Abstract

The dynamics of Bose-Einstein condensates trapped in a deep optical lattice is governed by a discrete nonlinear equation (DNL). Its degree of nonlinearity and the intersite hopping rates are retrieved from a nonlinear tight-binding approximation taking into account the effective dimensionality of each condensate. We derive analytically the Bloch and the Bogoliubov excitation spectra, and the velocity of sound waves emitted by a traveling condensate. Within a Lagrangian formalism, we obtain Newtonian-like equations of motion of localized wavepackets. We calculate the ground-state atomic distribution in the presence of an harmonic confining potential, and the frequencies of small amplitude dipole and quadrupole oscillations. We finally quantize the DNL, recovering an extended Bose-Hubbard model.
I. INTRODUCTION

Bose-Einstein condensates (BECs) trapped in periodic potentials are a new bedtest to investigate different and fundamental issues of quantum mechanics, ranging from quantum phase transitions [1] and atom optics [2,3] to the dynamics of Bloch and Josephson oscillations [4–6].

The key feature of these systems is the competition/interplay between the discrete translational invariance (introduced by the periodic potential) and the nonlinearity (due to the interatomic interaction). For instance, it has been pointed out that the excitation spectrum exhibits a band structure which has analogies with the electron Bloch bands in metals [7–9]. However, the coexistence of Bloch bands and nonlinearity allows for solitonic structures [10] and dynamical instabilities [11–13] which do not have an analog neither in metals, nor in Galilean invariant nonlinear systems.

The BEC in a periodic potential is described in mean field (or classical) approximation by the Gross-Pitaevskii equation (GPE) Eq.(4). When the interwell barriers of the periodic structure are high enough (see below), the relevant observables of the system are the number of particles \( N_j(t) \) and the relative phases \( \varphi_{j+1}(t) - \varphi_j(t) \) of the condensates in the lattice (the subscript \( j \) denotes the different wells of the array). In [10] it has been shown that the amplitudes \( \psi_j = \sqrt{N_j} e^{i\varphi_j} \) satisfy a discrete nonlinear Schrödinger equation (DNLS), recovered from the GPE (4) in the tight-binding approximation. Such a mapping has allowed the investigation of localized and extended excitations [10,14,15] in the framework of the nonlinear lattice theory [16], and has clarified the connection between such systems and an array of superconducting Josephson junctions. The relative phase dynamics of different condensates has been experimentally investigated looking at the interference patterns created by the atoms tunneling in the continuum from a vertical lattice [4], or by the overlapping condensates once the confining traps are removed [3,6,17].

In the “standard” tight-binding approximation, the condensate wavefunction localized in the \( j \)th well is factorized as a dynamical part \( \psi_j(t) = \sqrt{N_j(t)} e^{i\varphi_j(t)} \) and a spatial, real
wavefunction $\Phi_j(\vec{r})$ centered in the minimum $\vec{r}_j$ of the well. A crucial assumption, which will be discussed in detail, is that the shape of $\Phi_j(\vec{r})$ does not depend on the number of particles $N_j(t)$ in the same well. Under such conditions, the condensate order parameter $\Psi(\vec{r}, t)$ can be written as:

$$\Psi(\vec{r}, t) = \sum_j \psi_j(t) \Phi_j(\vec{r}). \quad (1)$$

The DNLS equation is recovered replacing Eq.(1) in the GPE Eq.(4), and integrating out the spatial degrees of freedom. Neglecting higher order terms, we get [10]:

$$i\hbar \frac{\partial \psi_j}{\partial t} = -K(\psi_{j-1} + \psi_{j+1}) + U_2 |\psi_j|^2 \psi_j + \epsilon_j \psi_j \quad (2)$$

with $K, U_2, \epsilon_j$ depending on the geometry of the trapping potentials and on the average number of atoms in each well [cfr. with Eqs.(8-11)].

II. A GENERALIZED TIGHT-BINDING APPROXIMATION

In this paper we stress the importance (and exploit the consequences) to generalize the “standard” tight-binding approximation Eq.(1). This generalization is imposed by the nonlinearity of the GPE Eq.(4), and largely extend the range of validity of the DNLS Eq.(2) in the study of the dynamics of weakly coupled BECs. The central argument is that the density profile of each condensate can strongly depend on the number of atoms present at a given instant in the same well. This introduce site- and time- dependent parameters in the DNLS Eq.(2), modifying, in particular, its effective degree of nonlinearity. Therefore, the tight-binding approximation of nonlinear systems has to be generalized as:

$$\Psi(\vec{r}, t) = \sum_j \psi_j(t) \Phi_j(\vec{r}, N_j(t)). \quad (3)$$

with $\Phi_j(\vec{r}, N_j(t))$ depending implicitly on time through $N_j(t) = |\psi_j(t)|^2$. We stress here, and discuss again later, that the spatial wavefunctions $\Phi_j$ (which are considered sufficiently localized in each well) can also depend explicitly on time due to the excitation of internal modes. In the present approach, however, we consider the adiabatic limit in which the
interwell number/phase dynamics is much slower that the typical time associated with the excitations of such internal modes (and, of course, the cases where such modes are not already present in the initial configuration of the system). In this limit, which can is well satisfied in typical experiments, the spatial wavefunctions in Eq.(3) will adiabatically follow the tunneling dynamics and can be approximate with the real wavefunction $\Phi_j(\vec{r};N_j(t))$.

