

# Dynamics of binary Bose–Einstein condensate via Ehrenfest like equations: appearance of almost shape invariant states

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**Abstract.** We derive Ehrenfest like equations for the coupled Gross Pitaevskii equations (CGPE) which describe the dynamics of the binary Bose–Einstein condensate (BBEC) both in the free particle regime and in the regime where condensate is well trapped. Instead of traditional variational technique, we propose a new Ehrenfest based approach to explore so far unrevealed dynamics for CGPE and illustrate the possibility of almost shape invariant states in both the regimes. In the absence of a trapping potential, when all the interactions present in the system are attractive, it is possible for an initially mixed Gaussian state to propagate with almost no change in width if the proper initial condition is satisfied. Even for repulsive intra-atomic and attractive inter-atomic interaction ( $g_{\alpha\beta}$ ) one can tune  $|g_{\alpha\beta}|$  such that the width of the propagating wave packet remains bounded within almost about 10%. We also discuss the dynamics of the initially phase separated condensate and have shown the breakdown of the Gaussian nature of the wave packets due to collisions. However, when the BEC is trapped in simple harmonic oscillator (SHO) potential, for  $g_{\alpha\beta} > 0$ , it is possible for an initially overlapping state to retain its initial shape if  $g_{\alpha\beta}$  is less than a critical value ( $g_{\alpha\beta}^c$ ). If  $g_{\alpha\beta}$  exceeds  $g_{\alpha\beta}^c$ , an overlapping state can become phase separated while keeping its shape unchanged.

## 1 Introduction and the Ehrenfest scenario

Over the last few decades the studies of Bose–Einstein condensates have revealed several interesting features arising from a nonlinearity that stems from a mean field picture of atomic interactions. This leads to a nonlinear Schrödinger equation which in this context is called the Gross Pitaevskii equation (GPE) since the condensates are produced in a trapping potential [1–3]. While the statics and dynamics of the single species condensate has been exhaustively researched, that of the binary condensate is somewhat more problematic and hence some questions remain at a fairly basic level when an analytic treatment is attempted. Some of these have to do with oscillation frequencies and dynamics of the condensate which is not in equilibrium [4]. A useful approximation scheme has been discussed by Navarro et al. [5], who have used a variational model [6] with a Gaussian trial function for each of the two condensates. The trap is actually three-dimensional. But one can vary the frequencies in different directions to produce very elongated (cigar shaped) or highly flattened (pancake shaped) condensate profile and thereby generating effectively one dimensional or effectively two dimensional condensate respectively. In this effective lower dimensional system, the shape of the condensates does not change in the other directions meaning the other

directions are frozen out. However, the dimensionality reduction is an approximation providing the effective one dimensional or two dimensional results instead of genuine one dimensional and two dimensional results. In principal, there are a number of techniques of reducing the relevant three dimensional GPE to an effectively one dimensional (quasi-low dimensional) dynamics [7,8]. This quasi-condensate [9] has the same density profile and local correlation properties as true condensates. We have recently found [10] that introducing an approximation, based on Ehrenfest equation, which is independent of the initial form of the wave function works well for the single component system and provides reliable results for initial shapes which are Gaussian or localized hyperbolic functions. However, our approach is complementary to that of Navarro et al. who use a generalization of the variational technique. In this present work, we show that a similar description using Ehrenfest relations can be set up for the binary condensates also and can be very effective in probing whether there can be a nearly shape invariant properties of initial wave packets.

Another interesting set of problems in dynamics of binary BEC involving Rabi switching of condensate wave functions and the interface instability has been considered by [11–15]. Following the works of McCarron et al. [16], it is possible to produce phase separated condensate and that should make the free expansion dynamics experimentally feasible. For the most part in Section 2, we focus on

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the following scenarios – an equilibrium situation exists for the binary condensate in a trapping potential and at  $t = 0$ , the trap is switched off. One would like to know how the dynamics will proceed. In particular, we are interested in exploring how closely does an initial wavepacket retains its shape, i.e., how much coherent it is. With this in mind, we introduce an Ehrenfest equation based approach for studying the dynamics and show that it is a reasonably versatile tool for handling several issues in the dynamics of the binary condensates which remained unexplored. We analyze the dynamics both in miscible (overlapping) and in phase separated regime with interesting combinations of parameters. In miscible domain, we indicate the appearance of almost coherent wave packet both for  $g_{\alpha\beta} < 0$  and  $g_{\alpha\beta} > 0$  if the proper initial conditions are satisfied. The possibility of breakdown of the wave packet due to the collisions between the wave packets in the phase separated regime is also presented. In Section 3, we discuss over the following framework – we consider the equilibrium binary BEC in a confining potential and at  $t = 0$ , the trap frequency is changed. Similar as in the Section 2, an interesting question then concerns the dynamics of the condensate in this framework. Thereafter, we proceed to investigate the existence of shape invariant states both in overlapping and phase separated initial conditions.

For two species  $\alpha$  and  $\beta$  CGPE can be written as

$$\begin{aligned} i\hbar\partial_t\psi_\alpha(x,t) &= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_\alpha(x,t) + V_{ext}(x)\psi_\alpha(x,t) \\ &\quad + (g_\alpha|\psi_\alpha|^2 + g_{\alpha\beta}|\psi_\beta|^2)\psi_\alpha \\ i\hbar\partial_t\psi_\beta(x,t) &= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_\beta(x,t) + V_{ext}(x)\psi_\beta(x,t) \\ &\quad + (g_\beta|\psi_\beta|^2 + g_{\alpha\beta}|\psi_\alpha|^2)\psi_\beta \end{aligned} \quad (1)$$

where we have considered identical masses ( $m$ ) for both the species for simplicity in analysis. The interaction strengths ( $g_\alpha$ ,  $g_\beta$  and  $g_{\alpha\beta}$ ) can be all positive (repulsive interaction) or all negative (attractive interaction) or combinations of them. In our study we have incorporated all the possibilities.

To write down the Ehrenfest equations, we write equation (1) as

$$\begin{aligned} i\hbar\partial_t\psi_\alpha(x,t) &= H\psi_\alpha + (g_\alpha P_\alpha + g_{\alpha\beta}P_\beta)\psi_\alpha \\ i\hbar\partial_t\psi_\beta(x,t) &= H\psi_\beta + (g_\beta P_\beta + g_{\alpha\beta}P_\alpha)\psi_\beta, \end{aligned} \quad (2)$$

where  $H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V_{ext}(x)$ ,  $P_\alpha = |\psi_\alpha|^2$  and  $P_\beta = |\psi_\beta|^2$ . The initial wave function is taken to be  $\psi_\alpha(x,0)\psi_\beta(x,0)$ , i.e., separable in the indices  $\alpha$  and  $\beta$ . We assume that this separability persists at later times and the wave function is  $\psi_\alpha(x,t)\psi_\beta(x,t)$ . Hence the average position of species  $\alpha$  is  $\langle\psi_\alpha|x|\psi_\alpha\rangle = \langle x\rangle_\alpha$  and that of species  $\beta$  is  $\langle\psi_\beta|x|\psi_\beta\rangle = \langle x\rangle_\beta$  with similar results holding for any other operator  $O$ . Taking the nonlinearity into account, consequently the Ehrenfest equation for species

$\alpha$  can be recast into the following form

$$i\hbar\langle\dot{O}\rangle_\alpha = \langle[O, H]\rangle_\alpha + \langle[O, (g_\alpha P_\alpha + g_{\alpha\beta}P_\beta)]\rangle_\alpha, \quad (3)$$

and a similar equation holds for species  $\beta$ . Equation (3) follows by noting

$$\langle O \rangle_\alpha = \int dx \psi_\alpha^* O \psi_\alpha \quad (4a)$$

since  $O$  does not have explicit time dependence

$$\begin{aligned} i\hbar\langle\dot{O}\rangle_\alpha &= \int dx i\hbar[\dot{\psi}_\alpha^* O \psi_\alpha + \psi_\alpha^* O \dot{\psi}_\alpha] \\ &= \int dx \psi_\alpha^* (OH - HO)\psi_\alpha \\ &\quad + \int dx \psi_\alpha^* [O(g_\alpha P_\alpha + g_{\alpha\beta}P_\beta)\psi_\alpha \\ &\quad - (g_\alpha P_\alpha + g_{\alpha\beta}P_\beta)O\psi_\alpha]. \end{aligned} \quad (4b)$$

A similar equation holds for  $\langle O \rangle_\beta$ .

We write the explicit answers for the first few moments for the species  $\alpha$  (with similar equation holding for species  $\beta$ )

$$\frac{d}{dt}\langle x \rangle_\alpha = \frac{\langle p \rangle_\alpha}{m} \quad (5a)$$

$$\frac{d}{dt}\langle p \rangle_\alpha = -\left\langle \frac{dV}{dx} \right\rangle_\alpha - g_{\alpha\beta} \int P_\alpha \frac{\partial P_\beta}{\partial x} dx \quad (5b)$$

$$\frac{d}{dt}\langle x^2 \rangle_\alpha = \frac{1}{m}\langle xp + px \rangle_\alpha \quad (5c)$$

$$\begin{aligned} \frac{d}{dt}\langle p^2 \rangle_\alpha &= -\left\langle p \frac{dV}{dx} + \frac{dV}{dx} p \right\rangle_\alpha - mg_\alpha \int \frac{\partial P_\alpha^2}{\partial t} dx \\ &\quad - 2mg_{\alpha\beta} \int P_\beta \frac{\partial P_\alpha}{\partial t} dx \end{aligned} \quad (5d)$$

$$\begin{aligned} \frac{d^2}{dt^2}\langle x^2 \rangle_\alpha &= \frac{1}{m} \frac{d}{dt}\langle xp + px \rangle_\alpha = \frac{2\langle p^2 \rangle_\alpha}{m^2} - 2\left\langle x \frac{dV}{dx} \right\rangle_\alpha \\ &\quad + \frac{g_\alpha}{m} \int P_\alpha^2 dx - \frac{2g_{\alpha\beta}}{m} \int x P_\alpha \frac{\partial P_\beta}{\partial x} dx \end{aligned} \quad (5e)$$

where  $\langle\psi_\alpha|p|\psi_\alpha\rangle = \langle p \rangle_\alpha$  denotes the average momentum for species  $\alpha$  and that of species  $\beta$  is  $\langle\psi_\beta|p|\psi_\beta\rangle = \langle p \rangle_\beta$ . These moment equations are exact and hold for all packets. Consequently, they can lead to exact conservation laws which are not found from any other approach. For a free particle of only one species, we note that

$$\langle p \rangle = \text{constant} \quad (6a)$$

$$\left\langle \frac{p^2}{2m} \right\rangle + \frac{g_\alpha}{2} \int P_\alpha^2 dx = \text{constant}. \quad (6b)$$

