Nonlinear tight-binding approximation for Bose-Einstein condensates in a lattice

A. Smerzi[1,2] and A. Trombettoni[3]
[1]*Istituto Nazionale di Fisica per la Materia BEC-CRS and Dipartimento di Fisica, Università di Trento, I-38050 Povo, Italy*
[2]*Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*
[3]*Istituto Nazionale per la Fisica della Materia and Dipartimento di Fisica, Università di Parma, parco Area delle Scienze 7A, I-43100 Parma, Italy*

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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 wave packets. We calculate the ground-state atomic distribution in the presence of a harmonic confining potential, the frequencies of small amplitude dipole, and quadrupole oscillations. We finally quantize the DNL, recovering an extended Bose-Hubbard model.

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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 [11,12], which do not have an analog neither in metals nor in Galilean invariant nonlinear systems.

The BEC in a periodic potential is described in the 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 Ref. [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 [10,13,14] in the framework of the nonlinear lattice theory [15], 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 [3,6,16].

In the ''standard'' tight-binding approximation, the condensate wave function localized in the jth well is factorized as a dynamical part $\psi_j(t)=\sqrt{N_j(t)}e^{i\varphi_j(t)}$ and a spatial, real wave function $\Phi_j(\vec{r})$ 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

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

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

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

with K, U_2, ϵ_j depending on the geometry of the trapping potentials and on the average number of atoms in each well [cf. with Eqs. (8)–(11)].

II. A GENERALIZED TIGHT-BINDING APPROXIMATION

In this paper, we stress the importance (and exploit the consequences) of generalizing the ''standard'' tight-binding approximation (1). This generalization is imposed by the nonlinearity of the GPE (4), and largely extends the range of validity of the DNLS (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 introduces site- and time-dependent parameters in the DNLS (2), modifying, in particular, its effective degree of nonlinearity. Therefore, the tight-binding approximation of nonlinear systems has to be generalized as

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

with $\Phi_j(\vec{r};N_j(t))$ depending *implicitly* on time through $N_j(t)\equiv|\psi_j(t)|^2$. We stress here, and discuss again later, that the spatial wave functions Φ_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 than 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 is well satisfied in typical experiments, the spatial wave functions in Eq. (3) will adiabatically follow the tunneling dynamics and can be approximated with the *real* wave function $\Phi_j(\vec{r};N_j(t))$.

III. THE DISCRETE NONLINEAR EQUATION

The BEC dynamics at $T=0$ satisfies the GPE [17]

$$i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\nabla^2\Psi+[V_{ext}+g_0|\Psi|^2]\Psi, \tag{4}$$

where V_{ext} is the external potential and $g_0=4\pi\hbar^2a/m$, 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 V_{ext} will be given by the optical periodic potential V_P superimposed on a harmonic magnetic field V_M. The periodic potential is

$$V_P=V_0\sin^2(kx), \tag{5}$$

where $k=2\pi/\lambda$ and λ 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 the units of the recoil energy $E_R=\hbar^2k^2/2m$. From Eq, (5), we see that the minima of the laser potential are located at the points $x_j=j(\lambda/2)$. Around these points, $V_P\approx(m/2)\tilde{\omega}_x^2(x-x_j)^2$, where

$$\tilde{\omega}_x=\sqrt{\frac{2V_0k^2}{m}}. \tag{6}$$

The magnetic potential is $V_M=(m/2)[\omega_x^2x^2+\omega_y^2y^2+\omega_z^2z^2]$, with $\tilde{\omega}_x\gg\omega_x$. It is convenient to write the external potential as $V_{ext}=V_L+V_D$, with the confining lattice potential $V_L=V_0\sin^2(kx)+(m/2)[\omega_y^2y^2+\omega_z^2z^2]$ and the "driving" field $V_D=(m/2)\omega_x^2x^2$. V_D has a simple physical meaning: $F=-(\partial V_D/\partial x)$ is the effective force acting on the center of mass of a condensate wave packet moving in the periodic potential, see Sec. VII.

