Classical and Quantum Dynamics of Bose-Einstein Condensates.

Generalized coherent states can be profitably employed in the study of dynamics of quantum systems. When a quantum Hamiltonian is a linear function of the generators of a dynamical Lee group, the generalized coherent states of the corresponding dynamical algebra, will give rise to the exact quantum solutions. However, when the Hamiltonian of a system is a nonlinear function of the generators of the dynamical group, the exact solutions are hardly obtained also by coherent states techniques. In these cases, suitable coherent states can be used in combination with appropriate *variational principles* in order to derive a semiclassical description of quantum-system dynamics. The nonlinear character, inherent the dynamics of *Bose-Einstein condensates* in periodic (optical) potentials, is at the base of many interesting *macroscopic phenomena* I have studied. The quantum dynamics of interacting Bose-Einstein condensates, can be explored in terms of coherent states, whereas the corresponding semiclassical description can be derived by means a *time dependent variational principle*.

The quantum dynamics of an ultracold dilute gas of bosonic atoms in an external trapping potential V_{ext} is described by the Hamiltonian operator

$$\hat{H}=\int d\mathbf{r}\,\hat{\psi}^{\dagger}(\mathbf{r})[-\frac{\hbar^2}{2m}\nabla^2+V_{ext}(\mathbf{r})]\,\hat{\psi}(\mathbf{r})+\frac{4\pi\hbar^2 a_s}{2m}\int d\mathbf{r}\,\hat{\psi}^{\dagger}(\mathbf{r})\hat{\psi}^{\dagger}(\mathbf{r})\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r})$$

For periodic potentials V_{ext}, the “single atom” Hamiltonian eigenstates are Bloch functions $\Phi_{\mathbf{q}}^{(n)}(r)$ of quasi-momentum $\mathbf{q}$ and the band index n. Already for moderate optical potential depths, a good approximation for the lowest energy gap is given by $\hbar\omega$, where ω is the oscillation frequency of a particle trapped in the harmonic approximation of the potential V_{ext} close to a minimum. One can assume that only the fundamental energy band is involved into the dynamics and describe the system using Wannier functions $u_j(\mathbf{r})$ localized at the minima of the optical potential. Accordingly, the boson-field operator can be expressed as $\hat{\psi}(\mathbf{r},t)=\sum_j u_j^*(\mathbf{r})\,\hat{a}_j(t)$ where the boson operator $\hat{a}_j\left(\hat{a}_j^{\dagger}\right)$ destroys (creates) an atom at the lattice site j. By substituting the latter expression for the field operators into the Hamiltonian, and by keeping the lowest order in the overlap between the single-well wave-functions, one obtains the effective *Bose-Hubbard Hamiltonian*

$$H=\sum\left[Un_j\left(n_j-1\right)+\xi_j n_j\right]-\frac{T}{2}\sum\left(a_j^{\dagger}a_{j+1}+h.c.\right)$$

In paper Int. Jour. of Mod. Phys. B Vol. **14**, No. 9 (2000) 943-961 it is shown that, by combining the description for the Bose-Hubbard model quantum states as product of site *Glauber coherent states* and, a time dependent variational principle, the semiclassical dynamics of Bose-Hubbard model is well described by a *discrete nonlinear Schroedinger equation* (that is the discrete version of the *Gross-Pitaevskii equation*). Furthermore, it is therein analysed the classical dynamics of two interacting Bose-Einstein condensates (*dimer*). In spite of the integrable character of the system's dynamics, due to non-linearity, its equations of motion admit interesting and unexpected dynamical behaviours. In fact, this system displays peculiar behaviours like the population *self-trapping*.

In part of paper Int. Jour. of Mod. Phys. B Vol. **14**, No. 9 (2000) 943-961 and, more deeply, in paper Phys. Rev. A **63**, 043609-1 (2001), it is considered the dimer quantum dynamics and it is analysed the link between classical trajectories and quantum energy levels. The spectrum structure is studied within the framework of the Schwinger realization of the angular momentum. The latter allows to recognize the symmetry properties of the system Hamiltonian and, then, to use them for characterizing the energy eigenstates. The dimer spectrum is characterised by the presence of nondegenerate doublets. It is really the existence of these nondegenerate doublets in the spectrum that allows to recover, in the classical limit, the symmetry-breaking (self-trapping) effect that characterizes the system classically.

