac{\partial H}{\partial \theta}, \dot{\theta} = \frac{\partial H}{\partial w}.$$

Therefore $w$ and $\theta$ are the canonically conjugate variables.
3. Solutions

3.1. Stationary solutions

We get stationary solutions by setting $\dot{w}$ and $\dot{\theta}$ equal to zero [10]. These are $w_{c_0} = 0$, $\theta_i = 2\pi n$ in which eigen energy is $E_i = -1 + \frac{\tilde{M}}{2}$ The next stationary state is $w_i = 0$, $\theta_i = (2n + 1)\pi$ with eigen energy $E_i = 1 + \frac{\tilde{M}}{2}$ In the case of non-interacting atoms in a symmetric DW potential, the eigenstates are always symmetric or anti-symmetric with $w_s = 0$. But due to the nonlinear interaction there is a symmetry breaking in $w$ corresponding to $\frac{\partial^2 H}{\partial w_1^2} \bigg|_{w_s,\theta_0} = 0$, where $H$ is the two mode Hamiltonian. Towards this end, we study the Hessian matrix for the system of $\theta_0 = 0$ and $\pi$. The Hessian matrix for this system is always diagonal and its eigenvalues are $\frac{\partial^2 H}{\partial w_1^2}$ and $\frac{\partial^2 H}{\partial w_0^2}$. The diagonal terms of the matrix are

$$\frac{\partial^2 H}{\partial w_1^2} = (M + \tilde{M}) - \tilde{M}\cos 2\theta + \frac{\cos \theta}{(1 - w^2)^2},$$

$$\frac{\partial^2 H}{\partial w_0^2} = \sqrt{1 - \tilde{M}} \cos 2\theta - 2\tilde{M} \cos 2\theta.$$

Depending on the sign of eigenvalues, a stationary point will be maxima, or minima or saddle point. In our case the eigenvalues depend on all interaction terms and the oscillations around a stationary point occur only if the stationary point is either minimum or maximum.

3.2. Stability analysis of stationary solutions

The linear stability of the condensate can be understood by analyzing the equations $\frac{\partial w}{\partial t} = 0; \frac{\partial \theta}{\partial t} = 0$, where $H$ is the two mode Hamiltonian. Through this analysis, we study the Hessian matrix of the form for $\theta_0 = 0$ and $\pi$. The Hessian matrix for this system is always diagonal and its eigenvalues are $\frac{\partial^2 H}{\partial w_1^2}$ and $\frac{\partial^2 H}{\partial w_0^2}$. The diagonal terms of the matrix are

$$\frac{\partial^2 H}{\partial w_1^2} = (M + \tilde{M}) - \tilde{M}\cos 2\theta + \frac{\cos \theta}{(1 - w^2)^2},$$

$$\frac{\partial^2 H}{\partial w_0^2} = \sqrt{1 - \tilde{M}} \cos 2\theta - 2\tilde{M} \cos 2\theta.$$

The small amplitude oscillations frequency around zero-phase mode is applicable only when $M > -1$ and $\tilde{M} < 0.5$. For $\pi$-phase mode it is applicable only $M < 1$ and $\tilde{M} > -0.5$. The oscillation frequency in $\pi$-mode is always less than that of the zero-mode. For positive $M$. But, for negative $M$, the oscillation frequency for $\pi$-mode is always greater than that of the zero-mode.

3.4. Macroscopic quantum self-trapping

The dynamics of the system changes drastically, when the initial population imbalance exceeds a critical value $w_i$. In that case, the tunneling is strongly suppressed, resulting in self-trapping. Once the critical value is reached, the tunneling current between two wells is such that the current gets reversed before even going to zero. This situation occurs because the phase exceeds $\pi$ before $w$ goes to zero. Consequently, the population imbalance remains non-zero throughout a complete cycle. This is the case where the population is trapped in a single-well although there is a Josephson current between two wells. To evaluate the condition for MQST, the initial energy for $w(0) = w_i$ and $\theta(0) = 0$ has to be large enough to reach $\theta_{final} = \pi$ at $w_{final} = 0$ which correspond to an energy

$$H_{final} = 1 + \frac{\tilde{M}}{2},$$

$$H_0 \equiv H(w(0) = w_i, \theta(0) = 0) = (M + \tilde{M}) \frac{w_i^2}{2} - \sqrt{1 - w_i^2} \cos \theta(0)$$

$$+ \frac{\tilde{M}}{2} (1 - w_i^2) \cos 2\theta(0) \equiv 1 + \frac{\tilde{M}}{2}.$$