III. THE DISCRETE NONLINEAR EQUATION

The BEC dynamics at $T = 0$ satisfies the Gross-Pitaevskii equation (GPE) [18]:

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + [V_{\text{ext}} + g_0 |\Psi|^2] \Psi$$

where $V_{\text{ext}}$ is the external potential and $g_0 = \frac{4\pi\hbar^2 a}{m}$, with $m$ the atomic mass and $a$ the s-wave scattering length: $a > 0$ ($a < 0$) corresponds to an effective interatomic repulsion (attraction). For the sake of clarity, we will focus on the case $a > 0$ (as for $^{87}$Rb atoms), and with $V_{\text{ext}}$ will be given by the optical periodic potential $V_P$ superimposed to a harmonic magnetic field $V_M$. The periodic potential is

$$V_P = V_0 \sin^2 (kx)$$

where $k = 2\pi/\lambda$ and $\lambda$ is the wavelength of the lasers (the lattice spacing is $\lambda/2$). The energy barrier between adjacent sites, $V_0 = sE_R$, is expressed in units of the recoil energy $E_R = \frac{\hbar^2 k^2}{2m}$. From (5) we see that the minima of the laser potential are located at the points $x_j = j \frac{\lambda}{2}$. Around these points, $V_P \approx \frac{m}{2} \tilde{\omega}_x^2 (x-x_j)^2$, where

$$\tilde{\omega}_x = \sqrt{\frac{2V_0 k^2}{m}}.$$  

The magnetic potential is $V_M = \frac{m}{2}[\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2]$, with $\tilde{\omega}_x >> \omega_x$. It is convenient to write the external potential as $V_{\text{ext}} = V_L + V_D$, with the confining lattice potential $V_L = V_0 \sin^2 (kx) + \frac{m}{2}[\omega_y^2 y^2 + \omega_z^2 z^2]$, and the “driving” field $V_D = \frac{m}{2} \omega_x^2 x^2$. $V_D$ has a simple physical meaning: $F = -\frac{\partial V_D}{\partial x}$ is the effective force acting on the center of mass of a condensate wave packet moving in the periodic potential, see Section VII.
Here we consider a one-dimensional optical lattice superimposed to an harmonic driving field, but the following considerations can be easily generalized to arbitrary $V_D$ and, in particular, extended to the case of two- [19] and three- [1] dimensional arrays created by several counterpropagating laser beams.

Replacing the nonlinear tight-binding approximation (3) in the GPE (4) and integrating out the spatial degrees of freedom we find the following DNL:

$$i\hbar\frac{\partial \psi_j}{\partial t} = \epsilon_j \psi_j - \chi [\psi_j (\psi_{j+1}^* + \psi_{j-1}^*) + c.c.] \psi_j + \mu_{j}^{\text{loc}} \psi_j$$

$$- [K + \chi (| \psi_j |^2 + | \psi_{j+1} |^2)] \psi_{j+1} - [K + \chi (| \psi_j |^2 + | \psi_{j-1} |^2)] \psi_{j-1}$$

(7)

(we use the normalization $\int d\vec{r} \Phi_j^2 = 1$, while the total number of atoms is $N_T = \sum_{j} |\psi_j|^2 \equiv \sum_{j} N_j$). In Eq.(7), the “local” chemical potential is the sum of three contributions

$$\mu_{j}^{\text{loc}} = \mu_{j}^{\text{kin}} + \mu_{j}^{\text{pot}} + \mu_{j}^{\text{int}} = \int d\vec{r} \left[ \frac{\hbar^2}{2m} (\nabla \Phi_j)^2 + V_L \Phi_j^2 + g_0 |\psi_j|^2 \Phi_j^4 \right].$$

(8)

$\mu_{j}^{\text{loc}}$ depends on the atom number $N_j$ through the condensed wavefunction $\Phi_j(\vec{r},N_j(t))$. The tunneling rates $K_{j,j\pm1}$ between the adjacent sites $j$ and $j \pm 1$ also depend, in principle, on the respective populations: $K_{j,j\pm1}(N_j;N_{j\pm1}) = -\int d\vec{r} \left( \frac{\hbar^2}{2m} \nabla \Phi_j \cdot \nabla \Phi_{j\pm1} + \Phi_j V_{\text{ext}} \Phi_{j\pm1} \right)$. In this case, however, we can expand the wavefunctions around an average number of atoms per site, $N_0$, and keep only the zero order term $\Phi_j(N_j) \simeq \tilde{\Phi}_j(N_0)$:

$$K \simeq -\int d\vec{r} \left[ \frac{\hbar^2}{2m} \nabla \tilde{\Phi}_j \cdot \nabla \tilde{\Phi}_{j\pm1} + \tilde{\Phi}_j V_{\text{ext}} \tilde{\Phi}_{j\pm1} \right].$$

(9)

We have checked numerically that higher order terms are negligible: for instance, with the experimental setup of [6], $V_0 = 10E_R$ and $N_0 = 1000$, we have $K_1 = \frac{\partial K}{\partial N_0} \delta N \sim 10^{-4} K$.

Similarly, the coefficient $\chi$ is given by:

$$\chi = -g_0 \int d\vec{r} \tilde{\Phi}_j^3 \tilde{\Phi}_{j\pm1}.$$  

(10)

The on-site energies arising from any external potential superimposed to the optical lattice are

$$\epsilon_j = \int d\vec{r} V_D \Phi_j^2;$$

(11)
\( \epsilon_j \propto j^2 \) (\( \epsilon_j \propto j \)) when the driving field is harmonic (linear). We notice that in the limit \( \tilde{\omega}_x >> \omega_x \) considered here, \( \epsilon_j \) does not depend on the on-site atomic populations.