Here we consider a one-dimensional optical lattice superimposed on a harmonic driving field, but the following considerations can be easily generalized to arbitrary V_D and, in particular, extended to the case of two- [18] and three- dimensional [1] 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:

$$\begin{aligned}i\hbar\frac{\partial\psi_j}{\partial t}=&\epsilon_j\psi_j-\chi[\psi_j(\psi_{j+1}^*+\psi_{j-1}^*)+\text{c.c.}]\psi_j+\mu_j^{loc}\psi_j\\&-[K+\chi\ (|\psi_j|^2+|\psi_{j+1}|^2)]\psi_{j+1}\\&-[K+\chi(|\psi_j|^2+|\psi_{j-1}|^2)]\psi_{j-1}\end{aligned} \tag{7}$$

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

$$\begin{aligned}\mu_j^{loc}&=\mu_j^{kin}+\mu_j^{pot}+\mu_j^{int}\\&=\int d\vec{r}\left[\frac{\hbar^2}{2m}(\vec{\nabla}\Phi_j)^2+V_L\Phi_j^2+g_0\left|\psi_j\right|^2\Phi_j^4\right],\end{aligned} \tag{8}$$

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

$$K\simeq-\int d\vec{r}\left[\frac{\hbar^2}{2m}\vec{\nabla}\tilde{\Phi}_j\cdot\vec{\nabla}\tilde{\Phi}_{j\pm1}+\tilde{\Phi}_jV_{ext}\tilde{\Phi}_{j\pm1}\right]. \tag{9}$$

We have checked numerically that higher-order terms are negligible: for instance, with the experimental setup of Ref. [6], $V_0=10E_R$ and $N_0=1000$, we have $K_1=(\partial K/\partial N_0)\delta N\sim10^{-4}$ K. Similarly, the coefficient χ is given by

$$\chi=-g_0\int d\vec{r}\tilde{\Phi}_j^3\tilde{\Phi}_{j\pm1}. \tag{10}$$

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

$$\epsilon_j=\int d\vec{r}V_D\Phi_j^2; \tag{11}$$

$\epsilon_j\propto j^2$ ($\epsilon_j\propto j$) when the driving field is harmonic (linear). We note that in the limit $\tilde{\omega}_x\gg\omega_x$ considered here, ϵ_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 wave functions $\int d\vec{r}\Phi_j\Phi_{j\pm1}\simeq0$. Moreover, we have verified numerically that spatial integrals involving condensates distant more than one site, as well as terms proportional to $\int d\vec{r}\Phi_j^2\Phi_{j\pm1}^2$, can be neglected. For example, with $V_0=10E_R$ and $N_0=1000$, $g_0N_0\int d\vec{r}\Phi_j^2\Phi_{j\pm1}^2/K\sim10^{-4}$, while $\chi N_0/K\sim10^{-2}$. For $V_0=20E_R$ and $N_0=10\,000$, $\chi N_0/K\sim10^{-1}$. In a double well with, e.g., $\tilde{\omega}_x=2\pi(100\text{ Hz})$ and $N_0=10\,000$, $\chi N_0\sim K$, while K_1 and $g_0N_0\int d\vec{r}\Phi_j^2\Phi_{j\pm1}^2$ can still be ignored. For these reasons, we do not neglect the χ terms in Eq. (7). A detailed account of the related numerical study will be presented elsewhere.

TABLE I. Effective dimensionality of the condensates trapped in each well of the lattice.

Case	Condition	
3D	$\mu_j^{int}(\sim N_j^{2/5}) \gg \omega_a, \omega_b, \omega_c$	(spherical)
2D	$\omega_a \gg \mu_j^{int}(\sim N_j^{1/2}) \gg \omega_b, \omega_c$	(pancake)
1D	$\omega_a, \omega_b \gg \mu_j^{int}(\sim N_j^{2/3}) \gg \omega_c$	(cigar)
0D	$\omega_a, \omega_b, \omega_c \gg \mu_j^{int}(\sim N_j)$	(spherical)

The atom number dependence in Eq. (8) introduces an effective *time-dependent, real*, local chemical potential $\mu_j^{loc}[N_j(t)]$. 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 $\Phi_j(\vec{r};N_j(t))$ 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 wave functions ($\sim \omega_r^{-1}, \tilde{\omega}_x^{-1}$). In this limit, well satisfied in realistic experiments, the spatial profile of the wave functions adapts adiabatically to the instantaneous number of atoms present in the respective wells [19].

