

## Nonspreading Wave Packets in Three Dimensions Formed by an Ultracold Bose Gas in an Optical Lattice

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(Received 22 May 2003; published 26 March 2004)

We predict that an ultracold Bose gas in an optical lattice can give rise to a new form of condensation, namely, nonspreading 3D wave packets that reflect the symmetry of the Laplacian with a negative effective mass along the lattice direction and are allowed to exist in the absence of any trapping potential even in the limit of noninteracting atoms. This result also has strong implications for optical propagation in periodic structures.

DOI: 10.1103/PhysRevLett.92.120404

PACS numbers: 03.75.Lm, 05.30.Jp, 42.65.Jx

Matter waves are a natural manifestation of large scale coherence of an ensemble of atoms populating a fundamental quantum state. The observation of Bose-Einstein condensates (BECs) in dilute ultracold alkalis [1] has initiated the exploration of many intriguing properties of matter waves, whose macroscopic behavior can be successfully described via a mean-field approach in terms of a single complex wave function with a well defined phase across the atom cloud [2]. Large scale coherence effects are usually observed by means of 3D magnetic or optical confining potentials (also 1D cigarlike or 2D disk-shaped BECs are possible [3]) in which BECs are described by their ground-state wave function. Trapping can also occur in free space (i.e., without a trap) through the mutual compensation of the leading-order (two-body) interaction potential and kinetic energy, leading to bright (dark) solitons for negative (positive) scattering lengths. This phenomenon, however, has been observed only in 1D [4]. In 2D and 3D, free-space localization cannot occur due to collapse instability of solitons, and even in a trap collapse usually prevents stable formation of BEC [5,6], needing stabilizing mechanisms [7].

A lot of attention was also devoted to periodic potentials due to optical lattices [8], where the behavior of atoms mimic those of electrons in crystals or photons in periodic media [9] and exhibit effects which stem from genuine atom coherence [10]. In 1D (elongated) lattices bright (gap) solitons can form also in the presence of repulsive interactions [11]. In this Letter we predict that a novel trapping phenomenon occurs when the full 3D dynamics is retained in a 1D lattice. Specifically, under conditions for which the Bloch state associated with the lattice has a negative effective mass, the natural state of BECs is a localized *matter X wave* characterized by a peculiar biconical shape [12–16]. The atoms are organized in this way in the absence of any trap, solely as the result of the strong anisotropy between the 1D modulation and the free motion in the 2D transverse plane. Furthermore, due to axial symmetry, the atoms can experience a collective motion with given velocity along the lattice, resulting in wave packets traveling (nearly) un-

distorted. Remarkably, matter *X waves* constitute also a general basis of expansion for physically realizable BECs, whose evolution preserves the initial atom number distribution.

We start from the mean-field Gross-Pitaevskii (GP) equation [2] with an optical standing wave potential and no additional trapping potential [we set  $\eta \equiv \hbar^2/(2m)$ ]

$$i\hbar\partial_t\psi = -\eta\nabla^2\psi + 4\Gamma\sin^2(kz/2)\psi + a|\psi|^2\psi = 0. \quad (1)$$

We assume axial symmetry around  $z$  and decompose the wave function  $\psi = \psi(r, z, t)$  ( $r^2 \equiv x^2 + y^2$ ) into its forward and backward components as  $\psi = [\psi_f(r, z, t)\exp(ikz/2) + \psi_b(r, z, t)\exp(-ikz/2)] \times \exp[i(k^2 - 8\Gamma)t/4\hbar]$ . For  $\psi_{f,b}$  varying slowly in  $z$ , dropping rapidly rotating terms, the GP equation (1) reduces to the coupled equations

$$\begin{aligned} \mathcal{L}_+\psi_f + \Gamma\psi_b - a(|\psi_f|^2 + 2|\psi_b|^2)\psi_f &= 0, \\ \mathcal{L}_-\psi_b + \Gamma\psi_f - a(|\psi_b|^2 + 2|\psi_f|^2)\psi_b &= 0, \end{aligned} \quad (2)$$