In the derivation of Eq.(7) we have exploited the (quasi-)orthogonality of the condensate wavefunctions \( \int d\vec{r} \Phi_j \Phi_{j\pm1} \approx 0 \). Moreover, we have verified numerically that spatial integrals involving condensates distant more than one site, as well as terms proportional to \( \int d\vec{r} \Phi_j^2 \Phi_{j\pm1}^2 / K \sim 10^{-4} \), can be neglected. E.g., with \( V_0 = 10E_R \) and \( N_0 = 1000 \), \( g_0 N_0 \int d\vec{r} \Phi_j^2 \Phi_{j\pm1}^2 / K \sim 10^{-4} \), while \( \chi N_0 / K \sim 10^{-2} \). For \( V_0 = 20E_R \) and \( N_0 = 10000 \), \( \chi N_0 / K \sim 10^{-1} \). In a double well with e.g. \( \tilde{\omega}_x = 2\pi \cdot 100Hz \) and \( N_0 = 10000 \), \( \chi N_0 \sim K \), while \( K_1 \) and \( g_0 N_0 \int d\vec{r} \Phi_j^2 \Phi_{j\pm1}^2 \) can still be ignored. For these reasons, we do not neglect the \( \chi \) terms in Eq.(7). A detailed account of the related numerical study will be presented elsewhere.

The atom number dependence in Eq.(8) introduces an effective time-dependent, real, local chemical potential \( \mu_j^{\text{loc}}[N_j(t)] \). This reflects an important approximation contained in the DNL: terms proportional to \( \partial \Phi_j / \partial t \) have been neglected. In other words, we have neglected the phases associated with the spatial dynamics of the \( \Phi_j(\vec{r}; N_j(t)) \) in Eq.(3). This adiabatic approximation is well satisfied when the tunneling time (\( \sim N_j / \dot{N}_j \)) is much longer than time scales associated with the change in shape of the wavefunctions (\( \sim \omega_r^{-1}, \tilde{\omega}_x^{-1} \)). In this limit, well satisfied in realistic experiments, the spatial profile of the wavefunctions adapts adiabatically to the instantaneous number of atoms present in the respective wells.

The dependence of the local chemical potential on the number of atoms depends on the effective dimensionality of the condensates trapped in each well of the lattice. This can be determined comparing the interaction chemical potential \( \mu_j^{\text{int}} = |\psi_j|^2 g_0 \int d\vec{r} \Phi_j^4 \) and the three frequencies, \( \tilde{\omega}_x, \omega_y, \omega_z \) obtained expanding the lattice potential around the minima of each well \( V_L \approx \frac{m}{2} [\tilde{\omega}_x^2 (x - x_j)^2 + \omega_y^2 y^2 + \omega_z^2 z^2] \). A sufficiently accurate calculation of \( \mu_j^{\text{int}} \) as a function of \( N_j \) can be obtained approximating the condensate order parameters with gaussians or Thomas-Fermi functions [21]. Here we first consider some limit cases which are particularly instructive.
When $\tilde{\omega}_x, \omega_y, \omega_z \gg \mu_j^{\text{int}}$, the spatial widths of each trapped condensate do not depend (in first approximation) on the number of particles $N_j$ in the same well, and the condensates wavefunctions are well approximated by gaussians. We consider this as a $0D$ (zero-dimensional) case ($nD$, with $n = 0, 1, 2, 3$, should not be confused with the spatial dimensionality of the lattice), and the ansatz Eq.(3) reduces to the ordinary TBA Eq.(1). The $1D$ case arises when two frequencies are greater than the interaction chemical potential. For instance, if $\tilde{\omega}_x, \omega_z \gg \mu_j^{\text{int}} \gg \omega_y$, the system realizes an array of weakly coupled cigar-shaped condensates oriented along the $y$-axis: the wavefunction $\Phi_j$ will be factorized as a product of two gaussians (in the $x$ and $z$ directions) and a Thomas-Fermi in the $y$ variable. In the $2D$ case only one frequency is smaller than the local interaction chemical potential. If $\tilde{\omega}_x \gg \mu_j^{\text{int}} \gg \omega_y, \omega_z$, we have an array of pancake-like condensates, with $\Phi_j$ factorized as a gaussian (along $x$) and a Thomas-Fermi in the $y$ and $z$ variables [see Eqs.(31-33)]. The $3D$ case is given by the condition $\mu_j^{\text{int}} \gg \tilde{\omega}_x, \omega_y, \omega_z$ and the wavefunction in the $j$th well $\Phi_j$ is simply given by a three-dimensional Thomas-Fermi function. To summarize:

$$3D \quad \mu_j^{\text{int}} (\sim N_j^{2/5}) \gg \omega_a, \omega_b, \omega_c \quad \text{[spherical]}$$

$$2D \quad \omega_a \gg \mu_j^{\text{int}} (\sim N_j^{1/2}) \gg \omega_b, \omega_c \quad \text{[pancake]}$$

$$1D \quad \omega_a, \omega_b \gg \mu_j^{\text{int}} (\sim N_j^{2/3}) \gg \omega_c \quad \text{[cigar]}$$

$$0D \quad \omega_a, \omega_b, \omega_c \gg \mu_j^{\text{int}} (\sim N_j) \quad \text{[spherical]}$$

with $a, b, c$ arbitrarily corresponding to the $x, y, z$ spatial directions, and among square brackets are specified the geometric shapes of the condensates in each well.