Clearly equation (6a) corresponds to momentum conservation. Similarly, equation (6b) corresponds to the conservation of energy where the energy of a free particle is its kinetic energy augmented by the ‘‘self energy’’ due to the interaction (the second term in Eq. (6b)). For

the two species problem in free particle regime with equal number of particles for both the species, we find from equation (5b) along with its counterpart for species  $\beta$ ,

$$\begin{aligned} \frac{d}{dt} [\langle p \rangle_\alpha + \langle p \rangle_\beta] &= -g_{\alpha\beta} \int_{-\infty}^{\infty} \left( P_\alpha \frac{\partial P_\beta}{\partial x} + P_\beta \frac{\partial P_\alpha}{\partial x} \right) dx \\ &= -g_{\alpha\beta} \int_{-\infty}^{\infty} \frac{\partial}{\partial x} (P_\alpha P_\beta) dx \\ &= 0 \end{aligned} \tag{7}$$

indicating

$$\langle p \rangle_\alpha + \langle p \rangle_\beta = \text{constant}. \tag{8}$$

This corresponds to the conservation of the total momentum of the two species. From equation (5d) along with its counterpart for species  $\beta$ , we deduce the following for equal number of particles of species  $\alpha$  and  $\beta$ ,

$$\begin{aligned} \frac{\langle p^2 \rangle_\alpha}{2m} + \frac{\langle p^2 \rangle_\beta}{2m} + \frac{g_\alpha}{2} \int P_\alpha^2 dx + \frac{g_\beta}{2} \int P_\beta^2 dx \\ + g_{\alpha\beta} \int P_\alpha P_\beta dx = \text{constant}. \end{aligned} \tag{9}$$

Furthermore, for an arbitrary external potential  $V(x)$ , we get

$$\begin{aligned} \frac{\langle p^2 \rangle_\alpha}{2m} + \langle V \rangle_\alpha + \frac{\langle p^2 \rangle_\beta}{2m} + \langle V \rangle_\beta + \frac{g_\alpha}{2} \int P_\alpha^2 dx \\ + \frac{g_\beta}{2} \int P_\beta^2 dx + g_{\alpha\beta} \int P_\alpha P_\beta dx = \text{constant} \end{aligned} \tag{10}$$

which for the single species problem reduces to

$$\frac{\langle p^2 \rangle}{2m} + \langle V \rangle + g \int \frac{P^2}{2} dx = \text{constant}. \tag{11}$$

Our equation (10) corresponds to the “energy” conservation for the system. The constraint of equal number of particles of the two species is a strong constraint. Also one needs to note the special case where  $g_\alpha = g_\beta = g_{\alpha\beta}$ , when the energy conservation looks identical to the single species case with the “self energy” included. In equation (11) the single species  $P$  is replaced by the sum of  $P_\alpha$  and  $P_\beta$ .

The advantage of using Ehrenfest’s equation for exploring the dynamics lies in being able to obtain constraining equations like equations (8)–(11) corresponding to conservation of energy.

It should be noted though that while the presence of the interaction term in the Gross-Pitaevskii still allows to write some conservation laws till the second moment, there is a clear complication for the higher moments. In this case it is clear that for the third and higher moments, the phase of the evolving wave function is going to play an important role. We point this out with the single species problem for the free particle which is the simplest to implement. We find for the third moment (now we have no subscript on

$g$  and  $g_{\alpha\beta} = 0$  for  $\alpha \neq \beta$ )

$$\frac{d}{dt} \langle x^3 \rangle = \frac{3}{2m} \langle x^2 p + p x^2 \rangle \tag{12}$$

$$\frac{d^2}{dt^2} \langle x^3 \rangle = \frac{3}{m^2} \langle x p^2 + p^2 x \rangle - \frac{3}{2} F(t) \tag{13}$$

where  $F(t) = \frac{g}{m} \int P x^2 \frac{dP}{dx} dx$

$$\frac{d^3}{dt^3} \langle x^3 \rangle = \frac{6}{m^3} \langle p^3 \rangle - \frac{dF}{dt} - \frac{12g}{m} \int x \frac{d}{dx} (P_\alpha) \frac{dP_\alpha}{dt} dx \tag{14}$$

In the above equation,  $\langle p^3 \rangle$  is not a constant of motion, as can be easily seen from its dynamics

$$\frac{d}{dt} \langle p^3 \rangle = -\frac{3g}{m} \int \left[ \frac{d^2 \psi^*}{dx^2} \frac{d}{dx} (P\psi) + \frac{d^2 \psi}{dx^2} \frac{d}{dx} (P\psi^*) \right] dx. \tag{15}$$

The above equation, apart from establishing that  $\langle p^3 \rangle$  is not constant for a free particle, also shows that development of  $\langle p^3 \rangle$  requires knowledge of amplitude and phase of  $\psi$  separately. This is a complication which shows that the higher order moments bring in the details of the dynamics of the wave function and are not determined by the moments alone. This is a fact that needs to be kept in mind while assessing the success in dealing with the low order moments. Once the inevitability of the existence of a phase in the wave-function is accepted, one needs to ask whether any further constraint can be imposed. These can come from the fact that the shape invariance would require the skewness, kurtosis of the distribution to be retained as well. This will sharpen the parameters for shape invariance and also help in relating to the integrable models where an infinite number of constants of motion exist.

Having pointed out a potential problem with higher moments, we now proceed to discuss specific time developments for the peaks and the widths of the initial wave packet. For  $V(x) = \frac{1}{2} m \omega^2 x^2$ , we find by straight forward algebra from equations (5a)–(5e)

$$\begin{aligned} \frac{d^2}{dt^2} (\Delta x) &= -\omega^2 (\Delta x) - \frac{g_{\alpha\beta}}{m} \int dx \left( P_\alpha \frac{dP_\beta}{dx} - P_\beta \frac{dP_\alpha}{dx} \right) \\ &= -\omega^2 (\Delta x) - \frac{2g_{\alpha\beta}}{m} \int dx P_\alpha \frac{dP_\beta}{dx} \end{aligned} \tag{16}$$

where  $\Delta x = \langle x \rangle_\alpha - \langle x \rangle_\beta$  is the separation between the two centers. Similarly the second moment  $S_2 = \langle x^2 \rangle - \langle x \rangle^2$  (in our entire analysis this second moment will be referred as the width of the distribution), is found to have the

dynamics (exact).

$$\begin{aligned} \frac{d^3}{dt^3} S_{2\alpha} + 4\omega^2 \frac{d}{dt} S_{2\alpha} - \frac{g_\alpha}{m} \frac{d}{dt} \int P_\alpha^2 dx &= -4 \frac{g_{\alpha\beta}}{m^2} \\ &\times \int P_\alpha \frac{dP_\beta}{dx} \langle P \rangle_\alpha dx - \frac{2g_{\alpha\beta}}{m} \frac{d}{dt} \\ &\times \int \frac{dP_\beta}{dx} (x - x_\alpha) P_\alpha dx \end{aligned} \quad (17)$$

with a similar equations for the species  $\beta$ . What about the probability distribution  $P_{\alpha,\beta}(x, t)$ ? The structure will be assumed to have the form

$$P_{\alpha,\beta}(x, t) = \frac{1}{\sqrt{S_{2\alpha,\beta}}} \mathcal{F}_{\alpha,\beta} \left( \frac{x - \langle x \rangle_{\alpha,\beta}}{\sqrt{S_{2\alpha,\beta}}} \right) \quad (18)$$

where  $\langle x \rangle_{\alpha,\beta}$  gives the position of the peak and  $S_{2\alpha,\beta}$  corresponds to the width of the distribution  $P_{\alpha,\beta}$  (for a Gaussian distribution  $S_{2\alpha,\beta}$  will be the standard deviation), which makes the strong supposition that an initial form of the probability distribution (provided through the initial condition for the GPE) will be preserved with the time dependencies appearing in  $\langle x \rangle$  and  $S_2$ . The primary issue will be to check whether this assumption is reasonable or not. In the next two sections we will use this technique to discuss the dynamics of the wave packets separately in the free particle regime and in a simple harmonic confining potential.

## 2 Dynamics in free particle regime

We consider the initial condition of equation (2) appropriate at  $t = 0$  when the trap is switched off. Subsequently the dynamics is that of a free system. The free system we consider does not imply that the condensate is non interacting. Rather the vital role of the entire dynamics is dictated by the inter and intra species interactions. After realizing the condensate in the trap, the trap is switched off and we study the condensate in absence of any external trapping potential.