where  $\mathcal{L}_\pm \equiv i\hbar\partial_t \pm i\eta k\partial_z + \eta\nabla_\perp^2$ , and  $\nabla_\perp^2 \equiv \partial_r^2 + r^{-1}\partial_r$ . In the linear limit  $a = 0$ , the plane-wave  $[\exp(i\kappa z - iEt/\hbar)]$  linear dispersion relation associated with Eqs. (2) has two branches  $E = E_\pm(\kappa) = \pm\Gamma\sqrt{1 + p^2}$  (we set  $p \equiv \kappa k\eta/\Gamma$ ), exhibiting an energy gap of width  $2\Gamma$ . The coupling between  $\psi_f$  and  $\psi_b$  causes the structure to be strongly dispersive near the band edge and the linear dynamics of atoms to be governed by strong Bragg reflection. Nevertheless, in the 1D limit ( $\eta = 0$ ), where Eqs. (2) were obtained previously [11], the nonlinearity (both attractive  $a < 0$  and repulsive  $a > 0$ ) induces self-transparency mediated by a two-parameter family of moving bright gap solitons, so-called because they exist in the gap seen in the soliton moving frame [17]. In the attractive case, one might think that the nonlinearity can balance also the kinetic transverse term  $\nabla_\perp^2$  leading to bell-shaped 3D atom wave packets [18]. We show in the following that, contrary to this expectation, close to the lower band edge  $E = E_-$ , the atomic wave function takes a completely different form. To this end we apply

a standard envelope function (or effective mass [19]) approximation [20], searching for spinor solutions  $\vec{\psi} = [\psi_f \psi_b]^T$  of the form

$$\vec{\psi} = \epsilon \phi(\epsilon r, \epsilon z, \epsilon t) \vec{\psi}_- \exp(i\kappa z - itE_-/\hbar) + O(\epsilon^2), \quad (3)$$

where  $\epsilon$  is a small expansion parameter,  $\phi$  is slowly modulating the Bloch state with amplitude  $\vec{\psi}_- = [\psi_{f-} \psi_{b-}]^T$  [eigenvector of Eqs. (2) with  $a = 0$  corresponding to the eigenvalue  $E_-$ ]. At the leading order we find that  $\phi$  obeys the following asymptotic equation:

$$i\hbar \partial_t \phi + iE'_- \partial_z \phi + E''_- \partial_z^2 \phi + \eta \nabla_\perp^2 \phi - \chi |\phi|^2 \phi = 0, \quad (4)$$

where  $\chi = \frac{a}{2} \frac{3+2p^2}{1+p^2}$ , and  $E'_- \equiv \frac{dE_-}{d\kappa}$ ,  $E''_- \equiv \frac{d^2 E_-}{d\kappa^2}$  account for dispersion. For the sake of simplicity we deal henceforth with the strict band-edge case  $\kappa = 0$ , which can be prepared by acting on the wave number and on the potential parameter [21]. In this case Eq. (4) reads explicitly as

$$i\hbar \partial_t \phi + \frac{\hbar^2}{2m} \left( \nabla_\perp^2 - \frac{m}{m_e} \partial_z^2 \right) \phi - \frac{3a}{2} |\phi|^2 \phi = 0, \quad (5)$$

where  $-m_e \equiv -m\Gamma/(\eta k^2)$  is the negative effective mass associated with the lattice, in turn determining the *hyperbolic* character of (GP) Eq. (5). The scaling transformation  $z, r, t, \phi \rightarrow z_0 z, r_0 r, t_0 t, c_0 \phi$  with  $r_0^2 = z_0^2 m_e/m$ ,  $t_0 = 2m_e z_0^2/\hbar$ ,  $c_0^2 = 2\hbar/(3|a|t_0)$ ,  $z_0$  being a length scale, allows us to use dimensionless variables.