The crucial point is that the effective dimensionality of the condensates gives a different scaling of the local interaction chemical potential Eq.(8) with the number of atoms:

$$\mu_j^{\text{loc}} = U_\alpha |\psi_j|^\alpha$$

$$\alpha = \frac{4}{2 + D}, \quad D = 0, 1, 2, 3.$$  

where $U_\alpha$ is a constant which does not depend on the number of atoms nor on the site index. In the following we will often consider, for the sake of clarity, the limit cases when
the local chemical potential is given by Eq. (12) (generalization to more complicate functional dependences of $\mu_{j \text{loc}}$ from $N_j$ are straightforward). The DNLS Eq. (2) is recovered from the DNL Eq. (7) in the case $D = 0$ (i.e. $\alpha = 2$) and neglecting terms proportional to $\chi$.

The derivation of the Hamiltonian of the system requires some care. The dynamical variables $\psi_j^{\star}, i\hbar \psi_j$ are canonically conjugate ($\dot{\psi}_j = \frac{\partial H_{\text{eff}}}{\partial (i\hbar \psi_j^{\star})}$) with respect to the effective Hamiltonian

$$H_{\text{eff}} = \sum_j \left\{ \epsilon_j \psi_j^{\star} \psi_j - K(\psi_j^{\star} \psi_{j+1} + \text{c.c.}) - \chi [ | \psi_j |^2 \psi_j (\psi_j^{\star} + \psi_{j-1}^{\star}) + \text{c.c.}] + \frac{2}{2+\alpha} U_\alpha |\psi_j|^{\alpha+2} \right\}$$

(14)

(with the nonlinear term $\frac{2}{2+\alpha} U_\alpha |\psi_j|^{\alpha+2}$ obtained from $\psi_j \int d\psi_j \mu_{j \text{loc}}^{\text{loc}}$).

The effective Hamiltonian $H_{\text{eff}}$ is an exact integral of motion, but differs from the “adiabatic” Hamiltonian retrieved simply replacing Eq. (3) in the Gross-Pitaevskii energy functional:

$$H_{\text{ad}} = \sum_j \left\{ \epsilon_j \psi_j^{\star} \psi_j - K(\psi_j^{\star} \psi_{j+1} + \text{c.c.}) + \right.$$

$$\left. - \chi [ | \psi_j |^2 \psi_j (\psi_j^{\star} + \psi_{j-1}^{\star}) + \text{c.c.}] + \frac{1}{2} U |\psi_j|^4 \right\},$$

(15)

with $U = g_0 \int d\bar{r} \bar{\phi}^4_j$. The $H_{\text{eff}}$ and $H_{\text{ad}}$ are identical only in the $0D$ case. In general, $H_{\text{ad}}$ is not exactly, but only “adiabatically”, conserved during the dynamics.

**IV. EXCITATION SPECTRA**

We now derive the Bloch excitation spectra and the Bogoliubov dispersion relation of the system (with $\epsilon_j = 0$), calculate the sound velocity and investigate the dynamical stability of condensate traveling waves. Eigenfunctions of the DNL are the plane waves $\psi_n = \psi_0 e^{i(pn-\mu t/\hbar)}$, with chemical potential and energy per site:

$$\mu = \mu_{\text{loc}} - 2 (K + 4 \chi N_0) \cos p$$

$$E = E_{\text{loc}} - 2 (K + 2 \chi N_0) N_0 \cos p$$

(16)
where $N_0 = |\psi_0|^2$, $\mu_{j}^{\text{loc}}|_{\psi_j=\psi_0} = U_\alpha |\psi_0|^\alpha$, and $E_{j}^{\text{loc}} = \psi_0 \int d\psi_j^* \mu_{j}^{\text{loc}}|_{\psi_j=\psi_0} = 2U_\alpha |\psi_0|^\alpha+2/(\alpha+2)$ [see Eq.(12)]. From Eq.(16) we can recover the group velocity of Bloch waves with quasimomentum $p$: $v_g \equiv \frac{1}{N_0} \frac{\partial E}{\partial p} = 2(2\chi N_0)\sin p$.

We remark that the Bloch energy $E$ and the chemical potential $\mu$ have the same $\cos p$ dependence on the quasimomentum $p$, but with different coefficients. This introduces different effective masses for the system (see also [23]), which will enter in peculiar ways in the equations discussed in this paper, as will be reported elsewhere [22]. Here we will write down our results only in terms of the DNL parameters.

In order to derive the Bogoliubov dispersion relation of the system, we perturb the large amplitude wave as $\psi_n = [\psi_0 + u(t)e^{iqn} + v^*(t)e^{-iqn}] e^{i(pn-\mu t/\hbar)}$. Retaining only first order terms proportional to $u/\psi_0$ and $v/\psi_0$, we get

$$i\hbar \frac{d}{dt} \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} a + b & c \\ -c^* & a - b \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = \omega \pm \begin{pmatrix} u \\ v \end{pmatrix}$$

(17)

with $a = 2(K + 4\chi N_0) \sin p \sin q$, $b = 2K \cos p - 2(K + 4\chi N_0) \cos p \cos q + N_0 \frac{\partial \mu_{\text{loc}}}{\partial N_0}$ and $c = -4\chi \psi_0^2 \cos p (1 + \cos q) + \psi_0^2 \frac{\partial \mu_{\text{loc}}}{\partial N_0} N_0 \cos p$. Up to the order $\chi^2 N_0^2 / K^2$, we get the eigenvalues:

$$\omega = 2(K + 4\chi N_0) \sin p \sin q \pm \frac{\sqrt{2(2(K + 2\chi N_0)) \frac{\partial \mu}{\partial N_0} N_0 \cos p \sin^2 \frac{q}{2}}}{2}$$

(18)