Using the above condition we find that the critical population imbalance for MQST for zero initial phase difference is given by

$$w_i = \frac{2}{M} \sqrt{M - 1}.$$

For zero initial phase difference, we get self-trapping only when $|M| > 2$ and for small values of $M$ ($> 2$) self-trapping occurs even at arbitrary large initial population imbalance $w(0)$. In order to reach self-trapping, one has to increase $w(0)$ above a critical value $w_i$ for fixed $M$ and $\tilde{M}$, or alternatively increase $M$ by changing the interaction parameters or total number of atoms keeping $w(0)$ fixed. We get an expression for scaled critical interaction energy

$$M_c = \frac{2 \left[ 1 + \sqrt{1 - w(0)^2} \cos(\theta(0)) + \frac{\tilde{M}}{2} \left( 1 - \cos(2\theta(0)) \right) \right]}{w(0)^2} \left[ 1 - \cos(2\theta(0)) \right].$$

In the zero or $\pi$-phase mode it gives same result [10]. The MQST is a nonlinear effect arising from inter-particle interactions in the individual wells. It is self-maintained in a closed system without an external drive.

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4. Results and discussion

4.1. Contact interaction

We consider three types of interatomic interactions: contact, long-range dipolar and finite-range interaction potential. We first discuss the case of delta potential \( V_0(r) = \rho \delta(r) \), where \( g = \frac{2\pi h}{\mu} a_s \) be the 3D s-wave scattering length and \( \mu = \frac{m}{2} \) is the reduced mass. For numerical illustration with realistic long-range dipolar and exchange terms are same. So, the number of interaction terms in the present case is three. The value of the tunneling coefficient is found to be \( J \approx 12.81 \text{ Hz} \) and total number of atoms is taken to be \( N = 1000 \).

From the left side of figure 1, it is clear that by changing the aspect ratio one can change the interaction energy keeping the scattering length \( a_s \) and \( N \) constant. We see that the value of the on-site interaction is large in the quasi-1D limit. When the trap is almost isotropic \( \lambda \approx 1 \) we get a situation where \( NU \approx J \) and in the quasi-1D limit \( \lambda \ll 1 \) \( NU \) is much greater than \( J \) leading to plasma regime [5]. We define average population imbalance \( \langle \omega \rangle_N \), as the average of \( \omega(t) \) over the time-period of oscillations. In the right side of figure 1 we plot \( \langle \omega \rangle_N \) as a function of \( \lambda \) for zero-phase mode. This figure shows that as \( \lambda \) decreases below a critical value, the system undergoes a transition from JO \( \langle \omega \rangle_N = 0 \) to MQST \( \langle \omega \rangle_N \neq 0 \). From this figure we notice that the transition point moves towards smaller value of \( \lambda \) as \( a_s \) increases.

To verify whether our quasi-1D contact interaction can yield similar results as given by 1D form of the regularized delta potential [22] \( V_0^{1D}(z) = g_0 \delta(z) \), where \( g_0 = \frac{2\pi h}{\mu_0} \left( 1 - \frac{\omega_s}{\omega_0} \right)^{-1} \), \( C \) is a constant, \( C = 1.4603 \) and \( a_p = \frac{\lambda}{\sqrt{\pi a_s}} \) is the size of the transverse harmonic potential. In figure 2 we show the comparison between the calculated values of the on-site interaction energy and time-averaged population imbalance as a function of \( \lambda \) for our quasi-1D contact interaction and 1D form of the regularized delta potential. We find that the transition point between JO and MQST differs almost by two times.

