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We formulate the dynamics of three coupled Bose-Einstein condensates within a semiclassical scenario based on the standard boson coherent states. We compare such a picture with that of Ref. [1] and show how our approach entails a simple formulation of the dimeric regime therein studied. This allows to recognize the parameters that govern the bifurcation mechanism causing self-trapping, and paves the way to the construction of analytic solutions. We present the results of a numerical simulation showing how the three-well dynamics has, in general, a cahotic behavior.

An increasing interest for the dynamics of coupled bosonic wells [known in the literature as the *dimer* (*trimer*) model in case of a pair (triplet) of coupled wells] has been prompted recently by the construction of devices where Bose-Einstein condensates (BEC) interact through the tunneling effect (see [2] and references therein). The theoretic work focused on such models, both in the atomic physics community and in other areas of theoretical physics, has supplied a large amount of results disclosing a quite structured interwell dynamics.

The two-well model (TWM) –used to represent two coupled BECs in a symmetric double-well potential– has been investigated within a picture based on the algebra su(2) in Refs. [3], where, after stemming the model from the many-body quantum theory of BECs, the initial state with the atomic population self-trapped in one well is shown to evolve in delocalized oscillations involving both the wells. The same model has been studied previously in Ref. [4], both at the quantum level and from the point of view of the dynamical system theory, to illustrate the level splitting that characterizes the dimer spectrum as a manifestation of the orbit bifurcation in the dimer phase space. In Refs. [5] the dynamics of the asymmetric TWM have been faced within the mean-field formulation relatively to the π-phase oscillations as well as the self-trapping effect. The latter was considered as well in Ref. [4] and therein interpreted as a symmetry breaking phenomenon. More recently, the TWM (and its S-well generalization) has been related [6,7] to the Bose-Hubbard model [8] and the two-well ground-states have been interpreted as insulator/superconducting regimes. In particular, reformulating the TWM in an effective single-boson realization –generalizable to any S-well system– has been shown to favour the use of the system symmetries as well as the recognition of the inner parameters controlling the occurrence of doublets in the energy spectrum.

In this paper we consider some recent results proving the existence of configurations with self-trapping within the dynamics of symmetric trimer (identical interwell couplings). These have been obtained in Ref. [1] by recasting the trimer Hamiltonian within a two-boson operators picture (introduced in the sequel) which involves the algebra su(3). Such a picture is the extension of the dimer case [3] based on the su(2) (the formal setup for S-well models involves [6,7] the algebra su(S)). The main contribution of this paper is to apply to the trimer an alternative approach that both reproduces the results of the su(3) picture and show how the dynamical mechanism causing self-trapping not only depends on the tunneling amplitude but also from the system initial conditions. Such an approach relies on a boson coherent state formulation previously developed for both boson and spin lattice models [9] which seems to be very simple and effective. The symmetric trimer is described by Hamiltonian

$$H = U\sum_{i=1}^{3} n_i^2 - vN - \frac{1}{2}\sum_{i<\ell} T_{i\ell}\,\left(a_i^+ a_\ell + a_\ell^+ a_i\right),$$

with $T_{i\ell} = T$, that one can derive from the many-body quantum theory of BECs through a three-mode expansion of the condensate field operator [1]. Parameters U, v, T, account for the interatomic scattering, the external potential and the tunneling amplitude, respectively; $n_i \doteq a_i^+ a_i$ count the bosons in the ith well ($N = \Sigma_i n_i$), while the destruction (creation) operators a_i (a_i^+) obey the canonical commutators $[a_i, a_\ell^+] = \delta_{i\ell}$. Preceding studies of the trimer dynamics have been focused on the asymmetric case characterized by tunneling amplitudes $T_{12} \gg T_{13}, T_{23}$. Classically ($a_i a_\ell^+ = a_\ell^+ a_i$, $a_\ell^+ \equiv a_\ell^*$), the asymmetric trimer has revealed [10] the presence of homoclinic chaos, while, at the quantum level, the survival of breather configurations [11] has been investigated on the trimer viewed as the smallest possible closed chain.