V. SOUND-WAVES AND INSTABILITIES

The small $q$ (large wavelength) limit of the Bogoliubov dispersion relation Eq.(18) is linear. Therefore, the system support (low amplitude) sound waves (propagating on top of the large amplitude traveling wave $\psi_0 e^{i(pn-\mu t/\hbar)}$) having velocity

$$v_s = \frac{\partial \omega}{\partial q} |_{q=0} = 2(K + 4\chi N_0) \sin p \pm \sqrt{2(2(K + 2\chi N_0)) \frac{\partial \mu}{\partial N_0} N_0 \cos p}$$

(19)

with $\mu$ given by Eq.(16). The $+$ (−) sign corresponds to a sound wave propagating in the same (opposite) direction of the large amplitude traveling wave. Notice that, contrary
to the case of a Galilean invariant system ($V_0 = 0$), the sound velocity depends on the quasimomentum $p$. Moreover, $v_s$ depends on the effective dimensionality of the condensates, since (from Eq. (12,13)) $\frac{\partial \mu}{\partial N_0} N_0 \sim \alpha U_\alpha N_0^{\alpha/2}$.

In the limit $V_0 = 0$, the system is energetically unstable if $\omega < 0$, namely when the group velocity is larger than the sound velocity (Landau criteria for superfluidity). This instability is present also when the system has a discrete translational invariance ($V_0 > 0$): from the Bogoliubov excitation spectrum Eq. (18) and the condition $\omega < 0$, we have that the system is not superfluid when

$$[2(K + 4\chi N_0) \sin p]^2 > 2(K + 2\chi N_0) \frac{\partial \mu}{\partial N_0} N_0 \cos p$$  \hspace{1cm} (20)

There is a further, different (dynamical) instability mechanism, which disappears in the translational invariant limit (when $a > 0$). This instability is associated with the appearance of an imaginary component in the Bogoliubov frequencies: from Eq. (18), this component appears if $\cos p < 0$. This reflects on an exponential increase of the amplitude of the perturbation modes, with the consequent strong dephasing and energy dissipation of the condensate traveling wave. The unstable modes $q$, for a given quasimomentum $p$, are given by:

$$2 \left( 1 + \frac{6\chi N_0}{K} \right) \left| \cos p \right| \sin^2 \frac{q}{2} < \frac{\partial \mu}{\partial N_0} N_0.$$  \hspace{1cm} (21)

For $\alpha = 2$ and $\chi = 0$ we recover the standard DNLS results [24,12]. The onset of energetic and dynamical instabilities with an arbitrary $V_0$ has been studied numerically in [11]. Experimental evidences are reported on [25]. A different manifestation of the instability is associated with the self-trapping of a condensate wavepacket at rest in an optical lattice [10]. First experimental results are reported in [26].

VI. GROUND-STATE ATOMIC DISTRIBUTION

We now consider a magnetic harmonic potential superimposed to the optical lattice $\epsilon_j = \Omega j^2$, with $\Omega = m\omega_x^2 \lambda^2 / 8$. For a large nonlinearity, the ground-state atomic distribution
can be calculated from the DNL (7) in Thomas-Fermi approximation, i.e. neglecting the kinetic terms proportional to $K$ and $\chi$ with respect to the nonlinear term:

$$N_j = \left(\frac{\nu - \Omega j^2}{U_\alpha}\right)^{2/\alpha} = \left(\frac{\nu}{U_\alpha}\right)^{2/\alpha} \left(1 - \frac{j^2}{j_{inv}^2}\right)^{2/\alpha}$$

where the inversion point is $j_{inv}^2 = \nu/\Omega$. Replacing sums with integrals, we get

$$\nu = \left(\frac{N_T\Omega^{1/2}U_\alpha^{2/\alpha}}{C_\alpha}\right)^{2\alpha/(\alpha+4)}$$

where $C_\alpha = 2^{4/\alpha+1}\Gamma(2/\alpha+1)^2/\Gamma(4/\alpha+2)$ is a numerical constant ($\Gamma$ is the Gamma function). For $\alpha = 2$ ($0D$), $C_2 = 4/3$, while for $\alpha = 1$ ($2D$), $C_1 = 16/15$.

VII. NEWTONIAN DYNAMICS AND SMALL AMPLITUDE OSCILLATION FREQUENCIES

We now study the wave-packet dynamics of a BEC in an optical lattice. We resort to a variational approach, previously considered in [10]. Here we use a general variational wavefunction

$$\psi_j = \sqrt{K(\sigma)} f\left(\frac{j - \xi}{\sigma}\right) e^{ip(j - \xi) + i\delta(j - \xi)^2}$$

(24)

where $\xi(t)$ and $\sigma(t)$ are, respectively, the center and the width of the wavepacket, $p(t)$ and $\delta(t)$ their associated momenta and $K(\sigma)$ a normalization factor (such that $\sum_j N_j = N_T$). $f$ is a generic function, even in the variable $X = (j - \xi)/\sigma$. E.g., we can choose $f(X) = e^{-X^2}$ or $f(X) = (1 - X^2)^{1/\alpha}$ (with $-1 \leq X \leq 1$) to describe, respectively, the dynamics of a gaussian or a Thomas-Fermi wave packet. With the Lagrangian $\mathcal{L} = i\hbar \sum_j \psi_j^* \dot{\psi}_j - \mathcal{H}_{eff}$ we can recover the equations of motions for the variational parameters $q_i(t) \equiv (\xi(t), \sigma(t), p(t), \delta(t))$, given by

$$\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}_i} = \frac{\partial \mathcal{L}}{\partial q_i}.$$ 