4.2. Dipole–dipole interaction

Next, we consider a dipolar atomic BEC with all the atoms being aligned in the \( y-z \) plane by an external field. Then the DDI is given by

\[
V_{dd}^{dd}(r) = \frac{d^2}{r^3} (1 - 3 \cos^2 \phi),
\]

where \( d^2 = \frac{\mu_0 h^2}{4\pi} / 4\pi \) with \( \mu_0 \) being the magnetic permeability of free space, \( \mu_0 \) is the magnetic dipole moment of each atom, \( r \) is interatomic position vector, \( \phi_{rd} \) is the angle between \( r \) and polarization direction. The effective 1D form of the DDI can be calculated by assuming that, in the strong radial confinement regime, all the atoms occupy the radial ground state \( \psi_r(\rho) \) and the condensed wave function is given by \( \psi(r, t) = \psi_{1D}(z, t) \psi_r(\rho) \). Putting this form of the wavefunction in the 3D GPE and then working in the center of mass (COM) frame of reference for a pair of atoms, and integrating over COM co-ordinates and in radial direction, one obtains a effective 1D DDI

\[
V_{dd}^{1D} = -\frac{\hbar}{4\pi} \left( 1 + 3 \cos 2\phi \right) \left\{ \frac{8}{3} \frac{|z|}{a_p} - 2 \frac{|z|}{a_p} + \sqrt{2\pi} \left[ 1 + \frac{|z|^2}{a_p^2} \right] \frac{8|z|}{a_p} \frac{4}{a_p} \right\}.
\]
where

\[ \cos \phi_d = \frac{r \cdot d}{|r||d|} = \left[ \frac{\rho \sin \theta_d}{\sqrt{z^2 + \rho^2}} \right] \sin \phi + \left[ \frac{z}{\sqrt{z^2 + \rho^2}} \right] \cos \phi. \]

The detailed derivation of the 1D DDI from the 3D dipolar interaction is available in [39, 40]. \(|z| = |z_1 - z_2|\) is the separation between two atoms 1 and 2 along the \(z\)-axis, where \(z_{1(2)}\) denotes the \(z\)-coordinate of atom 1(2); \(erfc\) is the complementary error function and \(\phi\) is the angle between direction of dipole polarization and \(z\) axis. Note that the \(V_{DD}^{1D}\), as defined by equation (12), is negative for angles \(0 \leq \phi < \phi_{crit}\) with \(\phi_{crit} = \cos^{-1}(1/\sqrt{3})\) and positive for \(\phi_{crit} < \phi \leq \pi/2\). For \(\phi = 0\), the 1D DDI is maximally attractive and for \(\phi = \pi/2\), it is maximally repulsive. Previously, the transition from JO to the MQST has been studied by changing the dipole orientation with respect to the \(z\)-axis [25]. But, here we find that one can also change or switch the interaction from repulsive to attractive by changing the aspect ratio of the trap for a fixed dipole orientation, and then if possible obtain a transition between JO and MQST.

Regarding two-mode approximation for a dipolar BEC in a DW trap, Xiong et al [25] have examined the validity of the two-mode approximation by numerically solving the full 3D GPE for a dipolar BEC in a DW trap for various dipolar orientations. They have found that, for predicting the transition between MQST and the Josephson regime, two-mode theory with the overlap between two site-specific wave functions being approximated to be zero is good, but the frequency of JO in the two-mode theory differs by two orders of magnitude. They have also discussed an effective two-mode treatment with input from numerical solution of the full 3D GPE for a better agreement. In our case, two-mode approximation is reasonably good because we have not used the zero-overlap approximation.

For numerical illustration, we consider a dipolar BEC of \(^{52}\text{Cr}\), which has magnetic moment \(\mu_d \approx 6\mu_B\) (\(\mu_B\) is Bohr magneton) and assume that the short-range forces do not affect the long-range DDI. We keep the total number of atoms \(N\) and DW trapping frequency same as used for contact potential interaction. Here we have to necessarily consider all four interaction terms \(U\) and DW trapping frequency same as used for contact potential interaction. Here we have to necessarily consider all four interaction terms We fix the value of \(\phi = 0.31\pi\), which is above the \(\phi_{crit} (=0.30\pi)\). As a result, our 1D DDI is repulsive and the effective on-site interaction \(NU\) lies well below band gap of the DW potential. The left side of figure 3 shows that as \(\lambda\) increases beyond \(\lambda = 0.58\), \(U\) changes from repulsive to attractive but all the other interaction parameters remain positive. The inter-site, partial exchange and exchange interactions are smaller than \(U\) by two or three orders of magnitude as shown in the right side of figure 3. However, because \(U\) switches its sign at \(\lambda = 0.58\) other interaction
terms also become important in the dynamics of JO and MQST near the zero crossing of $U$. The left side of figure 4 shows that by changing the aspect ratio of the trap one can get a transition from Rabi to Josephson regime in the small-amplitude oscillation limit, because of the confinement-induced sign change of $U$. To study the transition from JO to MQST, we choose the initial phase-difference between two condensates $\theta(0) = 0$. The right side of figure 4 we notice that when $\lambda > 0.28$ we get a transition from JO to MQST regime.

