Self-trapping mechanisms in the dynamics of three coupled Bose-Einstein condensates

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(Received 5 February 2001; published 4 December 2001)

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 K. Nemoto *et al.* [Phys. Rev. A **63**, 013604 (2001)] and show how our approach entails a simple formulation of the dimeric regime therein studied. This allows us to recognize the parameters that govern the bifurcation mechanism causing self-trapping, and paves the way to the construction of analytic solutions.

DOI: 10.1103/PhysRevA.65.013601 PACS number(s): 03.75.Fi, 05.45.−a, 03.65.Sq

I. INTRODUCTION

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 [1] 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 Ref. [2], 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. [3], 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.

The dynamics of the asymmetric TWM have been faced in Ref. [4] within the mean-field formulation relative to the π-phase oscillations as well as the self-trapping effect. The latter was considered as well in Ref. [3] and therein interpreted as a symmetry breaking phenomenon.

More recently, the TWM (and its *S*-well generalization) has been related [5,6] to the Bose-Hubbard model [7] and the ground states of the two-well system have been interpreted in terms of superconducting/insulator regimes. In particular, the reformulation of the TWM in an effective single-boson realization–generalizable to any S-well system—has been shown to favor the use of the system symmetries as well as the recognition of the inner parameters controlling the occurrence of doublets in the energy spectrum. Finally, the density matrix formalism has been used in Ref. [8] to include in the TWM mean-field picture the leading quantum corrections.

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. [9] by recasting the trimer Hamiltonian within a two-boson operators picture (introduced in the sequel) that involves the algebra su(3). Such a picture is the extension of the dimer case [2] based on the su(2) [the formal setup for *S*-well models involves [5,6] 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 [10] that seems to be very simple and effective. The symmetric trimer is described by Hamiltonian,

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

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 [9]. Parameters U, v, T, account for the interatomic scattering, the external potential, and the tunneling amplitude, respectively; $n_i \doteq a_i^\dagger a_i$ count the bosons in the ith well ($N=\Sigma_i n_i$), while the destruction (creation) operators a_i ($a_i^\dagger$) obey the canonical commutators $[a_i, a_\ell^\dagger] = \delta_{i\ell}$. 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 ($a_i a_\ell^\dagger = a_\ell^\dagger a_i, a_\ell^\dagger \equiv a_\ell^*$), the asymmetric trimer has revealed [11] the presence of homoclinic chaos, while, at the quantum level, the survival of breather configurations [12] has been investigated on the trimer viewed as the smallest possible closed chain.

II. CANONICAL FORM OF TRIMER DYNAMICS

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

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

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 Eq. (1) that, in fact, are also obtained from

$$\mathcal{H}(Z,Z^*)\equiv\sum_{j=1}^{3}[(U|z_j|^2-v)|z_j|^2-T(z_j^*z_{j+1}+\text{c.c.})/2],$$

by using the standard canonical brackets $\{z_k^*,z_j\}=i\delta_{kj}/\hbar$.

Another significant way to obtain Eq. (1) from H relies on applying the time-dependent variational principle on a suitable trial state $|\Psi\rangle=e^{i\theta}|Z\rangle$ with $Z=(z_1,z_2,\dots)$, where z_r's are time-dependent complex parameters accounting for the system evolution (see Refs. [13,14]). Performing the variation of $\langle\Psi|(i\partial_t-H)|\Psi\rangle=0$ furnishes a system of Hamiltonian equations for $Z=(z_1,\dots,z_r)$ and identifies θ with the action of the system. If the trial state is defined as [10]

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

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 Eq. (1) is recoverd (up to the shift $v\to v+U$) in which $z_i\equiv\langle z_i|a_i|z_i\rangle$, $z_i^*\equiv\langle z_i|a_i^\dagger|z_i\rangle$, $|z_i|^2\equiv\langle z_i|n_i|z_i\rangle$, 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.

III. su(3) FORM OF TRIMER DYNAMICS

In Ref. [9] 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, $a_i^\dagger$. Such an algebra is generated by the creation operators $\epsilon_1=a_1^\dagger a_2$, $\epsilon_2=a_2^\dagger a_3$, $\epsilon_3=a_3^\dagger a_1$, the destruction operators $\epsilon_i^\dagger=(\epsilon_i)^\dagger$, $i=1,2,3$ and the (so-called) Cartan operators $h_2=(D_2-D_3)/\sqrt{3}$, $h_1=D_1$, where