Depending upon the sign of  $D = g_\alpha g_\beta - g_{\alpha\beta}^2$ , we can have phase separated or overlapping initial densities of the two species [17,18]. For positive values of  $D$ , we have overlapping wave functions and for  $D < 0$ , we have separated wave functions. We accordingly write the initial wave packets for species  $\alpha$  and  $\beta$  having width  $\Delta_\alpha$  and  $\Delta_\beta$  respectively as

$$\begin{aligned} \psi_\alpha(x, t = 0) &= \frac{\sqrt{N_\alpha}}{(2\pi\Delta_{0\alpha}^2)^{1/4}} e^{-\frac{(x-x_{0\alpha})^2}{4\Delta_{0\alpha}^2}} e^{ip_{0\alpha}x} \\ \psi_\beta(x, t = 0) &= \frac{\sqrt{N_\beta}}{(2\pi\Delta_{0\beta}^2)^{1/4}} e^{-\frac{(x-x_{0\beta})^2}{4\Delta_{0\beta}^2}} e^{ip_{0\beta}x} \end{aligned} \quad (19)$$

with the understanding that  $|x_{0\alpha} - x_{0\beta}| < \sqrt{\Delta_{0\alpha}^2 + \Delta_{0\beta}^2}$  corresponds to overlapping initial condition. Whereas, the

initial condition in the phase separated domain is dictated by  $|x_{0\alpha} - x_{0\beta}| > \sqrt{\Delta_{0\alpha}^2 + \Delta_{0\beta}^2}$ ; where  $\Delta_{0\alpha}$  and  $\Delta_{0\beta}$  correspond to the initial widths and  $N_\alpha$  and  $N_\beta$  are the total number of atoms within the condensate for species  $\alpha$  and  $\beta$  respectively.  $x_{0\alpha}$  and  $p_{0\alpha}$  are the initial position and momentum for the wave packet of species  $\alpha$  and  $x_{0\beta}$  and  $p_{0\beta}$  are those of species  $\beta$ . In what follows, we will assume that it is possible to discuss the separate evolution of  $\psi_\alpha$  and  $\psi_\beta$ , although the parameters of one will influence those of the others.

With the help of equations (19) and (5a)–(5e), we derive the following dynamical equations for the width of the wave packets.

$$\begin{aligned} \ddot{\Delta}_\alpha^2 &= \frac{\hbar^2}{m^2 \Delta_\alpha^2} + \frac{g_\alpha}{m} \frac{1}{\sqrt{2\pi} \Delta_\alpha} + \frac{2g_{\alpha\beta}}{m} \frac{e^{-(x_d/\Delta)^2}}{\sqrt{\pi} \Delta^2} \\ &\times \left[ 1 - \left( \frac{x_d}{\Delta} \right)^2 \right] \left( \frac{\Delta_\alpha}{\Delta} \right)^2 \end{aligned} \quad (20a)$$

$$\begin{aligned} \ddot{\Delta}_\beta^2 &= \frac{\hbar^2}{m^2 \Delta_\beta^2} + \frac{g_\beta}{m} \frac{1}{\sqrt{2\pi} \Delta_\beta} + \frac{2g_{\alpha\beta}}{m} \frac{e^{-(x_d/\Delta)^2}}{\sqrt{\pi} \Delta^2} \\ &\times \left[ 1 - \left( \frac{x_d}{\Delta} \right)^2 \right] \left( \frac{\Delta_\beta}{\Delta} \right)^2 \end{aligned} \quad (20b)$$

$$\ddot{x}_d = \frac{4g_{\alpha\beta}}{\sqrt{\pi} m} \frac{e^{-(x_d/\Delta)^2}}{\Delta^3} x_d \quad (20c)$$

where  $x_d(t) = (x_{0\alpha}(t) - x_{0\beta}(t))$  is the distance between the peak of the wave packets at time  $t$  and we define  $\Delta^2(t) = \Delta_\alpha^2(t) + \Delta_\beta^2(t)$ . Without any ambiguity, for species  $\alpha$ , the symbol  $\ddot{\Delta}_\alpha^2$  implies  $\frac{d^2 \Delta_\alpha^2}{dt^2}$  and the same holds for species  $\beta$  also.

It should be noted that in the case of  $g_\alpha = g_\beta = g_{\alpha\beta} = 1 (D = 0)$ , our system reduces to exactly integrable Manakov model [19] whose single soliton solution [20,21] is of the variety  $\text{sech}[x - x_0(t)]/\Delta$  as opposed to the Gaussian chosen here. The importance of all the  $g$ 's being equal is now transparent. Among the infinite number of conservation laws for an exactly integrable model, the ‘‘momentum’’ and ‘‘energy’’ conservations should be there. The equality of all the  $g$ 's allows for the energy conservation here. In equation (19) we can take the  $\text{sech}(x)$  form and ask the question: what would be the value of  $\Delta$  for an almost shape invariant state. This will be the approximation to the exact bright soliton solutions found in [19–21].

### 2.1 Dynamics under overlapping initial condition ( $\frac{x_d}{\Delta} \ll 1$ )

At first, we consider the case of a strongly overlapping (completely mixed) initial state where  $x_d \ll \Delta$ . This situation will persist as can be seen from equation (20c), only if  $g_{\alpha\beta} < 0$ . Imposing this constraint

on equations (20a) and (20b) we get

$$\ddot{\Delta}_\alpha^2 = \frac{\hbar^2}{m^2 \Delta_\alpha^2} + \frac{g_\alpha}{m} \frac{1}{\sqrt{2\pi} \Delta_\alpha} + \frac{2g_{\alpha\beta}}{m} \frac{1}{\sqrt{\pi} \Delta} \left( \frac{\Delta_\alpha}{\Delta} \right)^2 \tag{21a}$$

$$\ddot{\Delta}_\beta^2 = \frac{\hbar^2}{m^2 \Delta_\beta^2} + \frac{g_\beta}{m} \frac{1}{\sqrt{2\pi} \Delta_\beta} + \frac{2g_{\alpha\beta}}{m} \frac{1}{\sqrt{\pi} \Delta} \left( \frac{\Delta_\beta}{\Delta} \right)^2. \tag{21b}$$

It is now relevant to ask whether the above dynamical system has a stable fixed point  $\Delta_{\alpha 0}, \Delta_{\beta 0}, \dot{\Delta}_{\alpha 0} = \dot{\Delta}_{\beta 0} = 0$ . If the form of the wave packet is preserved  $\dot{\Delta}_{\alpha 0} = \dot{\Delta}_{\beta 0} = 0$ . Solving equations (21a) and (21b) numerically with the constraint  $\dot{\Delta}_\alpha = 0 = \dot{\Delta}_\beta$  we obtain the critical value of the widths ( $\Delta_{\alpha c}$  and  $\Delta_{\beta c}$ ) of the wave packets for a particular set of coupling constants ( $g_\alpha, g_\beta, g_{\alpha\beta}$ ). If this fixed point exists and is stable, we will have a ‘‘coherent state’’ – a state which propagates without change of initial shape, i.e.,  $\psi(x, t) = \psi(x - x_0(t), 0)$ . At this point we stop the analysis and go through the numerics to check the validity of analytical findings. In particular, we consider the Gaussian wave packet with initial widths set at their critical value and observe whether the width changes with time or not.

**Numerical results:** For the dimensionless analysis of the theory all the coupling constants are rescaled as  $g = \sqrt{2\pi} \gamma \frac{\hbar p_0}{m}$ . All the concerned length and time units are rescaled by  $\frac{\hbar}{p_0}$  and  $\frac{p_0^2}{m\hbar}$  respectively.

### 2.1.1 Solving analytically obtained ODE

In dimensionless form equations (20a)–(20c) appear as following

$$\frac{d^2 \sigma_\alpha^2}{dt^2} = \frac{1}{\sigma_\alpha^2} + \frac{\gamma_\alpha}{\sigma_\alpha} + 2\sqrt{2} \gamma_{\alpha\beta} \sigma_\alpha^2 \frac{e^{-\frac{x_d^2}{\sigma_\alpha^2}}}{\sigma^3} \left[ 1 - \frac{x_d^2}{\sigma^2} \right] \tag{22}$$

$$\frac{d^2 \sigma_\beta^2}{dt^2} = \frac{1}{\sigma_\beta^2} + \frac{\gamma_\beta}{\sigma_\beta} + 2\sqrt{2} \gamma_{\alpha\beta} \sigma_\beta^2 \frac{e^{-\frac{x_d^2}{\sigma_\beta^2}}}{\sigma^3} \left[ 1 - \frac{x_d^2}{\sigma^2} \right] \tag{23}$$

$$\frac{d^2 x_d}{dt^2} = 4\sqrt{2} \gamma_{\alpha\beta} e^{-\frac{x_d^2}{\sigma^2}} \frac{x_d}{\sigma^3} \tag{24}$$

where  $\sigma$  corresponds to the width of the wave packets in dimensionless form and  $\sigma^2 = \sigma_\alpha^2 + \sigma_\beta^2$ . Before proceeding towards the numerical verification of our analysis, we consider the existence of such wave packets having width  $\sigma_{\alpha c}$  and  $\sigma_{\beta c}$  and we explore the behavior of the widths of the wave packets around these coherent widths. We do linear stability analysis by considering the width modulation  $\delta\sigma_\alpha(x, t)$  and  $\delta\sigma_\beta(x, t)$ .

$$\begin{aligned} \sigma_\alpha^2(x, t) &= \sigma_{\alpha c}^2 + \delta\sigma_\alpha^2(x, t) \\ \sigma_\beta^2(x, t) &= \sigma_{\beta c}^2 + \delta\sigma_\beta^2(x, t). \end{aligned} \tag{25}$$

Considering only the linear terms, with the help of equations (22)–(24) and taking the dimensionless argument of the theory into account, the flow equations for the width modulations takes the following dimensionless form

$$\begin{aligned} \delta\ddot{\sigma}_\alpha^2 &= \left[ \frac{\gamma_\alpha}{2\sigma_{\alpha c}^3} + 4\sqrt{2} \frac{\gamma_{\alpha\beta}}{\sigma_c^3} \left( 1 - \frac{3}{4} \left( \frac{\sigma_{\alpha c}}{\sigma_c} \right)^2 \right) \right] \delta\sigma_\alpha^2 \\ &\quad - 3\sqrt{2} \gamma_{\alpha\beta} \frac{\sigma_{\alpha c}^2}{\sigma_c^5} \delta\sigma_\beta^2 \\ \delta\ddot{\sigma}_\beta^2 &= \left[ \frac{\gamma_\beta}{2\sigma_{\beta c}^3} + 4\sqrt{2} \frac{\gamma_{\alpha\beta}}{\sigma_c^3} \left( 1 - \frac{3}{4} \left( \frac{\sigma_{\beta c}}{\sigma_c} \right)^2 \right) \right] \delta\sigma_\beta^2 \\ &\quad - 3\sqrt{2} \gamma_{\alpha\beta} \frac{\sigma_{\beta c}^2}{\sigma_c^5} \delta\sigma_\alpha^2. \end{aligned} \tag{26}$$