We look for stationary (shape-preserving) solutions of Eq. (5) in the form  $\phi = \varphi(r, z) \exp(i\mu t)$ .

According to Ref. [22], solutions that are strictly localized (i.e., with finite 3D norm  $\|\phi\| \equiv \langle \varphi | \varphi \rangle$  [23]) do not exist. Nevertheless, Eq. (5) possesses, in the attractive case ( $a < 0$ ), X-shaped solutions with slower than exponential decay (infinite norm, yet localized in a broader sense [12]), namely, matter X waves [16]. X waves, known

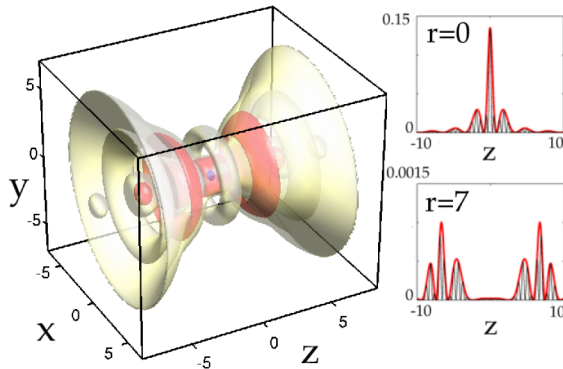


FIG. 1 (color online). Surfaces of constant envelope atom density  $|\phi|^2$  (increasing with darkness, or in color in the following order: bronze, red, and blue) of a matter envelope X wave solution ( $\mu = 0$ ) of Eq. (5). The insets show on axis ( $r = 0$ ) and off axis ( $r = 7$ ) longitudinal profiles of the overall ( $|\psi|^2$ , thin lines) and envelope ( $|\phi|^2$ , bold lines) densities. Here we set  $z_0 = 10/k$ .

in optics [12], acoustics [13], or microwaves [14], as nonspreading (in space and time) solutions of the *linear Helmholtz* wave equation [15], have been only recently discovered for Schrödinger-type models [such as Eq. (5)] related to the so-called paraxial regime of propagation [16]. A fundamental difference must be emphasized: while an optical or acoustic field retains a directly observable spatiotemporal X shape [12,16], in the case of a Bose gas, the local density of atoms  $|\psi|^2$  has an X-shaped spatial envelope  $|\phi|^2$  which modulates a periodic (with lattice period) term  $\cos^2(kz/2)$  owing to beating between  $\psi_f$  and  $\psi_b$  components (in other words, an atomic Bloch wave).

To assess further the regimes of observability of matter X waves, we discuss two crucial issues. First, by extending the analysis of Ref. [16], we are able to show that X wave solutions of Eq. (5) exist also in the (far more common) case of repulsive nonlinearity ( $a > 0$ ). As an example, we display in Fig. 1 the atom density corresponding to the stationary solution with eigenvalue  $\mu = 0$ , which shows a dense core accompanied by biconically shaped regions of lower density. As shown in the insets, the signature of the X shape is a single peak on axis ( $r = 0$ ) and a double peak off axis ( $r \neq 0$ ). The envelope  $|\phi|^2$  exhibits also slow oscillations and modulates the fast sinusoidal variation of the density  $|\psi|^2$ . In real-world units, the density scales with  $c_0^2 = \hbar^2/(3|a|m_e z_0^2)$ . For instance, the peak density in Fig. 1 ( $\sim 0.15$ ) yields 1 atom/ $\mu\text{m}^3$  in  $^{87}\text{Rb}$  (scattering length  $a_s = a(m/4\pi\hbar^2) \simeq 6$  nm) with a length scale  $z_0 = 10/k \sim 1 \mu\text{m}$  associated with a typical lattice pitch  $2\pi/k \sim 700$  nm.