4.3. Finite-range interaction

Next, to study the effects of relatively large scattering length and effective range of interaction we consider the finite-range interaction potential of Jost and Kohn [28]. The Jost–Kohn potential $V_r(r)$ [28] for positive $s$-wave scattering length $a_s$ is a three-parameter potential with the parameters being $a_s$, the effective range $r_0$ and another parameter $\Lambda$ which is related to the binding energy $E_b$ of the last $s$-wave bound state close to the threshold of the actual two-body interaction potential. Writing $E_b = -\hbar^2 \kappa^2 / 2\mu$ ($\kappa > 0$) where $\mu$ is the reduced mass and $\kappa$ is related to $\Lambda$ by

$$\kappa = \frac{1}{r_0} \left( 1 + \alpha \right) \frac{1 + \Lambda}{1 - \Lambda},$$

where $-1 < \Lambda < 1$, $\alpha = \sqrt{(1 - 2\kappa / a_s)}$ and $a_s > 2r_0$ for $r_0 > 0$. In terms of $a_s$, $r_0$, $\Lambda$, the potential is

$$V_r(r) = e^{-2(1-\alpha)\kappa} \frac{8\alpha \hbar^2}{\mu r_0^2} \{(1 + \alpha \Lambda)^2 (\alpha + \Lambda)^2 \times (\alpha - 1)^2 (1 - \Lambda^2 e^{-(\alpha + 1)\kappa} \right)^2

- \Lambda^2 (1 + \alpha)^2 [(1 + \Lambda^2 e^{-2\alpha \kappa} - (\alpha + \Lambda)^2 e^{-\kappa} \right] \times \{(1 + \alpha \Lambda)^2 (\alpha + \Lambda^2 e^{-2(\alpha + 1)\kappa})

- (\alpha + \Lambda)^2 (e^{-2(1-\alpha)\kappa} + \alpha^2 e^{-\kappa}) \right)^2. \tag{14}$$

The parameter $r_0$ used in equation (14) corresponds to the actual effective range only in the limit $\kappa \to \infty$ or equivalently $\Lambda \to 1$. As discussed in [41], when $\kappa$ is small, the modified effective range deviates from $r_0$. So, the parameter $\kappa$ or $\Lambda$ can be used to control the effective range at a low-energy $s$-wave scattering resonance such as a magnetic Feshbach resonance (MFR) which is extensively used to tune $a_s$ of ultracold atoms. It is experimentally observed that near a narrow MFR, the effective range $r_0$ sharply changes with magnetic field $B$ [30]. For instance, for the MFR of $^{39}$K near $B = 58.9$G, $r_0$ is found to be large negative [31]. For $^6$Li, near the narrow Feshbach resonance at $B = 543.3$G the similar results hold good [29]. So, near Feshbach resonances, the range becomes...
scattering-length or magnetic field dependent. With Jost-Kohn potential of equation (14) one can model this magnetic field dependence of $r_0$ by changing the parameter $\Lambda$ as discussed in [41].

The dependence of $U$ on $a_s$ and other parameters of the Jost-Kohn potential is discussed in some detail in the appendix, where we calculate $U$ using the wave-functions of interacting two-particle system in a harmonic well and compare it with that calculated using the single-particle wave-functions of non-interacting system. As shown in the appendix, the results for non-interacting case is underestimated by about one third of the results for interacting case. For numerical illustration of the dynamics of BJJ at relatively large scattering length, we fix the DW axis frequency $\omega_z = 2\pi \times 85$ Hz and the radial frequency $\omega_r = 2\pi \times 136$. So, $\lambda = 0.625$ then we fix the value of effective range $r_0 = 0.006a_z$ and $\kappa a_z = 1.2$. The left side of figure 5 shows that when scattering length nearly equals to the axial size of trap, on-site interaction energy changes from positive to negative value where the effective range is smaller by three orders of magnitude than axial size of the trap. Here we calculate the on-site interaction $U$ using the wave-functions of non-interacting two particle system in the DW. The inter-site interaction remains non-zero where the on-site interaction crosses zero as shown in the right side of figure 5. In order to maintain the two-mode approximation, we choose the small value of the repulsive and attractive on-site interaction energy near zero value. In figure 6 we show the variation of $U_i/U$, $I/U$, $2J - 2NI$ as a function of positive scattering length.