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

By using *imbalance* operators (3), the su(3) algebraic structure is specified by the commutators,

$$[\epsilon_i,\epsilon_i^\dagger]=2D_i,\quad [\epsilon_i,\epsilon_\ell]=\varepsilon_{i\ell k}\epsilon_k^\dagger,\quad [D_\ell,\epsilon_\ell]=\epsilon_\ell,$$

with $i,k,\ell\in[1,3]$ ($\varepsilon_{i\ell k}$ is the standard antisymmetric symbol), together with

$$[\epsilon_i,D_\ell]=\epsilon_i/2,\quad [\epsilon_i,\epsilon_\ell^\dagger]=0,$$

for $i\neq\ell$. Expressing Hamiltonian H through h_1 and h_2 one finds

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

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,

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

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

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

which leads to the reduced system of equations,

$$\begin{aligned}
i\dot\epsilon_1&=\frac{T}{2}(\epsilon_2^\dagger-\epsilon_2),\\
i\dot\epsilon_2&=\frac{T}{2}(\epsilon_2-\epsilon_1^\dagger-2D_2)-4UD_2\epsilon_2,\\
i\dot h_2&=\frac{T}{2}[\sqrt{3}\epsilon_2^\dagger-\text{c.c.}].
\end{aligned} \tag{6}$$

Their solutions have been calculated implicitly by geometric arguments and reproduced numerically for various choice of initial conditions in Ref. [9].

In the alternative solution scheme based on Eq. (1) the above constraints reduce to impose the condition $z_1=z_2$. This selects an integrable subdynamics. In fact, Eq. (1) becomes two:

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

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

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

make Eq. (7) integrable.

IV. DIMERLIKE REGIME AND SELF-TRAPPING ONSET

The dynamical behavior is obtained explicitly via a standard quadrature procedure (see Refs. [4,13]) which furnishes the phase-independent equation for D_3,

$$\dot{D}_3^2=\frac{9}{16}(4T^2n_1n_3-R^2), \tag{9}$$

by substituting $R:=[E+vN+Tn_1-U(2n_1^2+n_3^2)]=-T(z_3^*z_1+\text{c.c.})$ inside the (squared) equation $\dot{D}_3^2=-9T^2[z_3^*z_1-\text{c.c.}]^2/16$ 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

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

$$=\frac{2}{3}\{(A-D_2)[T+4U(A+D_2)]-TNK(P)\}$$

with

$$A:=D_3(0),\quad K(P):=\frac{1}{2}[(a+2)^2-9a^2]^{1/2}\cos\Delta,$$

$P:=(a,\Delta)$, $a=2A/N$, 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 $z_k=\sqrt{n_k}e^{i\theta_k}$. Equation (10) can be cast in the dimensionless form $(dx/ds)^2=-2V_\tau(x;P)$ with $s:=NUt$ and

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

$$-\frac{\tau^2}{2}(1-x)(1+2x),$$

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 non-negative, the further condition $(1-x)(1+2x)\geqslant 0$ must be accounted for which implies the restriction of the x range to $-1/2\leqslant x\leqslant 1$.

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 [15]. This will be enacted elsewhere. Operationally, our goal–the description of bifurcation 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.

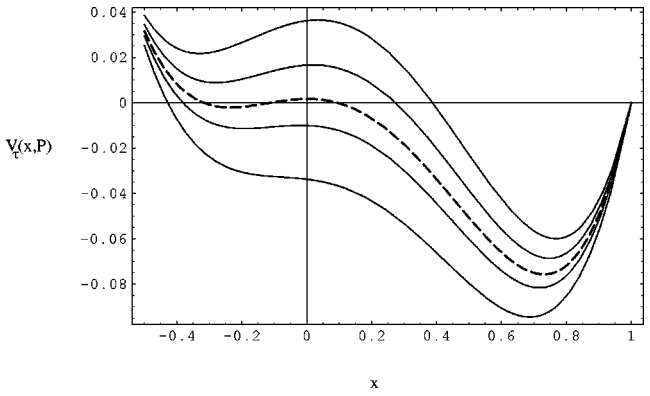

FIG. 1. By varying τ in $[-0.75,-0.63]$ with $a=1$, $V_\tau(x,P)$ generates a second (small) basin on the left (dashed potential corresponds to $\tau\simeq-0.66$). V_τ and x are dimensionless quantities.

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

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

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. [9] [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 non-negative, $V_\tau(x)$ generates two non-communicating basins with $V_\tau(x)\leqslant 0$ (separated by a forbidden interval where $V_\tau>0$) entailing two independent oscillatory motions. In each basin the motion has a periodic character. This represents the bifurcation effect reminescent of the behavior manifested by two-well dynamics [3,6].