With the variational wavefunction Eq.(24), the Lagrangian becomes:

$$\frac{\mathcal{L}}{N_T} = \hbar p\dot{\xi} - \hbar \sigma^2\dot{\delta}\frac{T_2}{2L_1} - V_D(\xi, \sigma) - \bar{U}_\alpha \frac{N_{\sigma^2/2}}{\sigma^{\alpha/2}} + \frac{2K}{L_1} \mathcal{I}_f(\sigma; \delta) \cos p + \frac{2\chi N_T}{\sigma L_1^2} \mathcal{I}_\chi(\sigma; \delta) \cos p$$

(25)

where $V_D(\xi, \sigma) = \frac{1}{L_1} \int dX f^2(X) \epsilon(\sigma X + \xi)$, $\bar{U}_\alpha = 2U_\alpha \mathcal{I}_{NL}/[(\alpha + 2)\mathcal{I}_{1/2}^{\alpha/2+1}]$, $\mathcal{I}_f(\sigma; \delta) = \int dX f(X + 1/2\sigma)f(X - 1/2\sigma)e^{i\sigma\delta X}$ and $\mathcal{I}_\chi(\sigma; \delta) = \int dX f(X + 1/2\sigma)f(X - 1/2\sigma)[f^2(X +
$1/2\sigma) + f^2(X - 1/2\sigma)e^{i\sigma\delta X}$. Furthermore $I_1 = \int dX f^2(X)$, $I_2 = \int dX X^2 f^2(X)$ and $I_{NL} = \int dX f^{\alpha+2}(X)$ are real numbers which depend on the particular choice of $f$. From the Lagrangian equation of motion we get the group velocity $\dot{\xi}$ and the effective force acting on the center of mass of the wavepacket:

$$\hbar \dot{\xi} = \frac{2K}{T_1} I_J(\sigma; \delta) + \frac{2\chi N_T}{\sigma T_2^2} I_X(\sigma; \delta) \sin p$$

$$\hbar \dot{\delta} = -\frac{\partial V_D}{\partial \xi}$$

(26)

The frequency of small amplitude oscillations of the wavepacket driven by an harmonic field $\epsilon_j = \Omega_j^2$ (which gives $V_D(\xi, \sigma) = \Omega(\xi^2 + \sigma^2/\tau_1^2)$), is:

$$\omega_{dip}^2 = \frac{2\Omega}{\hbar^2} \left( 2K + \frac{8\chi N_0 T_3}{T_1^2} \right)$$

(27)

where $N_0 = N_T/2\sigma$ [27]. Eq.(27) has been calculated in the limit of a large width $\sigma >> 1$, where $I_J(\sigma; 0) \approx I_1$ and $I_X(\sigma; 0) \approx 2I_3$, with $I_3 = \int dX f^4(X)$. The same results follow from the exact equation of motion for $\xi = \sum_j j N_j$ and $p = \varphi_{j+1} - \varphi_j$, with the latter assumed equal for each $j$ along the array (and using the fact that $\sum_j \sqrt{N_j N_{j+1}} \simeq N_T$ and $\sum_j N_j \sqrt{N_j N_{j+1}} \simeq \sum_j N_j^2$). For $\chi = 0$ Eq.(27) coincides with the result in [6].

To calculate the quadrupole oscillation frequency we need the equation of motion for the width $\sigma$ and the conjugate momentum $\delta$ (still with $V_D = \Omega \xi^2$):

$$-\hbar \dot{I_2} = \frac{2K}{\sigma T_1} \partial I_J \cos p + \frac{2\chi N_T}{\sigma^2 T_1^2} \partial I_X \cos p$$

$$\hbar \dot{\delta} \frac{I_2}{I_1} = -2\Omega \frac{I_2}{I_1} + \frac{\alpha U_\alpha N_T^\alpha/2}{2\sigma^{\alpha/2+2}} + \frac{2K}{\sigma T_1} \partial I_J \cos p + \frac{2\chi N_T}{\sigma^2 T_1^2} \left( \frac{\partial I_X}{\partial \sigma} - \frac{I_X}{\sigma} \right) \cos p$$

(28)

The equilibrium position is given by $\dot{\delta} = 0$, $\dot{\sigma} = 0$, $\xi = 0$ and $p = 0$. Linearizing around the equilibrium for the Thomas-Fermi ground-state (22), and after a lengthy calculation, we get the frequency of the quadrupole oscillations:

$$\omega_{quadr}^2 = \frac{\Omega (\alpha + 4) I_{NL}}{2\hbar^2 I_2(\alpha + 2)} \left( 2K + \frac{8\chi N_0 I_4}{I_1 I_2} \right)$$

(29)

where $I_4 = \int dX X^2 f^4(X)$ [28]. Eq.(29) shows that the quadrupole frequency explicitely depends on the effective dimensionality of the condensates in each well [29]. Collecting Eqs.(27) and (29) we get
\[
\frac{\omega_{\text{quadr}}^2}{\omega_{\text{dip}}^2} = \frac{\alpha(\alpha + 4)I_{NL}}{4(\alpha + 2)I_2}, \quad \frac{1 + 4\frac{\chi_0}{K}I_2}{1 + 4\frac{\chi_0}{K}I_2^3}.
\]

(30)

When \(\chi N_0 \ll K\), \(\frac{\omega_{\text{quadr}}^2}{\omega_{\text{dip}}^2} = 2\). In particular, \(\frac{\omega_{\text{quadr}}^2}{\omega_{\text{dip}}^2} = 3\) in the zero-dimensional case, \(D = 0\). The \(2D\), \(\chi = 0\) result, \(\frac{\omega_{\text{quadr}}^2}{\omega_{\text{dip}}^2} = \frac{5}{2}\), is in agreement with the results of [30].