If one derives the Heisenberg equations related to H for the boson operators a_i, a_i^+ and implements the random phase approximation in the equations for their expectation values $z_i = \langle a_i\rangle$, $z_i^* = \langle a_i^+\rangle$, the resulting equations for the three-well dynamics are ($j = 1, 2, 3$)

$$i\hbar\dot{z}_j = (2U|z_j|^2 - v + T/2)z_j - T(z_1 + z_2 + z_3)/2\,, \quad (1)$$

which entail $\Sigma_i|z_i|^2$ as a conserved quantity replacing the total boson number N such that $[N,H]=0$. The Hamiltonian structure of the Heisenberg equations is inherited by Eqs. (1) that, in fact, are also obtained from $\mathcal{H}(Z,Z^*) \equiv \Sigma_{j=1}^{3}[(U|z_j|^2-v)|z_j|^2 - T(z_j^* z_{j+1} + c.c.)/2]$, by using the standard Poisson brackets $\{z_k^*, z_j\} = i\delta_{kj}/\hbar$.

Another significant way to obtain Eqs. (1) from H relies on applying the time-dependent variational principle on a suitable trial state $|\Psi\rangle = e^{i\theta}|Z\rangle$ with $Z=(z_1,z_2,...)$, where z_r's are time-dependent complex parameters accounting for the system evolution. Performing the variation of $\langle\Psi|(i\partial_t - H)|\Psi\rangle = 0$ furnishes a system of hamiltonian equations for $Z=(z_1,...,z_r)$ and identifies θ with the action of the system. If the trial state is defined as [9]

$$|\Psi\rangle = e^{i\theta}|z_1\rangle \otimes |z_2\rangle \otimes |z_3\rangle\,, \tag{2}$$

where $|z_i\rangle$ are the standard bosonic coherent states that obey the defining equation $a_i|z_i\rangle = z_i|z_i\rangle$, then Eqs. (1) are recoverd (up to the shift $v \to v+U$) in which $z_i \equiv \langle z_j|a_i|z_i\rangle$, $z_i^* \equiv \langle z_j|a_i^+|z_i\rangle = z_i^*$, $|z_i|^2 \equiv \langle z_j|n_i|z_i\rangle$, and $d\theta/dt$ is the Lagrangian associated to $\mathcal{H}$. In addition to describing the system evolution through $|\Psi\rangle$, this approach also provides a natural way to find the quantum configuration (in terms of states) corresponding to the initial conditions of a given classical motion.

In Ref. [1] the semiclassical treatment of the trimer dynamics was based on deriving the equations of motion for the expectation values of the two-boson operators forming the basis of su(3) instead of a_i, a_i^+. Such an algebra is generated by the creation operators $\epsilon_1 = a_1^+ a_2$, $\epsilon_2 = a_2^+ a_3$, $\epsilon_3 = a_3^+ a_1$, the destruction operators $\epsilon_i^+ = (\epsilon_i)^+$, $i=1,2,3$ and the (so-called) Cartan operators $h_2 = (D_2 - D_3)/\sqrt{3}$, $h_1 = D_1$, where

$$D_1 = \frac{n_1 - n_2}{2}\,,\; D_2 = \frac{n_2 - n_3}{2}\,,\; D_3 = \frac{n_3 - n_1}{2}\,. \tag{3}$$