Considering  $\delta\sigma_j^2(x, t) = \delta\sigma_j^2(x) e^{-\Omega t}$  with  $j = \alpha, \beta$  we reach into the solution of  $\Omega$

$$\Omega^2 = -B \pm \sqrt{B^2 - 4C}$$

with

$$B = - \left[ 5\sqrt{2} \frac{\gamma_{\alpha\beta}}{\sigma_c^3} + \frac{1}{2} \left( \frac{\gamma_\alpha}{\sigma_{\alpha c}^3} + \frac{\gamma_\beta}{\sigma_{\beta c}^3} \right) \right]$$

and

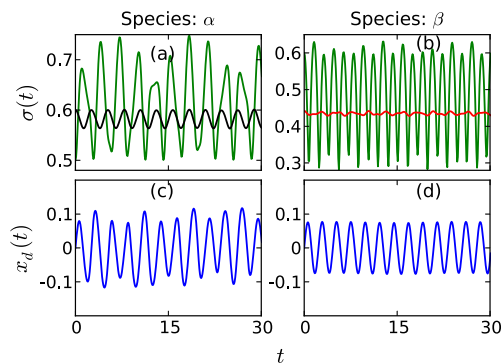
$$\begin{aligned} B^2 - 4C &= \left[ \frac{1}{2} \left( \frac{\gamma_\alpha}{\sigma_{\alpha c}^3} + \frac{\gamma_\beta}{\sigma_{\beta c}^3} \right) - 3\sqrt{2} \frac{\gamma_{\alpha\beta}}{\sigma_c^3} \right]^2 - \frac{\gamma_\alpha \gamma_\beta}{\sigma_{\alpha c}^3 \sigma_{\beta c}^3} \\ &\quad + 6\sqrt{2} \frac{\gamma_{\alpha\beta}}{\sigma_c^5} \left( \gamma_\alpha \frac{\sigma_{\beta c}^2}{\sigma_\alpha^3} + \gamma_\beta \frac{\sigma_{\alpha c}^2}{\sigma_\beta^3} \right). \end{aligned}$$

To have stable oscillatory solution  $\Omega^2$  must be less than zero. Considering  $\gamma_{\alpha\beta} < 0$ , one can have stable oscillatory solution if  $|\gamma_{\alpha\beta}| < \frac{\sigma_c^3}{10\sqrt{2}} \left( \frac{\gamma_\alpha}{\sigma_{\alpha c}^3} + \frac{\gamma_\beta}{\sigma_{\beta c}^3} \right)$ . Henceforth we proceed to analyze the following two scenarios under overlapping initial condition.

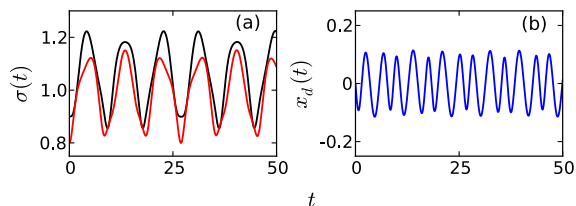
- All the coupling constants are considered negative

After solving equations (22) and (24) numerically, we observe the presence of shape invariant states. These are the states for which the widths of the wave packet remain almost constant with time. For free particle regime, where the free expansion of the wave packet is well known, our study has interesting implications. Considering  $\gamma_\alpha = -1.0, \gamma_\beta = -2.0, \gamma_{\alpha\beta} = -0.5$  we obtain the coherent widths  $\sigma_{\alpha c} = 0.6$  and  $\sigma_{\beta c} = 0.442$ . In Figure 1 we have shown the presence of shape invariant states when the initial widths  $\sigma_{0\alpha}$  and  $\sigma_{0\beta}$  are taken equal to the coherent widths. The black solid line in Figure 1a and the red solid line in Figure 1b indicate the presence of shape invariant states for species  $\alpha$  and  $\beta$  respectively. The green solid lines in Figures 1a and 1b represent the dynamics of width for species  $\alpha$  and  $\beta$  respectively under arbitrary initial conditions. The significant changes in the widths with time imply the absence of shape invariant states for both the species under any arbitrary initial condition.





**Fig. 1.** Dynamics of free particle wave packets under overlapping initial condition ( $\frac{x_d}{\Delta} \ll 1$ ) when both of them starts from same initial position  $x_d(0) = 0$  but possess different initial momentum  $\frac{dx_d}{dt}|_{t=0} \neq 0$ . (a) Dynamics of the width of the wave packet corresponding to the species  $\alpha$ . Black solid line indicates the presence of coherent states when appropriate initial condition ( $\gamma_\alpha = -1.0$ ,  $\gamma_\beta = -2.0$ ,  $\gamma_{\alpha\beta} = -0.5$ ,  $\sigma_{0\alpha} = 0.6 = \sigma_{\alpha c}$  and  $\sigma_{0\beta} = 0.442 = \sigma_{\beta c}$ .) is satisfied. Green solid line is obtained when the initial width of the wave packets are chosen arbitrarily ( $\sigma_{0\alpha} = 0.5$  and  $\sigma_{0\beta} = 0.6$ ). (b) Dynamics of the width of the wave packet corresponding to the species  $\beta$ . Red solid line corresponds to the coherent states and green solid line is for any arbitrary wave packets. In (c), the dynamics of  $x_d$  are shown for the wave packets when the widths are chosen arbitrarily (i.e., wave packets are not shape invariant) and (d) shows the dynamics of  $x_d$  for shape invariant case.



**Fig. 2.** Dynamics of the free particle wave packets with  $x_d(0) = 0$ .  $\gamma_\alpha = 0.66$ ,  $\gamma_\beta = 0.324$ ,  $\gamma_{\alpha\beta} = -1.5$ ,  $\sigma_{0\alpha} = 0.9 = \sigma_{\alpha c}$  and  $\sigma_{0\beta} = 0.8 = \sigma_{\beta c}$ . (a) Bounded oscillation of the widths (black for species  $\alpha$  and red for species  $\beta$ ) of the wave packets. This shows the existence of shape invariant states approximately even in case of repulsive interspecies interaction. (b) Dynamics of  $x_d$ .

Figures 1c and 1d display the dynamics of  $x_d$  in absence and presence of shape invariant states respectively.

- Intra species coupling constants are positive and interspecies coupling constant is considered negative

In this part of study, we consider two wave packets initially at the same position such that  $x_d(0) = 0$  and they are moving with equal momentum such that  $\frac{dx_d}{dt} = 0$  is satisfied. Both the species have repulsive interaction among themselves ( $\gamma_\alpha > 0$ ,  $\gamma_\beta > 0$ ) whereas the interspecies interaction is attractive, i.e.,  $\gamma_{\alpha\beta} < 0$ . For a free particle, the wave packet in generally expands with time indicating the delocalization in space. Figure 2 clearly shows that even if there is repulsive intraspecies interaction, there is a possibility of bounded oscillation of widths

of the wave packets in presence of attractive interspecies interaction provided the proper initial condition is satisfied, i.e., the initial widths are chosen equal to their corresponding coherent widths. Considering  $\gamma_\alpha = 0.66$ ,  $\gamma_\beta = 0.324$ ,  $\gamma_{\alpha\beta} = -1.5$ , we have obtained  $\sigma_{\alpha c} = 0.9$  and  $\sigma_{\beta c} = 0.8$ . However, in this case, Figure 2 displays that the presence of shape invariant state is approximate for both the species. This finding is in qualitative good agreement with the study of Pérez-García et al. [22] where the existence of bright solitons had been reported in quasi-one-dimensional heteronuclear multicomponent Bose–Einstein condensates with repulsive self-interaction and attractive interspecies interaction. In presence of a sufficiently attractive interspecies interaction, the presence of bright solitons in two-component repulsive BECs has also been observed in the study by Adhikari [23].

### 2.1.2 Solving the pair of CGPE

Numerically integrating the pair of coupled GP equations in equation (1) and considering the proper initial conditions, below we present the numerical results which reasonably agree with the analytical predictions of existence of coherent wave packets. For the numerical solution of nonlinear Schrödinger equation, spectral collocation method [24], time splitting spectral approximation [25] had been introduced. Pseudospectral and finite-difference methods [26] had also been adapted for solving three dimensional GP equations. However, we follow Crank-Nicolson scheme which has been developed and extensively used in numerical study of CGPE [27,28].

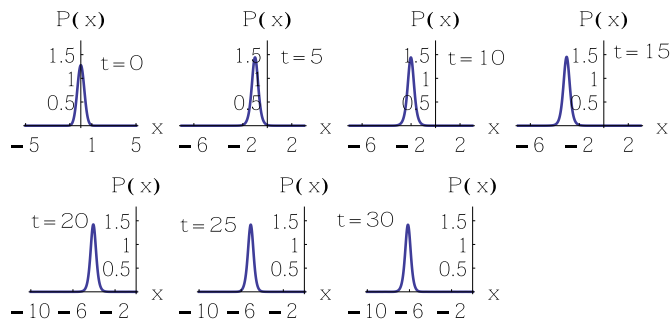
- All the coupling constants are negative

Considering the interaction parameters  $\gamma_\alpha = -1.0$ ,  $\gamma_\beta = -2.0$ ,  $\gamma_{\alpha\beta} = -0.5$  and the initial widths  $\sigma_{0\alpha} = 0.6 = \sigma_{\alpha c}$  and  $\sigma_{0\beta} = 0.442 = \sigma_{\beta c}$ , the dynamics of the wave packets have been shown in Figures 3 and 4. Both the wave packets start from the same initial position ( $x_{0\alpha} = x_{0\beta} = 0$ ) having initial momenta which are same in amplitude but opposite in direction ( $p_{0\alpha} = -0.2 = p_{0\beta}$ ). With time both the wave packets move together and retain their initial shapes. Hence the coherent state is discernible when the wave packets overlap with each other.