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 by comparing the interaction chemical potential $\mu_j^{int}=|\psi_j|^2 g_0 \int d\vec{r}\Phi_j^4$ and the three frequencies $\tilde{\omega}_x$, ω_y, ω_z obtained by expanding the lattice potential around the minima of each well $V_L \simeq (m/2)[\tilde{\omega}_x^2(x-x_j)^2+\omega_y^2 y^2 + \omega_z^2 z^2]$. A sufficiently accurate calculation of μ_j^{int} as a function of N_j can be obtained by approximating the condensate order parameters with Gaussians or Thomas-Fermi functions [20]. Here we first consider some limit cases which are particularly instructive.

When $\tilde{\omega}_x, \omega_y, \omega_z \gg \mu_j^{int}$, 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' wave functions 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 ansatz (3) reduces to the ordinary TBA (1). The 1D case arises when two frequencies are greater than the interaction chemical potential. For instance, if $\tilde{\omega}_x, \omega_z \gg \mu_j^{int} \gg \omega_y$, the system realizes an array of weakly coupled cigar-shaped condensates oriented along the y axis: the wave function Φ_j will be factorized as a product of two Gaussians (in the x and z directions) and a Thomas-Fermi function in the y variable. In the 2D case only one frequency is smaller than the local interaction chemical potential. If $\tilde{\omega}_x \gg \mu_j^{int} \gg \omega_y, \omega_z$, we have an array of pancakelike condensates, with Φ_j factorized as a Gaussian (along x) and a Thomas-Fermi function in the y and z variables [see Eqs. (31)–(33)]. The 3D case is given by the condition $\mu_j^{int} \gg \tilde{\omega}_x, \omega_y, \omega_z$ and the wave function in the jth well, Φ_j, is simply given by a three-dimensional Thomas-Fermi function. To summarize the above refer to Table I, 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 (8) with the number of atoms:

$$\mu_j^{loc} = U_\alpha |\psi_j|^\alpha, \tag{12}$$

$$\alpha = \frac{4}{2+D}, \quad D=0,1,2,3, \tag{13}$$

where U_α is a constant which depends neither 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 complicated functional dependences of μ_j^{loc} from N_j is straightforward). The DNLS (2) is recovered from the DNL (7) in the case $D=0$ (i.e., $\alpha=2$) and neglecting terms proportional to χ.

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

$$\mathcal{H}_{eff} = \sum_j \left\{ \epsilon_j \psi_j^* \psi_j - K(\psi_j^* \psi_{j+1} + \text{c.c.}) - \chi[|\psi_j|^2 \times \psi_j(\psi_{j+1}^* + \psi_{j-1}^*) + \text{c.c.}] + \frac{2}{2+\alpha} U_\alpha |\psi_j|^{\alpha+2} \right\} \tag{14}$$

[with the nonlinear term $(2/2+\alpha)U_\alpha|\psi_j|^{\alpha+2}$ obtained from $\psi_j \int d\psi_j^* \mu_j^{loc}$].