By using *imbalance* operators (3), the su(3) algebraic structure is specified by the commutators $[\epsilon_i, \epsilon_i^+] = 2D_i$, $[\epsilon_i, \epsilon_\ell] = \varepsilon_{i\ell k}\,\epsilon_k^+$, $[D_\ell, \epsilon_\ell] = \epsilon_\ell$ with $i,k,\ell \in [1,3]$ ($\varepsilon_{i\ell k}$ is the standard antisymmetric symbol), together with $[\epsilon_i, D_\ell] = \epsilon_i/2$, and $[\epsilon_i, \epsilon_\ell^+] = 0$, for $i \neq \ell$. Expressing Hamiltonian H through h_1 and h_2 one finds

$$H = 2U(h_1^2 + h_2^2) - f(N) - \frac{T}{2}(\epsilon_1 + \epsilon_2 + \epsilon_3 + h.c.)\,, \tag{4}$$

with $f(N) := UN^2/3 + vN$, where the operator N is a group invariant, namely $[N,g]=0$, $\forall g \in$ su(3). This implies that $[N,H]=0$. In this framework the Heisenberg equations are easily carried out. If the random phase approximation $\langle AB\rangle \equiv \langle A\rangle\langle B\rangle$ is also implemented Heisenberg's equations for the su(3) generators take the form

$$\begin{cases} i\dot{\epsilon_k} = -(T + 4U\epsilon_k)\,D_k + \frac{T}{4}\varepsilon_{ki\ell}(\epsilon_i^+ - \epsilon_\ell^+)\,, \\ i\dot{h_1} = \frac{T}{4}[(2\epsilon_1 - \epsilon_3 - \epsilon_2)\; -\; c.c.]\,, \\ i\dot{h_2} = \frac{T}{4}[\sqrt{3}(\epsilon_3 - \epsilon_2)\; -\; c.c.]\,. \end{cases} \tag{5}$$

where we have used the displacement operators D_j for simplifying the formulas. Notice that, in Eqs. (5) the approximation $\langle AB + BA\rangle \equiv 2\langle AB\rangle$ has been repeatedly applied to bilinear terms, and ϵ_ℓ, ϵ_ℓ^+, h_1, h_2 have been used in place of their expectation values $\langle\epsilon_\ell\rangle$, $\langle\epsilon_\ell^+\rangle$, $\langle h_1\rangle$, $\langle h_2\rangle$. A possible integrable regime is achieved by setting

$$h_1 = 0\;(\Leftrightarrow n_1 \equiv n_2)\,, \quad \epsilon_2 - \epsilon_3^+ = 0\,, \quad \epsilon_1 - \epsilon_1^+ = 0\,,$$

which leads to the reduced system of equations

$$\begin{cases} i\dot{\epsilon_1} = \frac{T}{2}(\epsilon_2^+ - \epsilon_2) \\ i\dot{\epsilon_2} = \frac{T}{2}(\epsilon_2 - \epsilon_1^+ - 2D_2) - 4U\,D_2\,\epsilon_2 \\ i\dot{h_2} = \frac{T}{2}[\sqrt{3}\epsilon_2^+ \;-\; c.c.]\,. \end{cases} \tag{6}$$

Their solutions have been calculated implicitly by geometric arguments and reproduced numerically for various choice of initial conditions in Ref. [1].

In the alternative solution scheme based on Eqs. (1) the above constraints reduce to impose the condition $z_1 = z_2$. This selects an integrable sub-dynamics. In fact, Eqs. (1) become two,

$$\begin{cases} i\hbar\dot{z}_1 = (2U|z_1|^2 - v)z_1 - \frac{T}{2}(z_1 + z_3) \\ i\hbar\dot{z}_3 = (2U|z_3|^2 - v)z_3 - Tz_1\,, \end{cases} \tag{7}$$

where the two costants of motion corresponding to the energy and the total boson number (we set $n_i \equiv |z_i|^2$)

$$\begin{cases} E = U(2n_1^2 + n_3^2) - vN - Tn_1 - T(z_3^* z_1 + z_1^* z_3) \\ N = 2n_1 \,+\, n_3 \end{cases} \tag{8}$$

make Eqs. (7) integrable. The dynamical behavior is obtained explicitly via a standard quadrature procedure (see Refs. [5,12]) which furnishes the phase-independent equation for D_3