The zero-phase mode oscillations describe the inter-well atomic tunneling dynamics with vanishing time-averaged value of the phase across the junction, $\theta(t) = 0$. For repulsive on-site interaction, we calculate the parameters $NU = 0.73$ $h\omega_z$, $NU = 0.03$ $h\omega_z$, $NI = 0.11$ $h\omega_z$, $NK = -1.8 \times 10^{-4}$ $h\omega_z$ with $N = 1000$. So the value of $M = -4.06$ and $\tilde{M} = 0.001$. For attractive on-site interaction, we have $NU = -0.86$ $h\omega_z$, $NU = -0.04$ $h\omega_z$, $NI = 0.13$ $h\omega_z$, $NK = -0.004$ $h\omega_z$ with $N = 1000$. Here the value of $M = 4.20$ and $\tilde{M} = 0.02$. For both cases the value of tunneling $J$ is 0.024 $h\omega_z$. The stationary point $(w_s, \theta_s) = (0, 0)$ is always a saddle point for repulsive on-site interaction but for attractive on-site interaction the point $(w_s, \theta_s) = (0, 0)$ is a maximum. So, the oscillations around a stationary point are possible only for the negative on-site interaction. From figure 7 it is clear that the system remains in self-trapped state for any initial value of the population imbalance in the repulsive on-site interaction due to the term $I$. Although the terms $U_i$, $I$ are typically one or two orders of magnitude smaller than on-site interaction as shown in figure 6, their collective contributions due to condensate have nontrivial effects on the oscillations of the population imbalance. From figure 8, we observe that for small population imbalance it oscillates around zero value. An increase of the initial population imbalance $w(0)$ adds higher harmonics to the sinusoidal oscillations. The oscillation period of the population imbalance $w$ increases with increasing $w(0)$ until, at a certain critical population imbalance $w(0) = 0.86$, the oscillation is suppressed and the system is self-trapped with the phase difference between two BEC’s in the left and right well evolves unbound as shown in figure 9.

In addition to zero-phase mode and MQST as discussed above, BJJ has another rich class of tunneling dynamics in which the system evolves with time-averaged phase value of $\theta = \pi$. For repulsive on-site interaction, $(w_s, \theta_s) = (0, \pi)$ is a minimum point whereas for attractive on-site interaction it is a saddle point. So, in the $\pi$ phase mode, the system remains
self-trapped for any value of the on-site attractive interaction owing to the symmetry breaking of population imbalance. As a result, we get two types of MQST characterized by the time-averaged value of population imbalance $\langle w \rangle$ with $w_s$ being the stationary value of $w$ at which the symmetry breaking occurs.

The various regimes of the finite-range BJJ discussed above can be summarized in terms of phase-plane portrait, where constant energy lines are plotted in $w$-$\theta$ diagram. Figure 10 shows the phase-plane plot for $M = -4.06$ and $M = 4.20$, obtained by numerically solving the coupled differential equation (7) and (8). The first plot in the left of figure 10 describes that all trajectories with initial value of the phase difference $\theta(0) = 0$ are self trapped (red lines) even for small population imbalances. The situation changes for $\theta(0) = \pi$, where for small population imbalances the trajectories are closed with no self-trapping (blue lines) but for higher population imbalance $w(0) = 0.88$, the system is self-trapped. In the second plot, the phase-plane diagram is shown for $M = 4.20$. In this plot when the initial value of the phase difference $\theta(0) = 0$, the system oscillates around zero value for small population imbalances, given by the closed energy lines. When the initial population imbalance increases above threshold $w(0) = 0.86$, the system goes to self-trapped state.
and for higher value of w(0) the system remains always self-trapped. The system also remains always self-trapped when the initial value of phase difference \( \theta(0) = \pi \).