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

$$\mathcal{H}_{ad} = \sum_j \left\{ \epsilon_j \psi_j^* \psi_j - K(\psi_j^* \psi_{j+1} + \text{c.c.}) - \chi[|\psi_j|^2 \psi_j(\psi_{j+1}^* + \psi_{j-1}^*) + \text{c.c.}] + \frac{1}{2} U |\psi_j|^4 \right\}, \tag{15}$$

with $U = g_0 \int d\vec{r}\tilde{\Phi}_j^4$. $\mathcal{H}_{eff}$ and $\mathcal{H}_{ad}$ are identical only in the 0D case. In general, $\mathcal{H}_{ad}$ 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:

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

$$E = E^{loc} - 2(K + 2\chi N_0)N_0 \cos p, \tag{16}$$

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

We remark that the Bloch energy E and the chemical potential μ have the same $\cos p$ dependence on the quasimomentum p, but with different coefficients. This introduces different effective masses for the system (see also Ref. [22]), which will enter in peculiar ways in the equations discussed in this paper, as will be reported elsewhere [21]. 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/ψ_0 and v/ψ_0, we get

$$i\hbar \frac{d}{dt}\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} a+b & c \\ -c^* & a-b \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix} = \omega_\pm \begin{pmatrix} u \\ v \end{pmatrix}, \tag{17}$$

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

$$\omega = 2(K + 4\chi N_0)\sin p \sin q \pm 2\sqrt{4K(K + 8\chi N_0)\cos^2 p \sin^4 \frac{q}{2} + 2(K + 2\chi N_0)\frac{\partial \mu}{\partial N_0} N_0 \cos p \sin^2 \frac{q}{2}}. \tag{18}$$

V. SOUND WAVES AND INSTABILITIES

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

$$v_s = \left.\frac{\partial \omega}{\partial q}\right|_{q=0} = 2(K + 4\chi N_0)\sin p \pm \sqrt{2(K + 2\chi N_0)\frac{\partial \mu}{\partial N_0} N_0 \cos p}, \tag{19}$$

with μ given by Eq. (16). The $+(-)$ sign corresponds to a sound wave propagating in the same (opposite) direction of the large amplitude traveling wave. Note 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 Eqs. (12) and (13)] $(\partial \mu/\partial N_0)N_0 \sim \alpha\, U_\alpha\, N_0^{\alpha/2}$.

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 (18) and the condition $\omega < 0$, we have that the system is not superfluid when

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

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

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

For $\alpha = 2$ and $\chi = 0$, we recover the standard DNLS results [12,23]. The onset of energetic and dynamical instabilities with an arbitrary V_0 has also been studied in Ref. [11]. Experimental evidences are reported in Ref. [24]. A different dynamical instability is associated with the self-trapping of a condensate wave packet at rest in an optical lattice [10]. First experimental results are reported in Ref. [25].

VI. GROUND-STATE ATOMIC DISTRIBUTION

We now consider a magnetic harmonic potential superimposed on 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 χ with respect to the nonlinear term:

$$N_j = \left(\frac{\nu - \Omega j^2}{U_\alpha}\right)^{2/\alpha} = \left(\frac{\nu}{U_\alpha}\right)^{2/\alpha}\left(1 - \frac{j^2}{j_{inv}^2}\right)^{2/\alpha}, \tag{22}$$

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

$$\nu=\left(\frac{N_T\Omega^{1/2}U_\alpha^{2/\alpha}}{C_\alpha}\right)^{2\alpha/(\alpha+4)}, \tag{23}$$

where $C_\alpha=2^{4/\alpha+1}[\Gamma(2/\alpha+1)]^2/\Gamma(4/\alpha+2)$ is a numerical constant (Γ 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 Ref. [10]. Here we use a general variational wave function

$$\psi_j=\sqrt{\mathcal{K}(\sigma)}f\left(\frac{j-\xi}{\sigma}\right)e^{ip(j-\xi)+i(\delta/2)(j-\xi)^2}, \tag{24}$$