$$\dot{D}_3^2 = \frac{9}{16}(4T^2 n_1 n_3 - R^2) \tag{9}$$

by substituting $R := [E + vN + Tn_1 - U(2n_1^2 + n_3^2)]$ $= -T(z_3^* z_1 + C.c.)$ inside the (squared) equation $\dot{D}_3^2 = -9T^2[z_3^* z_1 - c.c.]^2/16$ for D_3. Introducing the further constant of motion N to obtain $\dot{D}_3^2$ written in terms of the unique variable D_3 requires that n_1 and n_2 are expressed as $n_1 = (N - 2D_3)/3$ and $n_3 = (N + 4D_3)/3$. These, in turn, substituted in Eq. (9) give the equation

$$\dot{D}_3^2 = \frac{T^2}{4}(N - 2D_3)(N + 4D_3) \;-\; \frac{9}{16}\,R^2(D_3)\,, \tag{10}$$

for the imbalance variable $D_3 = (n_3 - n_1)/2$, in which

$$R(D_3) \equiv E + vN + \frac{T}{3}(N - 2D_3) - \frac{U}{3}(N^2 + 8D_3^2) =$$

$$= \frac{2}{3}\left\{(A-D_2)[T+4U(A+D_2)] - TN\,K(P)\right\}$$

with $A := D_3(0)$, $K(P) := \frac{1}{2}[(a+2)^2 - 9a^2]^{\frac{1}{2}}\cos\Delta$, $P := (a, \Delta)$, $a = 2A/N$, and $\Delta := \theta_3(0) - \theta_1(0)$. The second version of $R(D_3)$ is obtained by writing E in terms of the initial conditions $D_3(0)$, $\theta_k(0)$. Phases θ_j are defined by $z_k = \sqrt{n_k}e^{i\theta_k}$. Eq. (10) can be cast in the dimensionless form $(dx/ds)^2 = -2V_\tau(x;P)$ with $s := NUt$ and

$$V_\tau(x;P) := \frac{1}{2}\Big[(a-x)(a+x+\tau/2) - \tau K\Big]^2 - \frac{\tau^2}{2}(1-x)(1+2x)$$

where $x := 2D_3/N$ ($x \in [-1,1]$), $\tau := T/NU$. In view of the fact that both the squared term in V_τ (namely R^2) and $(dx/ds)^2$ are nonnegative, the further condition $(1-x)(1+2x) \geq 0$ must be accounted for which implies the restriction of the x range to $-1/2 \leq x \leq 1$.

The reduction of Eq. (7) to Eq. (10) allows one to construct explicit solutions in terms of elliptic functions by recasting the quartic term via standard transformation methods [14]. This will be enacted elsewhere. Operationally, our goal –the description of biforcation mechanism inherent in Eq. (10)– can be achieved as well through the equivalent potential problem $\mathcal{E} = \frac{1}{2}(dx/ds)^2 + V_\tau(x;P)$ at $\mathcal{E} = 0$, where parameters N, K and $x(0)$ in V_τ are fixed by setting the initial conditions.

With negative τ and a suitable choice of the other parameters, V_τ can exhibit an asymmetric double-well. In general, three solutions are obtained by annihilating

$$\frac{dV_\tau}{dx} = 2x^3 + \frac{3\tau}{2}x^2 + \frac{1}{4}\Big[9\tau^2 - 8\beta_\tau(P)\Big]x - \frac{\tau}{2}\Big[\tau + \beta_\tau(P)\Big],$$

where $\beta(\tau,P) := (a+\tau/4)^2 - \tau(K+\tau/16)$, that correspond to a maximum of $V_\tau(x;P)$ with two side minima.

In particular, setting $a = 1$ reproduces the conditions under which dynamics was studied in Ref. [1] (depleted twin wells, that is $n_3(0) \equiv 1$), and leads to the potential

$$V_\tau(x) = \frac{1}{2}(1-x)^2\left(x + \frac{\tau}{2} + 1\right)^2 - \frac{\tau^2}{2}(1-x)(1+2x)$$

whose maximum is such that $V_\tau(x_m) = 0$ with $x_m = 0$ when $\tau = -2/3$. For $\tau > -2/3$ one has $V_\tau(x_m) > 0$. The important feature thus emerging (see Fig. 1) is that, whenever the potential maximum is nonnegative, $V_\tau(x)$ generates two noncommunicating basins with $V_\tau(x) \leq 0$ (separated by a forbidden interval where $V_\tau > 0$) entailing two independent oscillatory motions. In each basins the motion has a periodic character. This represents the bifurcation effect reminescent of the behavior manifested by two-well dynamics [4,7].