VIII. NUMERICAL ESTIMATES

We now consider a specific example to further clarify the calculation of the DNL coefficients Eqs.(8-11). Considering the experimental apparatus of [6], we put: \(\omega_x = 2\pi \times 9 Hz\), \(\omega_y = \omega_z = 2\pi \times 90 Hz\), \(\lambda = 795 \text{ nm}\), \(E_R/h = 3.6 \text{ kHz}\) and \(V_0/E_r\) from 2 to 15. From Eq.(6), we obtain \(\tilde{\omega}_x/2\pi = \sqrt{s} \cdot 7.2 \text{ kHz}\).

Since \(\tilde{\omega}_x >> \omega_r\), we find \(\mu_j^{\text{kin}} + \mu_j^{\text{f orm}} \approx \hbar \tilde{\omega}_x/2\). With an average value of atoms in each well \(N_0 \sim 1000\) and with \(V_0 = 5E_r\), we obtain an interaction chemical potential \(\mu_j^{\text{int}} \sim \hbar \cdot 2kHZ\), which corresponds, according to the table in Section III, to the \(2D\) case. The system can be seen as a horizontal pile of pankakes, having a smaller diameter at the border of the pile, dense at the center and more dilute at the surface. In this limit we have:

\[
\Phi_j(\vec{r}, N_j(t)) \simeq \phi_G^{(j)}(x - x_j)\phi_{TF}^{(j)}(y, z)
\]

(31)

where \(\phi_G^{(j)} = (\sigma\sqrt{\pi})^{-1/2} e^{-(x-x_j)^2/2\sigma^2}\) is a gaussian with width \(\sigma\) (we impose \(\int dx (\phi_G^{(j)})^2 = \int dydz (\phi_{TF}^{(j)})^2 = 1\)). A variational calculation shows that there is a very weak dependence of \(\sigma\) on \(N_j\); we therefore assume it as site-independent [17,31]: \(\sigma = \frac{\lambda}{2\pi \sigma^{1/4}}\). Replacing Eq.(31) in Eq.(4) and integrating out along the \(x\) direction, we obtain an equation for \(\phi_{TF}^{(j)}(y, z)\):

\[
[-\frac{\hbar^2}{2m} \nabla_{\vec{R}}^2 + \mathcal{V}(\vec{R}) + \tilde{g}_0 N_j(\phi_{TF}^{(j)})^2]\phi_{TF}^{(j)} = \mu_j^{\text{int}}\phi_{TF}^{(j)}
\]

(32)

with \(\tilde{g}_0 = g_0/\sqrt{2\pi \sigma}\); \(\vec{R} = (y, z)\) is the vector expressing the position in the \(y\)-\(z\) radial plan and \(\mathcal{V}(\vec{R}) = \frac{m}{2}\omega_r^2 R^2\). In Thomas-Fermi approximation (i.e. neglecting the kinetic terms in Eq.(32)), we find
\[ \phi_{TF}^{(j)}(\vec{R}) = \left( \frac{\mu_j^{\text{int}} - \mathcal{V}(\vec{R})}{g_0 N_j} \right)^{1/2}. \] (33)

The inversion point is \( R_\perp^2 = 2\mu_j^{\text{int}}/m \omega_\perp^2 \). Replacing Eq.(33) in Eqs.(8) we obtain

\[ \mu_j^{\text{loc}} = \sqrt{\frac{m \omega_r^2 g_0}{2 \pi \pi \sigma}} N_j^{1/2}. \] (34)

The on-site energies (11) are given by \( \epsilon_j = \Omega j^2 \), where \( \Omega = \frac{m}{2} m \omega_\perp^2 (\lambda^2) \). We have neglected the kinetic terms \( \epsilon_j^{(\text{kin})} = \frac{\hbar^2}{2m} \int d\vec{R} (\vec{\nabla} \phi_{TF}^{(j)}) \), consistent with the Thomas-Fermi approximation (33). Using Eqs.(34) we get the DNL (7) with \( D = 2 \) (\( \alpha = 1 \)) and [see Eq.(12)]

\[ U_1 = \sqrt{\frac{m \omega_r g_0}{2 \pi \pi \sigma}}. \] (35)

The population distribution in the ground state, according to Eq.(22), is given by

\[ N_j = \left( \frac{\nu}{U_1} \right)^2 \left( 1 - \frac{j^2}{j_{\text{inv}}^2} \right)^2. \] (36)

The inversion point is \( j_{\text{inv}} = \sqrt{\frac{\pi}{\nu}} \) and the discrete chemical potential (23) is is \( \nu = (15 N_T U_1^2 \sqrt{\Omega}/16)^{2/5} \). Therefore

\[ j_{\text{inv}}^2 = \frac{2 \hbar \bar{\omega}}{m \omega_x^2 d^2} \left( \frac{15}{8 \sqrt{\pi}} N_T \frac{ad}{a_{ho} \sigma} \right)^{2/5} \] (37)

where \( d = \lambda/2, a_{ho} = \sqrt{\hbar/m \bar{\omega}} \) and \( \bar{\omega} = (\omega_r^2 \omega_x)^{1/3} \). The \( D = 2 \) ground state Eqs.(36-37) is in agreement with [17], previously calculated with a different approach.

**IX. QUANTUM CASE: AN EXTENDED BOSE-HUBBARD MODEL**

The quantization of the DNL equation requires some care. The quantum equation for the bosonic gas in an external potential is:

\[ i\hbar \frac{\partial}{\partial t} \hat{\Psi} (\vec{r}, t) = [T + V_{\text{ext}} + g_0 \hat{\Psi}^\dagger \hat{\Psi}] \hat{\Psi}, \] (38)

The Gross-Pitaevskii equation (4) can be retrieved introducing the classical field \( \Psi = \langle \hat{\Psi} \rangle \) and with \( \langle \hat{\Psi}^\dagger \hat{\Psi} \rangle \approx \langle \hat{\Psi}^\dagger \rangle \langle \hat{\Psi} \rangle \langle \hat{\Psi} \rangle \).