In Phys. Rev. A **65**, 013601-1 (2001); Phys. Rev. E, **67**, 046227 (2003) and Phys. Rev. Lett., **90**, 050404 (2003)**,** it has been shown that the apparently harmless addition of a further coupled condensate to the dimer system, is sufficient to make the dynamics of three coupled Bose-Einstein condensates (*trimer*) non-integrable. Indeed, in Phys. Rev. A 65, 013601-1 (2001); Phys. Rev. E, **67**, 046227 (2003) and Phys. Rev. Lett., **90**, 050404 (2003)**,** is investigated the trimer classical dynamics in different inequivalent, and experimentally meaningful, configurations, showing that it displays instabilities in extended regions of the phase space. Besides the chaotic nature of the trimer dynamics, in the latter papers is investigated the collective modes associated with the system's equations and the non-linear self-trapping that emerges in the super-fluid regime.

The non-linear character of the classical equations of motion of Bose-Einstein condensates in arrays of arbitrary length, is at the base of the self-localization phenomenon that, in Phys. Rev. Lett. **97**, 060401 (2006)**,** I have predicted to take place in condensates loaded in dissipative optical lattices (see Fig. 5.). The dynamical configurations that in Phys. Rev. Lett. **97**, 060401 (2006) has been shown to spontaneously appear, have the nature of (static or moving) "breathing dynamical solutions" (see Fig. 5) that are the very genuine non-linear discrete dynamical states. These macroscopic effects are, and have been, of primary importance in leading toward their experimental observation also in small (few interacting condensates) systems.

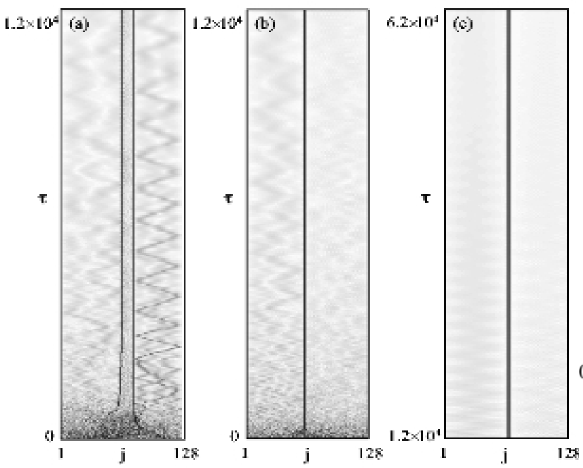

Fig. 4 Evolution of the atomic density in the optical lattice with losses at the ends of the trapping potential

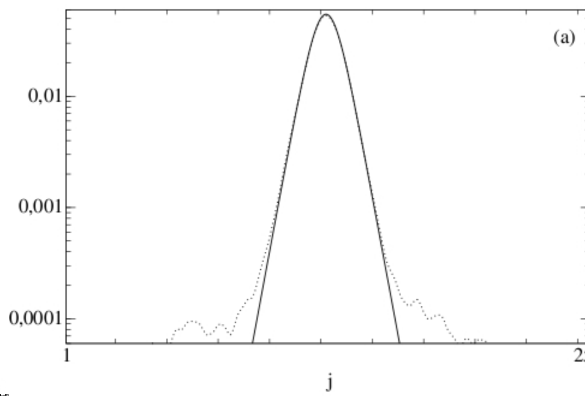

Fig. 5 Static breathers, continuous from analytic solution, dotted line from dissipative procedure.

In paper J. Stat. Phys. (2011) 143: 824–830 I have considered a generic classical many particle system described by an autonomous Hamiltonian $H(x_1,\ldots,x_{N+2})$ which, in addition, has a conserved quantity $V(x_1,\ldots,x_{N+2})$, so that the Poisson bracket $\{H,V\}$ vanishes. I have derived in detail the microcanonical expressions for entropy and temperature. I have shown that both of these quantities depend on multidimensional integrals over submanifolds given by the intersection of the constant energy hypersurfaces with those defined by $V(x_1,\ldots,x_{N+2})=v$. I have shown that temperature and higher order derivatives of entropy are microcanonical observable that, under the hypothesis of ergodicity, can be calculated as time averages of suitable functions. Finally I have derived the explicit expression of the function that gives the temperature.

In paper [S. Iubini, R. Franzosi, R. Livi, G.-L. Oppo and A. Politi, "*Discrete breathers and* *negative-temperature states",* New J. Phys. **15** (2013) 023032] we have shown how **negative temperature nonequilibrium states** can be obtained in the Nonlinear Discrete Schroedinger Equation. The definition of the microcanonical temperature given by me in paper J. Stat. Phys. (2011) 143: 824–830, associated with the corresponding Hamiltonian, allows to obtain a consistent thermodynamic description for both positive and negative temperature states. We have also described how one can pass from positive to negative temperatures by applying energy dissipation to the Nonlinear Discrete Schroedinger Equation chain boundaries. We have found that the microscopic evolution in thermalized negative temperature states is characterized by the mechanism of focusing of particle density (and energy), characterized by the formation of localized breather states.

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