What we emphasize here, based on our z_j description, is that the onset of separated motions can be caused by varying the other parameters of the problem. In particular, a high sensitivity is manifested relatively to the initial phases incorporated in Δ. Suitable changes of the latter are capable of switching on the bifurcation mechanism even for $a \neq 1$. Such a situation is represented in Fig. 2 for $a = 0.99$ (twin wells almost empty) and $\tau = -2/3$, where various potential wells are generated by varying $\cos\Delta$ in $[-1,1]$. For sufficiently low values of $\cos\Delta$ the presence of the maximum is ensured. The 'opposite' case $a = -0.49$ and $\tau = -1/3$ (corresponding to twin wells almost half-filled and $n_3(0) \simeq 0$) of Fig. 3 confirms the presence of isolated basins as well as the case with a more negative coupling $\tau = -0.7 < -2/3$ and $a = 0.99$.

Decreasing sufficiently the value of τ (Fig. 4 illustrates the case $\tau = -0.8$ with $a = 0.99$) by keeping the same range for $\cos\Delta$ entails situations where wells never exhibit a local maximum. This can be proved analitically in the special case $\tau = -1$ in which the potential becomes

$$V_\tau(x;P) \equiv \frac{1}{2}\Big[(a-1/4)^2 + K - X^2\Big]^2 - \frac{9}{16} + X^2$$

with $X = x - 1/4$, and the stationary points can be calculated explicitly. One finds a maximum at $x_m = 1/4$ with $V_\tau(x_m) < 0$ so that no bifurcation effect occurs. The side minima are placed at $x_{r,\ell} = 1/4 \pm [K - 1 + (a-1/4)^2]^{1/2}$. These are real provided $K - 1 + (a-1/4)^2 \geq 0$ namely if

$$\cos\Delta \geq [1 - (a-1/4)^2]/[(1-a)(1+2a)]^{\frac{1}{2}}\,.$$

For a generic τ, the maximum depends on a and Δ in a complicated way which makes difficult the analytic calculation of $V_\tau(x_m)$ and of its sign. Nevertheless, some necessary conditions ensuring its existence can be obtained explicitly. As suggested by Figs. 1-3, increasing Δ with both τ and a constant implies that the maximum at $x = x_m$ and the left minimum at $x = x_\ell$ reach the (flex) point $x = c$ for critical value $\Delta \equiv \Delta^*$. Since the interval $[x_\ell, x_m]$ where $dV_\tau/dx > 0$ vanishes for $x_\ell, x_m \to c$ then

$$\lim_{\Delta\to\Delta^*}\big(dV_\tau/dx\big)_{x_l,x_m} = 0 = \big(d^2V_\tau/dx^2\big)_c\,. \qquad (11)$$

The derivation of the roots of $d^2V_\tau/dx^2 = 0$ at $x = c$

$$x_\pm = \frac{\tau}{4}\left\{-1 \pm [8(2a^2 + a\tau - 2K\tau)/(3\tau^2) - 5]^{1/2}\right\},$$

from $d^2V_\tau/dx^2 = 6x^2 + 3\tau x - 2\beta_\tau(P) + 9\tau^2/4$ allows one to exploit the fact that the lowest one, x_-, is a maximum of dV_τ/dx corresponding to the V_τ flex point at $x = c$. When

$$\big(dV_\tau/dx\big)_c \equiv \frac{8\tau}{3^{3/2}|\tau|}\,[\beta_\tau(P)]^{\frac{3}{2}} - \tau(\tau+1) \geq 0 \qquad (12)$$

becomes negative the maximum disappears (see, e. g., Figs. 1-3). The bifurcation condition $V_\tau(x) > 0$ must be searched within the parameter space domain where a, Δ, τ satisfy formula (12).