In tight-binding approximation
\( \hat{\Psi}(\vec{r}, t) = \sum_j \hat{\psi}_j(t) \Phi_j(\vec{r}) \)  \hspace{1cm} (39)

(with \( \hat{\psi}_j^\dagger \hat{\psi}_j \) the bosonic number operator), we obtain the Bose-Hubbard model (BHM) [32,33]

\[
\hat{H} = \sum_j \left\{ -K(\hat{\psi}_j^\dagger \hat{\psi}_{j+1} + h.c.) + \frac{U}{2}(\hat{\psi}_j^\dagger \hat{\psi}_j^\dagger \hat{\psi}_j \hat{\psi}_j) + \epsilon_j \hat{\psi}_j^\dagger \hat{\psi}_j \right\} \hspace{1cm} (40)
\]

We now discuss the case in which the localized wavefunction \( \Phi_j \) in the \( j \)th well adiabatically depends on the average number of particles in the same well: the generalization to the quantum case of (3) is

\[
\hat{\Psi}(\vec{r}, t) = \sum_j \hat{\psi}_j(t) \Phi_j(\vec{r}; N_j(t)) \hspace{1cm} (41)
\]

where

\[
N_j = \langle \hat{\psi}_j^\dagger \hat{\psi}_j \rangle. \hspace{1cm} (42)
\]

Replacing the ansatz (41) in (38), it is easy to recover the quantum equation of motion for bosonic operators \( \hat{\psi}_j \). Such equations are generated, with the standard bosonic commutation relations, from the extended Bose-Hubbard Hamiltonian:

\[
\hat{H} = \sum_j \left\{ \epsilon_j \hat{\psi}_j^\dagger \hat{\psi}_j + \frac{1}{2} U(\hat{\psi}_j^\dagger \hat{\psi}_j^\dagger \hat{\psi}_j \hat{\psi}_j) - K(\hat{\psi}_j^\dagger \hat{\psi}_{j+1} + h.c.) - \chi[\hat{\psi}_j^\dagger \hat{\psi}_j \hat{\psi}_j(\hat{\psi}_j^\dagger + \hat{\psi}_{j-1}) + h.c.] \right\} \hspace{1cm} (43)
\]

with the parameter \( K, \chi, \epsilon_j, U \) expressed as in the classical DNL Eq.(7). Notice that the extended BHM can be alternatively recovered quantizing the classical adiabatic Hamiltonian \( \mathcal{H}_{ad} \) Eq.(15) (and not the effective Hamiltonian Eq.(14)).

X. CONCLUSIONS

The Gross-Pitaevskii dynamics of a Bose-Enstein condensate trapped in a deep periodic potential can be studied in terms of a discrete, nonlinear equation. This mapping allows a clear and intuitive picture of the main dynamical properties of the system, which can be calculated analytically. We have shown that the slopes of the energy and chemical
potential Bloch excitation spectra, with respect to the quasimomentum of the condensate, are different. We have calculated the Bogoliubov dispersion relation, and studied the sound-wave velocity as a function of i) the effective dimensionality of each condensate, and ii) the quasimomentum of the carrier wave. Through a Lagrangian formalism, we have recovered Newtonian-like equation of motion of localized wavepackets, and the frequencies of dipole and quadrupole small amplitude oscillations. We have finally quantized the discrete nonlinear Hamiltonian recovering an extended Boson-Hubbard model.

Note added in proof: An equation similar to the DNL (7) (with $\alpha = 2$, and including the term proportional to $\int d\vec{r} \tilde{\Phi}_j^2 \tilde{\Phi}_{j\pm1}^2$) has been derived by Öster, Johansson, and Eriksson [34] to describe the amplitude of an electric field in an array of coupled waveguides embedded in a material with Kerr nonlinearities.

Acknowledgements. We thank C. Menotti for several valuable comments. We acknowledge discussions with S. Giorgini, M. Krämer, L. P. Pitaevskii, and S. Stringari. A.T. thanks the CRS-BEC of Trento, where part of this work was completed, for the kind hospitality. This work has been partially supported by the DOE.
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with $\alpha = 1$, $\mathcal{I}_1 = 16/15$, $\mathcal{I}_2 = 16/105$, $\mathcal{I}_{NL} = 32/35$, $\mathcal{I}_3 = 256/315$ and $\mathcal{I}_4 = 256/3465$;

with $\alpha = 2$, $\mathcal{I}_1 = 4/3$, $\mathcal{I}_2 = 4/15$, $\mathcal{I}_{NL} = 16/15$, $\mathcal{I}_3 = 16/15$ and $\mathcal{I}_4 = 16/105$.

[29] Eqs.(27,29) can be expressed in terms of the atom populations $N_j$ as $\omega_{\text{dip}}^2 = \frac{2\Omega}{\hbar^2} \left( 2K + \frac{4\chi}{N_T} \sum_j N_j^2 \right)$, $\omega_{\text{quadr}}^2 = \frac{U_\alpha}{25^2(\alpha+2)} \cdot \frac{\sum_j N_j^{\alpha/2+1}}{\sum_j j^2 N_j^2} \cdot \left( 2K + 4\chi \frac{\sum_j j^2 N_j^2}{\sum_j j^2 N_j} \right)$.

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