where $\xi(t)$ and $\sigma(t)$ are, respectively, the center and the width of the wave packet, $p(t)$ and $\delta(t)$ their associated momenta, and $\mathcal{K}(\sigma)$ a normalization factor (such that $\Sigma_j N_j=N_T$). f is a generic function, even in the variable $X=(j-\xi)/\sigma$. For example, we can choose $f(X)=e^{-X^2}$ or $f(X)=(1-X^2)^{1/\alpha}$ (with $-1\leqslant X\leqslant 1$) to describe, respectively, the dynamics of a Gaussian or a Thomas-Fermi wave packet. With the Lagrangian $\mathcal{L}=i\hbar\Sigma_j\psi_j^*\dot{\psi}_j-\mathcal{H}_{eff}$, 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 $(d/dt)(\partial\mathcal{L}/\partial\dot{q}_i)=(\partial\mathcal{L}/\partial q_i)$. With the variational wave function (24), the Lagrangian becomes

$$\frac{\mathcal{L}}{N_T}=\hbar p\dot{\xi}-\hbar\sigma^2\dot{\delta}\frac{\mathcal{I}_2}{2\mathcal{I}_1}-V_D(\xi,\sigma)-\tilde{U}_\alpha\frac{N_T^{\alpha/2}}{\sigma^{\alpha/2}}+\frac{2K}{\mathcal{I}_1}\mathcal{I}_J(\sigma;\delta)\cos p+\frac{2\chi N_T}{\sigma\mathcal{I}_1^2}\mathcal{I}_\chi(\sigma;\delta)\cos p, \tag{25}$$

where

$$V_D(\xi,\sigma)=\frac{1}{\mathcal{I}_1}\int dX f^2(X)\epsilon(\sigma X+\sigma),$$

$$\tilde{U}_\alpha=2U_\alpha\mathcal{I}_{NL}/[(\alpha+2)\mathcal{I}_1^{\alpha/2+1}],$$

$$\mathcal{I}_J(\sigma;\delta)=\int dX f(X+1/2\sigma)f(X-1/2\sigma)e^{i\sigma\delta X},$$

and

$$\mathcal{I}_\chi(\sigma;\delta)=\int dX f(X+1/2\sigma)f(X-1/2\sigma)\times[f^2(X+1/2\sigma)+f^2(X-1/2\sigma)]e^{i\sigma\delta X}.$$

Furthermore, $\mathcal{I}_1=\int dX f^2(X)$, $\mathcal{I}_2=\int dX X^2 f^2(X)$, and $\mathcal{I}_{NL}=\int dX f^{\alpha+2}(X)$ 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 wave packet:

$$\hbar\dot{\xi}=\left[\frac{2K}{\mathcal{I}_1}\mathcal{I}_J(\sigma;\delta)+\frac{2\chi N_T}{\sigma\mathcal{I}_1^2}\mathcal{I}_\chi(\sigma;\delta)\right]\sin p,$$

$$\hbar\dot{p}=-\frac{\partial V_D}{\partial\xi}. \tag{26}$$

The frequency of small amplitude oscillations of the wave packet, driven by a harmonic field $\epsilon_j=\Omega j^2$ (which gives $V_D(\xi,\sigma)=\Omega[\xi^2+\sigma^2(\mathcal{I}_2/\mathcal{I}_1])$, is

$$\omega_{dip}^2=\frac{2\Omega}{\hbar^2}\left(2K+\frac{8\chi N_0\mathcal{I}_3}{\mathcal{I}_1^2}\right), \tag{27}$$

where $N_0=N_T/2\sigma$ [26]. Equation (27) has been calculated in the limit of a large width $\sigma\gg 1$, where $\mathcal{I}_J(\sigma;0)\simeq\mathcal{I}_1$ and $\mathcal{I}_\chi(\sigma;0)\simeq 2\mathcal{I}_3$, with $\mathcal{I}_3=\int dX f^4(X)$. The same results follow from the exact equation of motion for $\xi=\Sigma_j jN_j$ and $p=\varphi_{j+1}-\varphi_j$, with the latter assumed equal for each j along the array (and using the fact that $\Sigma_j\sqrt{N_jN_{j+1}}\simeq N_T$ and $\Sigma_j N_j\sqrt{N_jN_{j+1}}\simeq\Sigma_j N_j^2$). For $\chi=0$, Eq. (27) coincides with the result in Ref. [6].