The analysis just developed shows that changing Δ can modify deeply the system dynamics and that, in general, the onset of the bifurcation effect is governed by the

complex interplay of all parameters a, Δ, τ. A complete study of the dynamics requires that one considers any possible initial condition for the dynamics and thus, e. g., the situations in which $n_1(0) \neq n_2(0)$, excluded in the present paper. In this case the nonintegrable character of the system crops up in a dramatic way as illustrated in Fig. 5. The systematic analysis of fixed points for the symmetric three-well dynamics and thus the emergence of chaos close to the hyperbolic points is in progress at this moment. It will be discussed in a separate paper.

[1] K. Nemoto *et al.*, Phys. Rev. A **63**, 13604 (2001).

[2] A. S. Parkins, D. F. Walls, Phys. Rep. 303, 1 (1998), F. Dalfovo *et al.*, Rev. Mod. Phys. **71**, 463 (1999).

[3] G. J. Milburn *et al.*, Phys. Rev. A **55**, 4318 (1997); J. F. Corney and G. J. Milburn, Phys. Rev. A **58**, 2399 (1998).

[4] S. Aubry *et al.*, Phys. Rev. Lett. **76**, 1607 (1996).

[5] A. Smerzi *et al.*, Phys. Rev. Lett. **79** , 4950 (1997); S. Raghavan *et al.*, Phys. Rev. A **59**, 620 (1999).

[6] R. Franzosi *et al.*, Int. J. Mod. Phys. B **14**, 943 (2000).

[7] R. Franzosi, V. Penna, Spectral Properties of Coupled Bose-Einstein Condensates, cond-mat/0006446 (to appear on PRA).

[8] The Bose-Hubbard model for a bosonic fluid on an S-site lattice [9] is interpreted as S coupled bosonic wells (representing a chain of interacting condensate in the mean field approximation) by means of the time-dependent variational principle and the coherent state method.

[9] L. Amico and V. Penna, Phys. Rev. B **62** , 1224 (2000).

[10] D. Henning *et al.*, Phys. Rev. A **51**, 2870 (1997).

[11] S. Flach and V. Fleurov, J. Phys.: Condens. Matter 9, 7039 (1997).

[12] A. Montorsi, V. Penna, Phys. Rev. B **62** , 1224 (1997).

[13] W.M. Zhang *et al.*, Rev. Mod. Phys. **62**, 867 (1990).

[14] H.T. Davis, *Introduction to Nonlinear Differential and Integral Equations*, (Dover, New York, 1970).

FIG. 1. By varying τ in $[-0.75, -0.63]$ with $a = 1$, $V_\tau(x, P)$ generates a second (small) basin on the left (dashed potential corresponds to $\tau \simeq -0.66$).

FIG. 2. By varying Δ in $[0, \pi]$ with $a = 0.99$, $V_\tau(x, P)$ generates a second (small) basin on the left (dashed potential corresponds to $\Delta \simeq 1.40$).

FIG. 3. Representation of bifurcation mechanism by varying $\Delta \in [0, \pi]$ in $V_\tau(x, P)$ with $a = -0.49$, $\tau = -1/3$.

FIG. 4. $V_\tau(x, P)$ with $a = 0.99$ and $\tau = 0.8$: a sufficiently negative τ involves a single basin for any $\Delta \in [0, \pi]$.

FIG. 5. Poincaré section of the $\xi_1 - \phi_1$ plane, where $\xi_1 := 1 - 2n_1/N$ and $\phi_1 = \theta_2 - \theta_1$, obtained by setting $n_3 \simeq 6.85$; this is derived by numerical integration of Eqs. (1) with energy $E \simeq 92.33$, $N = 10$, $T = U = 1$.