5. Conclusions

In conclusion, we have shown that, it is possible to induce transitions from JO to MQST by changing the aspect ratio of the trap keeping the scattering length fixed. For DDI, we have shown the possibility of the Rabi to Josephson transitions in small-amplitude oscillations. It is also possible to get JO and MQST in DDI by changing the aspect ratio. We have shown the possibility of the Rabi to Josephson transitions in resonantly coupled atomic and molecular BEC. In such atom-molecule coupled systems, the effects of trap-confinement and finite-range of interactions as studied in this paper will become important.

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Appendix. Jost–Kohn potential

Using the Jost–Kohn potential of equation (14) as shown in section 4.3, even if the scattering length is positive, one can generate attractive interaction due to confinement induced effects in a finite-range interaction. This is unlike the contact interaction where the sign of the scattering length determines the nature of interaction.

Though \( V_s(r) \) does not support any bound state, it explicitly depends on the parameter \( \kappa \). In the limit \( \kappa \rightarrow \infty \), the interaction is described by scattering length \( a_s \) and the effective range \( r_0 \) which can be obtained from the well-known effective range expansion

\[
k \cot \eta(k) = -\frac{1}{a_s} + \frac{1}{2}r_0 k^2 + ...,\]

where \( \eta(k) \) is the scattering phase shift associate with the wave-vector \( k \). However, for small \( \kappa \), the effective range expansion is modified with modified scattering length and modified effective range [41]

\[
\tilde{a}_s = a_s - \frac{2}{\kappa}, \quad \tilde{r}_0 = \frac{a_s}{\tilde{a}_s} (\frac{1}{2\kappa a_s} + \frac{1}{4\kappa^2 a_s} - 2r_0 \kappa). \quad (A.1)
\]

It is clear that \( \tilde{r}_0 \) is negative but \( \tilde{a}_s > 0 \) for \( \kappa r_0 \ll 1 \) and \( \kappa a_s > 2 \) with \( r_0 > 0 \). Negative effective range occurs for a narrow resonance [29, 32] and may be interpreted as the breakdown of the standard effective range expansion [41]. On the other hand \( \tilde{a}_s < 0 \) for \( \kappa a_s < 2 \). Here we choose \( \lambda = 0.625 \) then we fix the value of the effective range \( r_0 = 0.001 a_s \). We vary \( \kappa \) to different values to see how the interaction parameters behave as a function of \( a_s \). The left side of figure A1 describes the variation of on-site interaction \( U \) as a function of \( a_s \) when \( \kappa a_s = 1 \), showing that when scattering length is large (\( a_s = 0.65 a_s \)), on-site interaction changes from positive to negative value. Here we calculate the on-site interaction using the wave-functions of interacting (dashed-red) two-particle system in a harmonic well and compare the results with that using the wave-functions of non-interacting (dashed-blue) two particle system. Though

**Figure A1.** Variation of \( U \) (in unit of \( \hbar \omega_c \)) as a function of \( a_s \) (in unit of \( a_s \)) for \( r_0 = 0.001 a_s \), \( \lambda = 0.625 \) and \( \kappa a_s = 1 \) (left), \( \kappa a_s = 5 \) (right) for interacting (dashed-red) and non-interacting (dashed-blue) cases.
both results are qualitatively similar, the results with the wave-functions of non-interacting system is underestimated by about one-third of that with the wave-function of interacting system as shown in figure A1 for which $\bar{r}_0$ and $\bar{a}_s$ are always negative. Next if we consider the value $\kappa a_z = 5$ then from the right side of figure A1 we have a situation where $\bar{a}_s > 0$ and $\bar{a}_s < 0$. Here also $\bar{r}_0$ is negative always. For larger values of $\kappa a_z = 500$, as shown in figure A2, the variation of $U$ as a function of $a_z$ is almost linear in the small scattering length limit. But in the large scattering length limit $U$ becomes constant. The values of $\bar{r}_0$ and $\bar{a}_s$ are always positive in this case. For higher values of $k = a_500$, as shown in figure A3, we plot the on-site interaction energy as a function of $a_z$ for two different values of aspect ratio $\lambda$. When $\lambda = 0.001$, we have quasi-1D regime for which $U$ becomes saturated in the large scattering length limit when $\kappa a_z = 5$. When $\lambda = 0.625$, the value of $U$ is larger compare to the quasi-1D regime. So, to study the BJJ at large scattering length we have to choose the values of $\kappa a_z$ small so that our $NU$ lies well below the gap between ground and first excited state of the single well.

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