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

$$-\hbar\dot{\sigma}\frac{\mathcal{I}_2}{\mathcal{I}_1}=\frac{2K}{\sigma\mathcal{I}_1}\frac{\partial I_J}{\partial\delta}\cos p+\frac{2\chi N_T}{\sigma^2\mathcal{I}_1^2}\frac{\partial I_\chi}{\partial\delta}\cos p,$$

$$\hbar\dot{\delta}\frac{\mathcal{I}_2}{\mathcal{I}_1}=-2\Omega\frac{\mathcal{I}_2}{\mathcal{I}_1}+\frac{\alpha\tilde{U}_\alpha N_T^{\alpha/2}}{2\sigma^{\alpha/2+2}}+\frac{2K}{\sigma\mathcal{I}_1}\frac{\partial I_J}{\partial\sigma}\cos p+\frac{2\chi N_T}{\sigma^2\mathcal{I}_1^2}\left(\frac{\partial I_\chi}{\partial\sigma}-\frac{I_\chi}{\sigma}\right)\cos p. \tag{28}$$

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 lenghty calculation, we get the frequency of the quadrupole oscillations:

$$\omega_{quadr}^2=\frac{\Omega\alpha(\alpha+4)\mathcal{I}_{NL}}{2\hbar^2\mathcal{I}_2(\alpha+2)}\left(2K+\frac{8\chi N_0\mathcal{I}_4}{\mathcal{I}_1\mathcal{I}_2}\right), \tag{29}$$

where $\mathcal{I}_4=\int dX X^2 f^4(X)$ [27]. Equation (29) shows that the quadrupole frequency explicitly depends on the effective dimensionality of the condensates in each well [28]. Collecting Eqs. (27) and (29), we get

$$\frac{\omega^2_{quadr}}{\omega^2_{dip}}=\frac{\alpha(\alpha+4)\mathcal{I}_{NL}}{4(\alpha+2)\mathcal{I}_2}\frac{1+4\dfrac{\chi N_0}{K}\dfrac{\mathcal{I}_4}{\mathcal{I}_1\mathcal{I}_2}}{1+4\dfrac{\chi N_0}{K}\dfrac{\mathcal{I}_3}{\mathcal{I}_1^2}}. \tag{30}$$

When $\chi N_0 \ll K$, $(\omega^2_{quadr}/\omega^2_{dip})=2(D+3)/(D+2)$. In particular, $\omega^2_{quad}/\omega^2_{dip}=3$ in the zero-dimensional case, D=0. The 2D, $\chi=0$ result, $(\omega^2_{quadr}/\omega^2_{dip})=\frac{5}{2}$, is in agreement the results of [29].

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 Ref. [6], we put $\omega_x=2\pi(9\text{ Hz})$, $\omega_y=\omega_z\equiv\omega_r=2\pi(90\text{ Hz})$, $\lambda=795$ nm, $E_R/h=3.6$ kHz, and V_0/E_r from 2 to 15. From Eq. (6), we obtain $\tilde{\omega}_x/2\pi=\sqrt{s}(7.2\text{ kHz})$.

Since $\tilde{\omega}_x \gg \omega_r$, we find $\mu_j^{kin}+\mu_j^{harm}\approx\hbar\tilde{\omega}_x/2$. 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 $\mu_j^{int}\sim h(2\text{ kHz})$, which corresponds, according to Table I, to the 2D case. The system can be seen as a horizontal pile of panakes, 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

$$\Phi_j(\vec{r},N_j(t))\simeq\phi_G^{(j)}(x-x_j)\phi_{TF}^{(j)}(y,z), \tag{31}$$

where $\phi_G^{(j)}=(\sigma\sqrt{\pi})^{-1/2}e^{-(x-x_j)^2/2\sigma^2}$ is a Gaussian with width σ [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 σ on N_j; we therefore assume it as site independent [16,30]: $\sigma=(\lambda/2\pi s^{1/4})$. Replacing Eq. (31) by Eq. (4) and integrating out along the x direction, we obtain an equation for $\phi_{TF}^{(j)}(y,z)$:

$$\left[-\frac{\hbar^2}{2m}\nabla^2_{\vec{R}}+\mathcal{V}(\vec{R})+\tilde{g}_0N_j(\phi_{TF}^{(j)})^2\right]\phi_{TF}^{(j)}=\mu_j^{int}\phi_{TF}^{(j)}, \tag{32}$$