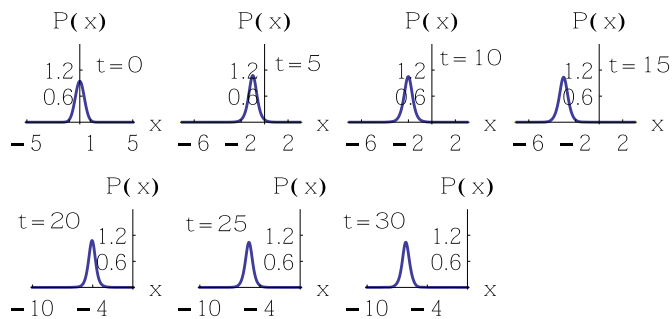
Figures 5 and 6 show that even in the presence of positive intra species interaction, the widths of the wave packets remain approximately constant if the proper initial conditions are satisfied. This is in good agreement with the solution of analytically obtained ODE in Figure 2 where bounded oscillations of widths of the wave packets have been observed. We have considered  $\gamma_\alpha = 0.66$ ,  $\gamma_\beta = 0.324$ , and  $\gamma_{\alpha\beta} = -1.5$  which provides  $(\sigma_{\alpha c}) = 0.9$  and  $(\sigma_{\beta c}) = 0.8$  for shape invariance condition to be satisfied. The presence of nearly shape invariant states in this case confirms the robustness of the coherent nature of the wave packets in case of binary BEC when intraspecies interaction are repulsive.

- Intra species coupling constants are positive

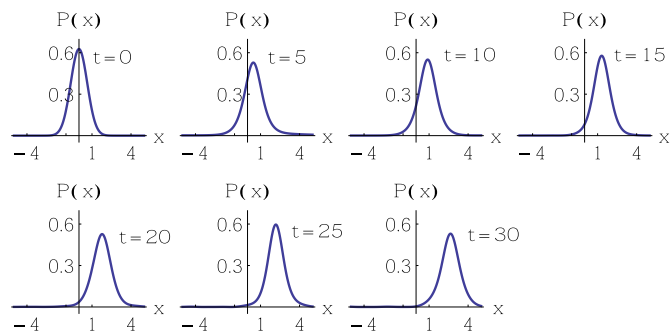
The dynamics in Figures 5 and 6 show that both of the wave packets move in the same direction in spite of having the momentum in opposite direction. This behavior



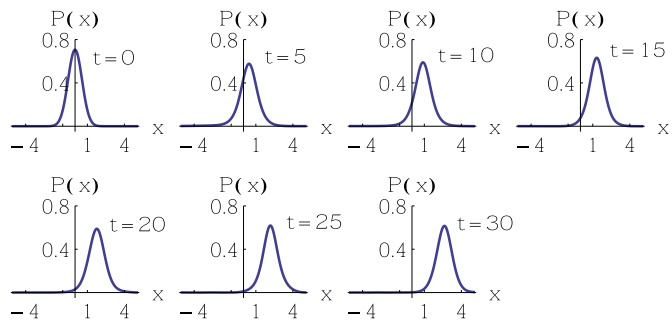
**Fig. 3.** Dynamics of the wave packet for species  $\beta$  in free particle regime. With the evolution of time, the wave packet retains its initial shape. For  $\gamma_\alpha = -1.0$ ,  $\gamma_\beta = -2.0$  and  $\gamma_{\alpha\beta} = -0.5$ , the initial widths  $\sigma_{0\alpha} = 0.6 = \sigma_{\alpha c}$  and  $\sigma_{0\beta} = 0.442 = \sigma_{\beta c}$  are considered. The initial momentums for both the wave packets are taken equal ( $p_{0\alpha} = -0.2 = p_{0\beta}$ ).



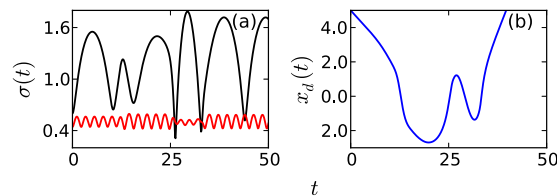
**Fig. 4.** Dynamics of the wave packet for species  $\alpha$  in free particle regime. The figure shows that the wave packet retains its initial shape. The initial widths of the wave packets are considered to be equal to their coherent widths (as obtained from analytics), i.e.,  $\sigma_{0\alpha} = 0.6 = \sigma_{\alpha c}$  and  $\sigma_{0\beta} = 0.442 = \sigma_{\beta c}$  to keep the wave packets shape invariant. The coupling constants are:  $\gamma_\alpha = -1.0$ ,  $\gamma_\beta = -2.0$ ,  $\gamma_{\alpha\beta} = -0.5$ . The initial momentum of the wave packets for each of the species is taken equal  $p_{0\alpha} = -0.2 = p_{0\beta}$ .



**Fig. 5.** Dynamics of the wave packet for species  $\alpha$  in free particle regime. The interaction parameters are  $\gamma_\alpha = 0.66$ ,  $\gamma_\beta = 0.324$ ,  $\gamma_{\alpha\beta} = -1.5$  and we considered the initial widths ( $\sigma_{0\alpha} = 0.9 = \sigma_{\alpha c}$  and ( $\sigma_{0\beta} = 0.8 = \sigma_{\beta c}$ ). The initial momentums are considered different:  $p_{0\alpha} = -0.2$ ;  $p_{0\beta} = 0.4$  for species  $\alpha$  and  $\beta$  respectively.



**Fig. 6.** Dynamics of the wave packet for species  $\beta$  in free particle regime. All the parameters and initial conditions are the same as Figure 5.



**Fig. 7.** Dynamics of the free particle wave packets in the phase separated regime. The wave packets are initially at a fairly large distance from each other ( $x_d(0) \gg \sigma_{\alpha,\beta}$ ). (a) Dynamics of the widths of the wave packets. Black curve is for species  $\alpha$  and red is that for species  $\beta$ . We have considered  $x_d(0) = 5.0$  and  $\frac{dx_d}{dt}|_{t=0} = -0.25$ , i.e., the wave packet of species  $\beta$  has greater initial momentum than that of  $\alpha$  and in course of time both of the wave packet will merge and then the wave packet with higher momentum will overtake the other one. All other parameters are same as in Figure 1a. The wave packet for species  $\alpha$  lose its coherence nature although that for species  $\beta$  somehow retains its initial shape.

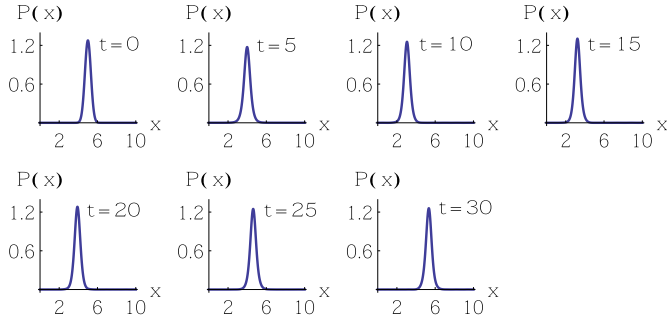
can be understood taking the flow equations into account. We note from equation (5b) that for negative  $g_{\alpha\beta}$ ,  $\frac{d\langle p \rangle}{dt}$  is always positive. Hence an initially negative  $\langle p \rangle$  will become positive after a short time and will remain positive. With  $\frac{d\langle x \rangle}{dt}$  being determined by  $\langle p \rangle$  (Eq. (5a)), both species will have positive  $\langle p \rangle$  after an initial phase and the average  $\langle x \rangle$  remains to the right of the origin.

## 2.2 Dynamics when $x_d/\Delta$ is not small

In this part of study, since  $x_d/\Delta$  is not small, we take the wave packets to be initially separated by a moderate distance such that they can belong to the initially phase separated regime.

### – Solving set of ODE

The numerical findings suggest that this case is the very interesting one since it can have the possibility of mixing the two wave packets starting from initially phase separated regime. Initially the wave packets are apart from each other ( $x_d(0) = 5.0$ ), and in course of time when  $x_d$  becomes zero, the two wave packets indeed enter into the mixed regime around  $t \approx 12$ . This possibility is shown in Figure 7b. However, the widths of the wave packets start behaving peculiarly as shown in Figure 7a and coherence



**Fig. 8.** Dynamics of the wave packet for species  $\beta$  in phase separated regime. Wave packets are initially at a fairly large distance from each other such that  $(x_d(0) \gg \sigma_{\alpha,\beta})$ . We have considered  $x_{0\alpha} = 0.0$  and  $x_{0\beta} = 5.0$ .  $\frac{dx_d}{dt}|_{t=0} < 0$ , i.e., the wave packet of species  $\beta$  has greater magnitude of initial momentum ( $p_{0\beta} = -0.2$ ) than that of  $\alpha$  ( $p_{0\alpha} = 0.1$ ). All other parameters are same as in Figure 1a. The wave packet somehow manages the coherent nature.

property of the wave packet for species  $\alpha$  is completely lost in this case.

#### – Solving CGPE

Solving pair of coupled GP equations numerically under phase separated initial condition we observe in Figures 8 and 9 that it is very hard to retain the coherent nature of both of the wave packets simultaneously when the wave packets have a possibility of collision with each other. To investigate the possibility in Figures 8 and 9 we set  $p_{0\alpha} = 0.1$  and  $p_{0\beta} = -0.2$  while  $x_{0\alpha} = 0.0$  and  $x_{0\beta} = 5.0$  such that two of them can undergo collision while moving. In fact, we observe the breakdown of the Gaussian nature of the  $\alpha$  wave packet though the wave packet for species  $\beta$  remains approximately shape invariant.

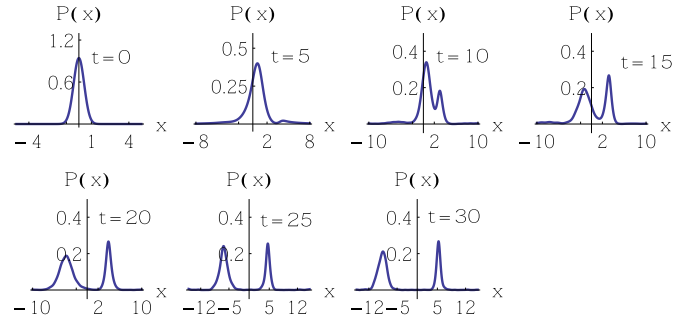
On the other hand, in the phase separated domain, if the directions of the motions of the wave packets are such that they do not have a possibility to collide with each other, then in absence of collision, we observe the coherent states (not shown in figure).