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 relative 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

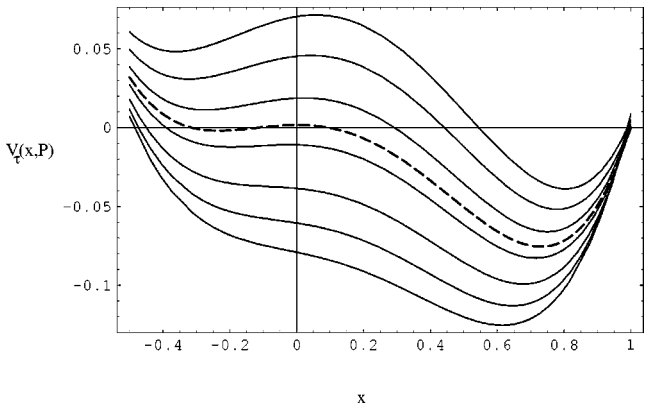

FIG. 2. By varying Δ in $[0,\pi]$ with $a=0.99$, $V_\tau(x,P)$ generates a second (small) basin on the left (dashed potential corresponds to $\Delta\simeq 1.40$).

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 by keeping the same range for $\cos\Delta$ entails situations where the potential wells never exhibit a local maximum responsible for the self-trapping. This can be proved analytically in the special case $\tau=-1$ in which the potential becomes

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

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 $K-1+(a-1/4)^2\geqslant 0$ namely if

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

For a generic τ, the maximum depends on a and Δ in a complicated way that 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

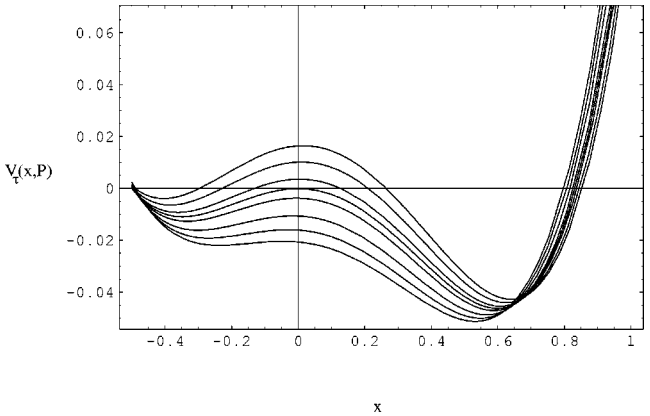

FIG. 3. Representation of bifurcation mechanism by varying $\Delta\in[0,\pi]$ in $V_\tau(x,P)$ with $a=-0.49$, $\tau=-1/3$.

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

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

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

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

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

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

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).

V. CONCLUSIONS

Based on a variational technique developed previously [10,5], we have reformulated the dynamics of the bosonic trimer in terms of the expectation values z_i and z_i^* of operators a_i and $a_i^\dagger$, respectively (canonical description). Such a picture is quite simple and provides a useful alternative to the formulation based on the algebra su(3) of Ref. [9] when one investigates the trimer dynamics. In particular, the description of dynamics via z_i's [such coherent states' labels are introduced by state (2)] both allows one to relate quantum states to initial conditions of classical motions, and to stem in a direct way the integrable dimeric subregime already obtained within the su(3) description.

The main advantage entailed by the canonical description becomes evident, in particular, when Eq. (7) are used to reduce the dimeric dynamics to a one-dimensional potential problem via a systematic use of constant of motions. This has allowed us to explore thoroughly (namely for initial conditions a, Δ, and values of τ chosen in a general way) the self-trapping effect pointed out in Ref. [9] (and therein studied for a particular choice of initail conditions) and to recognize the general circumstances able to cause it. The change of Δ, for example, is shown to be sufficient to initiate the appearence of separated periodic motions with the same energy.

If the analysis developed reproduces consistently the self-trapping of the pure dimer, it shows as well how the onset of the bifurcation effect is governed, in general, by the complex interplay of all parameters a, Δ, τ. These turn out to undergo condition (12). A complete study of trimer dynamics requires that one considers any possible initial condition for the dynamics and thus the situations in which $n_1(0)\neq n_2(0)$, ex-

cluded in the present paper. In this case the nonintegrable character of the system is expected to crop up in a dramatic way. The systematic analysis of fixed points for the symmetric three-well dynamics and the emergence of possible chaotic behavior close to the hyperbolic points is in progress at this moment. It will be discussed in a separate paper.

ACKNOWLEDGMENTS

The work of R.F. has been supported by an INFN grant. V.P. gratefully acknowledges the financial support of INFM (Italy) and of MURST within the project ''Theory of Coherent Fluids.''

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