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 plane, and $\mathcal{V}(\vec{R})=(m/2)\omega_r^2R^2$. In Thomas-Fermi approximation [i.e., neglecting the kinetic terms in Eq. (32)], we find

$$\phi_{TF}^{(j)}(\vec{R})=\left(\frac{\mu_j^{int}-\mathcal{V}(\vec{R})}{\tilde{g}_0N_j}\right)^{1/2}. \tag{33}$$

The inversion point is $R_\perp^2=2\mu_j^{int}/m\omega_r^2$. Replacing Eq. (33) by Eq. (8), we obtain

$$\mu_j^{loc}=\sqrt{\frac{m\omega_r^2g_0}{\sqrt{2\pi}\pi\sigma}}N_j^{1/2}. \tag{34}$$

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

$$U_1=\sqrt{\frac{m\omega_rg_0}{\sqrt{2\pi}\pi\sigma}}. \tag{35}$$

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

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

The inversion point is $j_{inv}=\sqrt{(\nu/\Omega)}$ and the discrete chemical potential (23) is $\nu=(15N_TU_1^2\sqrt{\Omega}/16)^{2/5}$. Therefore

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

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 (36) and (37) is in agreement with Ref. [16], previously calculated with a different approach.

IX. QUANTUM CASE: AN EXTENDED BOSE-HUBBARD MODEL

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

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

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

In the tight-binding approximation,

$$\hat{\Psi}(\vec{r},t)=\sum_j\hat{\psi}_j(t)\Phi_j(\vec{r}) \tag{39}$$

(with $\hat{\psi}_j^\dagger\hat{\psi}_j$ the bosonic number operator), we obtain the Bose-Hubbard model (BHM) [31,32],

$$\hat{H}=\sum_j\left\{-K(\hat{\psi}_j^\dagger\hat{\psi}_{j+1}+\text{H.c.})+\frac{U_2}{2}(\hat{\psi}_j^\dagger\hat{\psi}_j^\dagger\hat{\psi}_j\hat{\psi}_j)+\epsilon_j\hat{\psi}_j^\dagger\hat{\psi}_j\right\}. \tag{40}$$

We now discuss the case in which the localized wave function Φ_j in the jth well adiabatically depends on the average number of particles in the same well: the generalization to the quantum case of Eq. (3) is

$$\hat{\Psi}(\vec{r},t)=\sum_j \hat{\psi}_j(t)\Phi_j(\vec{r};N_j(t)), \tag{41}$$

where

$$N_j=\langle \hat{\psi}_j^\dagger \hat{\psi}_j \rangle. \tag{42}$$

Replacing ansatz (41) in Eq. (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

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

with the parameters K,χ,ϵ_j,U expressed as in the classical DNL (7). Note that the extended BHM can be alternatively recovered quantizing the classical *adiabatic* Hamiltonian $\mathcal{H}_{ad}$ (15) [and not the *effective* Hamiltonian (14)].

X. CONCLUSIONS

The Gross-Pitaevskii dynamics of a Bose-Einstein 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 wave packets, and the frequencies of dipole and quadrupole small amplitude oscillations. We have finally quantized the discrete nonlinear Hamiltonian recovering an extended Bose-Hubbard model.

Note added in proof. An equation similar to DNL (7) (with $\alpha=2$, and including the term proportional to $\int d\vec{r}\tilde{\Phi}_j^2\tilde{\Phi}_{y\pm1}^2$), has been derived by Öster, Johansson, and Eriksson [33] to describe the dynamics of an electric field in an array of coupled waveguides embedded in a material with Kerr nonlinearities.

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