### 3 Dynamics when system is trapped in SHO

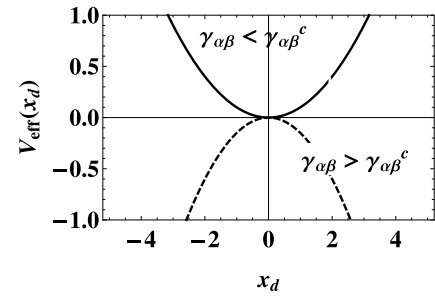
In this section, we consider the condensate in a harmonic oscillator potential,  $V(x) = \frac{1}{2}m\omega^2x^2$  and with the help of equations (19) and (5a)–(5e), we obtain the following equation of motion for the width of the wave packets.

$$\begin{aligned} \ddot{\Delta}_\alpha^2 &= \frac{\hbar^2}{m^2\Delta_\alpha^2} - 2\omega^2\Delta_\alpha^2 + \frac{g_\alpha}{m} \frac{1}{\sqrt{2\pi}\Delta_\alpha} \\ &+ \frac{2g_{\alpha\beta}}{m} \frac{e^{-\frac{x_d^2}{\Delta^2}}}{\sqrt{\pi}\Delta} \left[ 1 - \frac{x_d^2}{\Delta^2} \right] \frac{\Delta_\alpha^2}{\Delta^2} \end{aligned} \quad (27a)$$

$$\begin{aligned} \ddot{\Delta}_\beta^2 &= \frac{\hbar^2}{m^2\Delta_\beta^2} - 2\omega^2\Delta_\beta^2 + \frac{g_\beta}{m} \frac{1}{\sqrt{2\pi}\Delta_\beta} \\ &+ \frac{2g_{\alpha\beta}}{m} \frac{e^{-\frac{x_d^2}{\Delta^2}}}{\sqrt{\pi}\Delta} \left[ 1 - \frac{x_d^2}{\Delta^2} \right] \frac{\Delta_\beta^2}{\Delta^2} \end{aligned} \quad (27b)$$



**Fig. 9.** Dynamics of the wave packet for species  $\alpha$  in phase separated regime. All the initial conditions are same as in Figure 8 and all the parameters are the same as in Figure 1a. The wave packet not only lose its coherent nature but due to the collision with other wave packet, it loses its initial Gaussian shape also.



**Fig. 10.** Schematic diagram of the effective potential as a function of  $x_d$  when  $\gamma_{\alpha\beta} > 0$ . Solid black curve is obtained when  $\gamma_{\alpha\beta} < \frac{1}{4\sqrt{2}}(\sigma_{\alpha c}^2 + \sigma_{\beta c}^2)^{\frac{3}{2}}$  is satisfied. Under this type of potential  $x_d$  will have bounded oscillation around minima ( $x_d = 0$ ). Dashed black curve shows unbounded motion of  $x_d$  implying a possibility of transition from overlapping state to phase separated state.

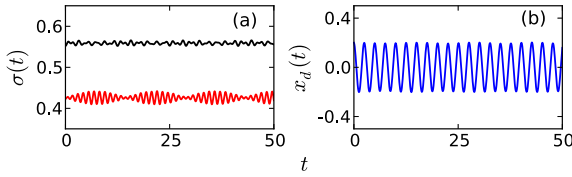
$$\ddot{x}_d = -\omega^2x_d + \frac{4g_{\alpha\beta}}{\sqrt{\pi}m} \frac{e^{-\frac{x_d^2}{\Delta^2}}}{\Delta^3}x_d \quad (27c)$$

where  $x_d = x_{0\alpha} - x_{0\beta}$ . As in the case of free particle, here also the wave packet dynamics can be studied both in the completely overlapping state with initial condition  $|x_{0\alpha} - x_{0\beta}| < \sqrt{\Delta_\alpha^2 + \Delta_\beta^2}$  and in the phase separated state for  $|x_{0\alpha} - x_{0\beta}| > \sqrt{\Delta_\alpha^2 + \Delta_\beta^2}$ . Hereafter we will analyze the dynamics of the wave packets under these two initial conditions in detail.

#### 3.1 Dynamics under overlapping initial condition ( $\frac{x_d}{\Delta} \ll 1$ )

Like free particle case, here also we assume the existence of coherent wave packets having width  $\Delta_{\alpha c}$  and  $\Delta_{\beta c}$  and we proceed to explore the behavior of the widths of the wave packets around the coherent widths. Following the same analysis as we did for free particle case, here in the harmonic oscillator domain, the flow equations for the width





**Fig. 11.** Dynamics of the wave packets in SHO under attractive interspecies interaction when overlapping initial condition is satisfied. (a) Dynamics of the widths of the wave packets for species  $\alpha$  (solid black) and  $\beta$  (dashed red) with initial condition  $x_d(t = 0) = 0.2$  and  $\frac{d}{dt}x_d = -0.05$ .  $\gamma_\alpha = -1.0$ ,  $\gamma_\beta = -2.0$ ,  $\gamma_{\alpha\beta} = -0.336$ ,  $\sigma_{0\alpha} = 0.552 == \sigma_{\alpha c}$  and  $\sigma_{0\beta} = 0.423 == \sigma_{\beta c}$ . Both the wave packets remains almost shape invariant. (b) Dynamics of  $x_d$ .

modulations take the following dimensionless form

$$\begin{aligned} \delta\ddot{\sigma}_\alpha^2 &= -\left[3 + 3\sqrt{2}\gamma_{\alpha\beta}\frac{\sigma_{\alpha c}^2}{\sigma_c^5} - \frac{\gamma_\alpha}{2\sigma_{\alpha c}^3}\right]\delta\sigma_\alpha^2 \\ &\quad - 3\sqrt{2}\gamma_{\alpha\beta}\frac{\sigma_{\alpha c}^2}{\sigma_c^5}\delta\sigma_\beta^2 \\ \delta\ddot{\sigma}_\beta^2 &= -\left[3 + 3\sqrt{2}\gamma_{\alpha\beta}\frac{\sigma_{\beta c}^2}{\sigma_c^5} - \frac{\gamma_\beta}{2\sigma_{\beta c}^3}\right]\delta\sigma_\beta^2 \\ &\quad - 3\sqrt{2}\gamma_{\alpha\beta}\frac{\sigma_{\beta c}^2}{\sigma_c^5}\delta\sigma_\alpha^2 \end{aligned} \quad (28)$$

where  $\sigma_{\alpha c}$  and  $\sigma_{\beta c}$  are the magnitudes of the coherent widths such that  $\Delta_{\alpha c} = \sigma_{\alpha c}\sqrt{\frac{\hbar}{m\omega}}$  and  $\Delta_{\beta c} = \sigma_{\beta c}\sqrt{\frac{\hbar}{m\omega}}$ . Like free particle case in Section 2, here also all the coupling constants are rescaled as  $g = \sqrt{2\pi}\gamma\hbar\omega\sqrt{\frac{\hbar}{m\omega}}$ , all the concerned length and time unit are rescaled by  $\sqrt{\frac{\hbar}{m\omega}}$  and  $\omega^{-1}$  respectively. Considering  $\delta\sigma_j^2(x, t) = \delta\sigma_j^2(x)e^{-\Omega t}$  with  $j = \alpha, \beta$  we reach into the solution of  $\Omega$

$$\Omega^2 = -B \pm \sqrt{B^2 - 4C} \quad (29)$$

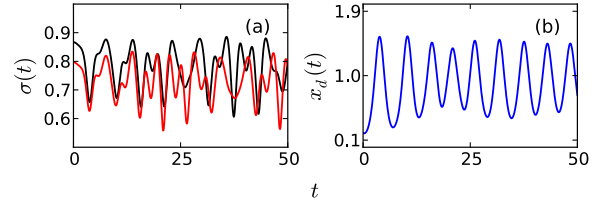
with

$$B = \left[3\sqrt{2}\frac{\gamma_{\alpha\beta}}{(\alpha^2 + \beta^2)^{3/2}} - \frac{(\gamma_\alpha + \gamma_\beta)}{2} + 6\right]$$

and

$$\begin{aligned} B^2 - 4C &= \left[\left(3\sqrt{2}\frac{\gamma_{\alpha\beta}}{(\alpha^2 + \beta^2)^{3/2}} - \frac{(\gamma_\alpha + \gamma_\beta)}{2}\right)^2\right. \\ &\quad \left.+ (6\sqrt{2}\gamma_{\alpha\beta}\frac{(\gamma_\alpha\beta^2 + \gamma_\beta\alpha^2)}{(\alpha^2 + \beta^2)^{5/2}} - \gamma_\alpha\gamma_\beta)\right]. \end{aligned}$$

To have stable oscillatory solution  $\Omega^2$  must be less than zero which can be possible if  $B > 0$  along with the condition  $\gamma_{\alpha\beta} < \frac{1}{6\sqrt{2}}\frac{\gamma_\alpha\gamma_\beta\sigma_c^5}{\sigma_{\alpha c}^3\sigma_{\beta c}^3\left[\gamma_\alpha\frac{\sigma_{\beta c}^2}{\sigma_{\alpha c}^3} + \gamma_\beta\frac{\sigma_{\alpha c}^2}{\sigma_{\beta c}^3}\right]}$ .



**Fig. 12.** Dynamics of the wave packets in SHO under repulsive interspecies interaction when overlapping initial condition is satisfied. (a) Dynamics of the width of the wave packets for species  $\alpha$  (solid black) and  $\beta$  (dashed red) with initial condition  $x_d(t = 0) = 0.2$  and  $\frac{d}{dt}x_d = -0.05$ .  $\gamma_\alpha = -0.5$ ,  $\gamma_\beta = -0.75$ ,  $\gamma_{\alpha\beta} = 0.577$ ,  $(\sigma_{0\alpha}) = 0.867 == \sigma_{\alpha c}$  and  $(\sigma_{0\beta}) = 0.797 == \sigma_{\beta c}$ . The widths of both of the wave-packets remain localized and shows bounded oscillation in presence of positive  $\gamma_{\alpha\beta}$ . Whereas, the dynamics of  $x_d$  in (b) High amplitude oscillation indicating a possibility of transition from overlapping to phase separated state as is expected from the corresponding effective potential in Figure 10.

Considering the limit  $x_d \ll \Delta$  and following the same analysis as was done earlier in case of free particle, we obtain pair of equation (30) for the coherent wave packets.

$$\begin{aligned} \frac{1}{\sigma_{\alpha c}^2} - 2\sigma_{\alpha c}^2 + \frac{\gamma_\alpha}{\sigma_{\alpha c}} &= -2\sqrt{2}\frac{\gamma_{\alpha\beta}}{\sqrt{(\sigma_{\alpha c}^2 + \sigma_{\beta c}^2)}} \\ &\quad \times \left(\frac{\sigma_{\alpha c}^2}{\sigma_{\alpha c}^2 + \sigma_{\beta c}^2}\right) \\ \frac{1}{\sigma_{\beta c}^2} - 2\sigma_{\beta c}^2 + \frac{\gamma_\beta}{\sigma_{\beta c}} &= -2\sqrt{2}\frac{\gamma_{\alpha\beta}}{\sqrt{(\sigma_{\alpha c}^2 + \sigma_{\beta c}^2)}} \\ &\quad \times \left(\frac{\sigma_{\beta c}^2}{\sigma_{\alpha c}^2 + \sigma_{\beta c}^2}\right). \end{aligned} \quad (30)$$

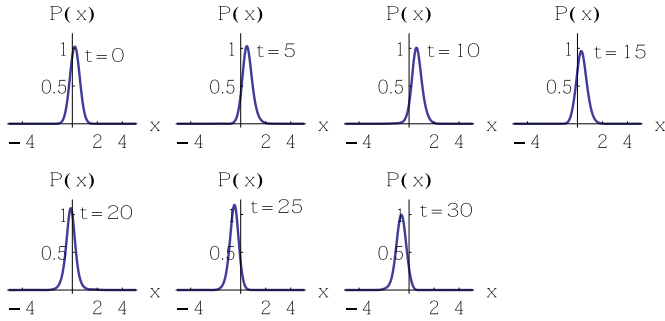
From equation (27c), we can further comment on the dynamics of  $x_d$ . To analyze in detail we will separately consider the cases for  $\gamma_{\alpha\beta} > 0$  and  $\gamma_{\alpha\beta} < 0$  in the following.

– Dynamics of  $x_d$  with  $\gamma_{\alpha\beta} > 0$

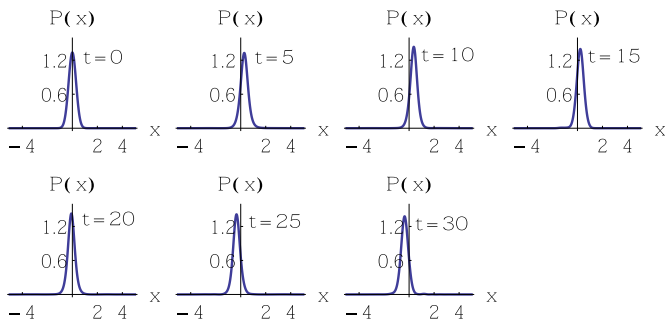
In this case, the dynamics of  $x_d$  is governed by an effective potential of the following form (quadratic in  $x_d$ )

$$V_{eff}(x_d) = \left(\frac{1}{2} - 2\sqrt{2}\frac{\gamma_{\alpha\beta}}{(\sigma_{\alpha c}^2 + \sigma_{\beta c}^2)^{3/2}}\right)x_d^2. \quad (31)$$

Equation (31) and Figure 10 clearly imply that for the bounded dynamics of  $x_d$ , we require  $\gamma_{\alpha\beta} < \gamma_{\alpha\beta}^c$ . Where  $\gamma_{\alpha\beta}^c = \frac{1}{4\sqrt{2}}(\sigma_{\alpha c}^2 + \sigma_{\beta c}^2)^{3/2}$ . If this condition is satisfied (solid black curve in Fig. 10),  $x_d$  will oscillate around zero with very small amplitude and the overlapping wave packets will remain overlapping for all the time. But if  $\gamma_{\alpha\beta} > \gamma_{\alpha\beta}^c$  (dashed black curve in Fig. 10), the overlapping state can have the possibility of phase separation since  $x_d$  will increase unboundedly under this condition. Here we



**Fig. 13.** Dynamics of the wave packet for species  $\alpha$  trapped in SHO with initial condition  $x_d(t=0) = 0.2$  and  $p_{0\alpha} = 1.0$ . We consider  $\gamma_\alpha = -1.0$ ,  $\gamma_\beta = -2.0$ ,  $\gamma_{\alpha\beta} = -0.336$ ,  $\sigma_{0\alpha} = 0.552 = \sigma_{\alpha c}$  and  $\sigma_{0\beta} = 0.423 = \sigma_{\beta c}$ . The wave packet oscillates inside the confining potential while retaining its initial width.



**Fig. 14.** Dynamics of the wave packet for species  $\beta$  trapped in SHO with initial condition  $x_d(t=0) = 0.2$  and  $p_{0\beta} = 0.9$ . All other parameters are same as Figure 13. The wave packet oscillates inside the confining potential while initial width remains invariant.

assume that all the  $\sigma$ s remain fixed at their coherent values.

– Dynamics of  $x_d$  with  $\gamma_{\alpha\beta} < 0$

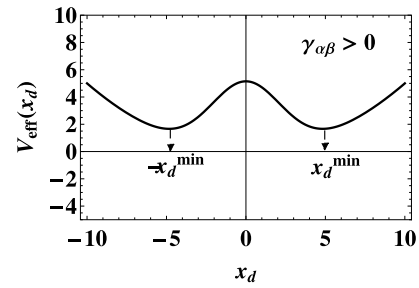
In this case, the expression for effective potential becomes  $V_{eff}(x_d) = \left(\frac{1}{2} + 2\sqrt{2} \frac{|\gamma_{\alpha\beta}|}{(\sigma_{\alpha c}^2 + \sigma_{\beta c}^2)^{\frac{3}{2}}}\right)x_d^2$  and hence its schematic diagram will be similar as shown in the solid black curve of Figure 10 for the case of  $|\gamma_{\alpha\beta}| < |\gamma_{\alpha\beta}^c|$ . This form of the effective potential supports bounded oscillation of  $x_d$  around zero for all values of  $\gamma_{\alpha\beta}$ , i.e., an overlapping state will remain overlapping. There is no possibility of transition from an overlapping state to phase separated state as shown in Figure 11 which supports our numerical findings in Figures 11, 13 and 14.

## Numerical results

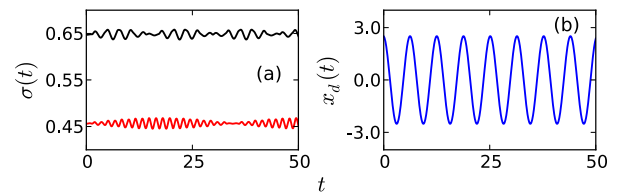
### 3.1.1 Solving analytically obtained ODE

– For  $\gamma_{\alpha\beta} < 0$

Like the free particle, here also the shape invariant states for both the wave packets exist if initial widths are chosen to be equal to their coherent widths depending



**Fig. 15.** Schematic diagram of the effective potential as a function  $x_d$  for  $\gamma_{\alpha\beta} > 0$  under phase separated initial condition. The curve shows two equidistant minima from  $x_d = 0$ . With time  $x_d$  will oscillate around any one of these minima depending upon the initial  $x_d$  at  $t = 0$ .

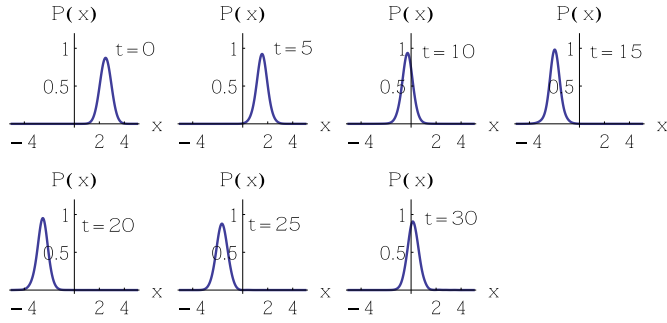


**Fig. 16.** Dynamics of the wave packets in SHO under phase separated regime. (a) Dynamics of the widths of the wave packets for species  $\alpha$  (solid black) and  $\beta$  (dashed red).  $\gamma_\alpha = -1.0$ ,  $\gamma_\beta = -2.0$ ,  $\gamma_{\alpha\beta} = 0.029$ ,  $\sigma_{0\alpha} = 0.647 = \sigma_{\alpha c}$  and  $\sigma_{0\beta} = 0.456 = \sigma_{\beta c}$ . The presence of shape invariant state in phase separated regime is the key point to observe. (b) Dynamics of  $x_d$  with  $x_d(t=0) = 2.5$  and  $\frac{d}{dt}x_d = -0.25$  indicates a small relative velocity of the wave packets.  $x_d$  oscillates with the mean value of  $x_d^{mean} = 0$  which is expected from analytical calculation ( $x_d^{min} = 0$ ) also.

on the interaction parameters of the system. For  $\gamma_\alpha = -1.0$ ,  $\gamma_\beta = -2.0$  and  $\gamma_{\alpha\beta} = -0.336$ , the initial widths are found to be  $\sigma_{0\alpha} = 0.552 = \sigma_{\alpha c}$  and  $\sigma_{0\beta} = 0.423 = \sigma_{\beta c}$ . Considering this set of parameters and solving the set of equations (27b) and (27c), the dynamics of the wave packets are shown in Figure 11. The wave packets for both the species remain shape invariant for all the time.

– For  $\gamma_{\alpha\beta} > 0$

On the other hand, by considering repulsive interspecies interaction  $\gamma_{\alpha\beta} = 0.577$  and attractive intraspecies interactions  $\gamma_\alpha = -0.5$ ,  $\gamma_\beta = -0.75$  we obtain  $(\sigma_{\alpha c}) = 0.867$  and  $(\sigma_{\beta c}) = 0.797$ . In Figure 12, we have shown the dynamics of the widths (at left) of the wave packets and the dynamics of  $x_d$  (at right) when the initial widths are chosen equal to their corresponding coherent widths.  $x_d$  grows with time and oscillates. This case is quite interesting in the sense that it opens up the possibility of transition from overlapping to phase separated state in SHO. However, for  $\gamma_{\alpha\beta} > 0$ , the bounded oscillation of widths with very small amplitude are noticeable and hence the presence of shape invariant states in this case is approximate. Also the oscillatory dynamics of  $x_d$  opens up the possibility for the wave packets to transit between overlapping state and phase separated state.



**Fig. 17.** Wave packet dynamics for species  $\alpha$  in simple harmonic confining potential. For  $\gamma_\alpha = -1.0$ ,  $\gamma_\beta = -2.0$ ,  $\gamma_{\alpha\beta} = 0.029$ , the initial widths are  $\sigma_{0\alpha} = 0.647$  and  $\sigma_{0\beta} = 0.456$ . Wave packets are initially separated by moderately large distance such that the phase separated initial condition ( $x_d/\Delta \gg 1$ ) is satisfied.  $x_d(0) = 2.5$  and  $p_{0\alpha} = -0.5$  are chosen. The wave packet starts from  $x_{0\alpha}(t = 0) = 2.5$  and oscillates with reasonable magnitude while retaining its initial shape.

### 3.1.2 Solving CGPE

This part of study contains two initially overlapping wave packets, i.e.,  $x_d(t = 0) = 0.2$  moving in the same direction ( $p_{0\alpha} = 1.0$  and  $p_{0\beta} = 0.9$ ). Considering  $\gamma_\alpha = -1.0$ ,  $\gamma_\beta = -2.0$ ,  $\gamma_{\alpha\beta} = -0.336$ , the coherent widths for both the wave packets have already been shown to be  $\sigma_{\alpha c} = 0.552$  and  $\sigma_{\beta c} = 0.423$ . After solving CGPE given in equation (1) with proper initial widths equal to their corresponding coherent widths like other previous cases, we observe almost shape invariant states (coherent states) for both the wave packets in Figures 13 and 14. Being in the overlapping state, the wave packets remain stick together and oscillate collectively inside the trapping potential with time. However, we refrain from showing same qualitative figures for  $\gamma_{\alpha\beta} > 0$ , where the approximate shape invariant states have also been found.

### 3.2 Wave packet dynamics under phase separated initial condition

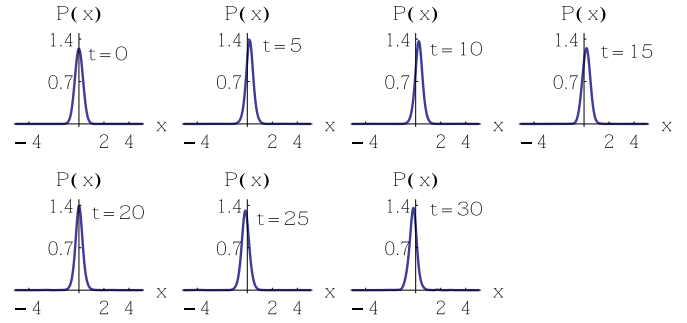
With the help of equation (27c), we can recast equations (27b) and (27c) in the following dimensionless form

$$\frac{1}{\sigma_{\alpha c}^2} - \frac{3}{2}\sigma_{\alpha c}^2 + \frac{\gamma_\alpha}{\sigma_{\alpha c}} = \frac{\sigma_{\alpha c}^2}{2} \left[ 1 - \ln \left( \frac{4\sqrt{2}\gamma_{\alpha\beta}}{\sigma_c^3} \right) \right], \quad (32a)$$

$$\frac{1}{\sigma_{\beta c}^2} - \frac{3}{2}\sigma_{\beta c}^2 + \frac{\gamma_\beta}{\sigma_{\beta c}} = \frac{\sigma_{\beta c}^2}{2} \left[ 1 - \ln \left( \frac{4\sqrt{2}\gamma_{\alpha\beta}}{\sigma_c^3} \right) \right]. \quad (32b)$$

Solving equations (32a) and (32b) numerically we obtain  $\sigma_{\alpha c} = 0.647$  and  $\sigma_{\beta c} = 0.456$  for  $\gamma_\alpha = -1.0$ ,  $\gamma_\beta = -2.0$ ,  $\gamma_{\alpha\beta} = 0.029$ . In this case,  $x_d > \sigma$  and hence the effective potential for  $\gamma_{\alpha\beta} > 0$  turns out to be

$$V_{eff}(x_d) = \frac{x_d^2}{2} + 2\sqrt{2} \frac{\gamma_{\alpha\beta}}{\sqrt{\sigma_{\alpha c}^2 + \sigma_{\beta c}^2}} e^{-\frac{x_d^2}{(\sigma_{\alpha c}^2 + \sigma_{\beta c}^2)}} \quad (33)$$



**Fig. 18.** Wave packet dynamics for species  $\beta$  in SHO. The initial widths are  $\sigma_{0\alpha} = 0.647$  and  $\sigma_{0\beta} = 0.456$  for  $\gamma_\alpha = -1.0$ ,  $\gamma_\beta = -2.0$ ,  $\gamma_{\alpha\beta} = 0.029$ . To keep the initial wave packets in phase separated regime, here we choose  $x_d(0) = 2.5$  and  $p_{0\beta} = 0.4$ . The wave packet oscillates with very small magnitude around the initial position  $x_{0\beta}(t = 0) = 0$  keeping its initial shape invariant.

which has minima at  $x_d^{min}$

$$x_d^{min} = \pm \sqrt{(\sigma_{\alpha c}^2 + \sigma_{\beta c}^2) \ln \left[ \frac{4\sqrt{2}\gamma_{\alpha\beta}}{(\sigma_{\alpha c}^2 + \sigma_{\beta c}^2)^{\frac{3}{2}}} \right]}. \quad (34)$$

Thus, for the existence of this minimum value,  $\gamma_{\alpha\beta}$  must be greater than zero. In Figure 15 we have shown the possible form of effective potential.

On the other hand, if  $\gamma_{\alpha\beta}$  becomes attractive, the effective potential for  $x_d$  shows a single minima and consequently  $x_d$  will oscillate around this minima with time.

### Numerical results

#### 3.2.1 Solving analytically obtained equations

Solving equations (27b) and (27c) and considering  $\sigma_{\alpha c} = 0.647$  and  $\sigma_{\beta c} = 0.456$  for  $\gamma_\alpha = -1.0$ ,  $\gamma_\beta = -2.0$ ,  $\gamma_{\alpha\beta} = 0.029$ , we obtain Figure 16 where we have shown the dynamics of the width of the wave packets and the dynamics of  $x_d$  respectively. Figure 16 (left) shows the shape invariance for both the wave packets (black is for species  $\alpha$  and red is for species  $\beta$ ). Figure at right shows the oscillatory behavior of  $x_d$  around zero as is expected from equation (34).

#### 3.2.2 Solving CGPE

Considering the wave packets with equal but opposite initial momentum, we numerically study CGPE. Wave packets with initial width equal to those required by the coherence condition, support the shape invariant states as is shown in Figures 17 and 18. The widths of the wave packets remain approximately invariant leading to the existence of shape invariant states.

Being in the phase separated domain each of the wave packets oscillates individually. Unlike the free particle case in SHO, the shape invariant states are quite robust in this case.

## 4 Conclusion and discussions

In this article, we have analyzed the dynamics of initial Gaussian wave packets in the presence of intra species and inter species interaction. Like single species BEC, here also we have observed that for free particle when the delocalization of the wave packet in space is natural, the attractive nature of interactions can make the wave packets localized under certain condition. We investigated the generation of coherent wave packets or the shape invariant states followed by CGPE. In free particle regime, whatever be the nature of intraspecies interaction (repulsive or attractive), when there is attractive interspecies interaction ( $g_{\alpha\beta} < 0$ ), we have always obtained almost shape invariant states for both the species under proper initial conditions. Depending upon the initial conditions, an overlapping state during the course of evolution can remain overlapping ( $x_d \simeq \Delta_{\alpha,\beta}$ ) or can have a transition into phase separated ( $x_d \gg \Delta_{\alpha,\beta}$ ) while the shape invariant state persists approximately. On the other hand, if the initial state belongs to the phase separated domain, there can have the possibility of breaking its initial Gaussian form due to collision between the wave packets.

Unlike free particle, in case of system trapped in SHO potential, shape invariant states (coherent wave packets) can be supported by both  $g_{\alpha\beta} > 0$  and  $g_{\alpha\beta} < 0$ , i.e., irrespective of the nature of interspecies interaction. In the phase separated regime, for small and positive  $g_{\alpha\beta}$ , shape invariant states have been observed. But it may approximately exist or may cease to exist for large positive values of  $g_{\alpha\beta}$ . However, under the overlapping initial condition, the shape invariant state can exist for comparatively large positive values of  $g_{\alpha\beta}$  while the system may enter from overlapping domain to phase separated domain. This situation has been analyzed and the corresponding effective potential supports this possibility. In particular, for  $g_{\alpha\beta} > 0$ , it is possible for an initially overlapping state to retain its initial shape if  $g_{\alpha\beta} < g_{\alpha\beta}^c$ . If  $g_{\alpha\beta}$  exceeds this value, an overlapping state can become phase separated while keeping its shape unchanged. Our findings are of quite importance while searching for the disturbances propagating with almost no change in shape in two component BEC.

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## Author contribution statement

All authors have contributed equally.

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