Second, our aim is to show that nonspreading atom X-shaped BECs can be formed also in an *ideal noninteracting gas* ( $a = 0$ , realizable by exploiting Feshbach resonance [4]). This is in contrast with other known settings where BECs need either a confining potential (as in pioneering experiments [1]), or nonlinearities to balance kinetic spreading. Ultimately, this stems from the fact that X waves have a finite linear limit, unlike solitons of standard (elliptic) GP equation whose amplitude vanishes as  $a \rightarrow 0$ . To show the importance of *linear* matter X waves, however, we need to address their observability with a finite number of atoms (i.e., finite norm). To this end, we start by solving Eq. (5) with  $a = 0$

$$(i\partial_t + \nabla_\perp^2 - \partial_z^2)\phi = 0, \quad (6)$$

seeking for shape-preserving solutions of the kind (i.e., generalized to move with velocity  $v$ )

$$\phi(r, z, t) = \varphi(r, \zeta) \exp(-ivz/2 + itv^2/4), \quad (7)$$

where  $\zeta \equiv z - vt$ , and  $\varphi$  turns out to obey the equation

$$\partial_r^2 \varphi + r^{-1} \partial_r \varphi - \partial_\zeta^2 \varphi = 0. \quad (8)$$

The general solution of Eq. (8)

$$\varphi(r, \zeta) = \int_0^\infty f(\alpha) J_0(\alpha r) e^{i\alpha \zeta} d\alpha, \quad (9)$$

represents a class of envelope  $X$  waves specified by their spectrum  $f(\alpha)$ , which generalize to (Schrödinger-type) Eq. (6) the  $X$  wave solutions of the Helmholtz equation [15]. An exponentially decaying (with arbitrary inverse width  $\Delta$ ) spectrum  $f_x(\alpha) = \exp(-\alpha\Delta)$  yields the simplest (or fundamental)  $X$  wave  $\varphi_x = [r^2 + (\Delta - i\zeta)^2]^{-1/2}$ , while  $f_x^{(n)} = \alpha^n \exp(-\alpha\Delta)$  ( $n = 1, 2, \dots$ ) defines the *derivative*  $X$  waves  $\varphi_x^{(n)} = d^n \varphi_x / d\Delta^n$ . In general, from Eq. (9), we obtain the full envelope  $X$  wave solution of Eq. (6) as

$$\phi(r, z, t) = \int_0^\infty f(\alpha) J_0(\alpha r) e^{i[\alpha - (v/2)]z + i[(v^2/4) - \alpha v]t} d\alpha, \quad (10)$$

where  $|\phi|^2$  travels clearly undistorted along  $z$ . However, we face the pitfall that these  $X$  waves do not represent physical objects since their norm diverges. This follows from the *transverse scalar product*  $\langle \phi | \hat{\phi} \rangle_\perp(z, t)$ , which yields for any pair of solutions  $\phi, \hat{\phi}$  of Eq. (6) with different spectra  $f, \hat{f}$  (but equal velocity  $v$ ),

$$\langle \phi | \hat{\phi} \rangle_\perp = 2\pi \int_0^\infty f(\alpha) \hat{f}^*(\alpha) \alpha^{-1} d\alpha. \quad (11)$$

Since  $\langle \phi | \hat{\phi} \rangle_\perp$  does not depend on  $z, t$ , the 3D norm  $\langle \phi | \phi \rangle$  of any  $X$  wave  $\phi$  diverges, thus requiring an (unphysical) infinite number of atoms. Remarkably, however, finite norm beams can be generally constructed by introducing new orthogonal  $X$  waves [24]. Inspired by Eq. (11), we exploit the orthogonality of associated Laguerre polynomials  $L_q^{(1)}(x)$  ( $q = 0, 1, 2, \dots$ ), with respect to the function  $x \exp(-x)$ , to introduce a numerable class of (transversally) orthogonal  $X$  waves  $\phi_q^\perp(r, z, t|v)$  defined by the spectra (and parametrically by their velocity  $v$ )

$$f_q^\perp(\alpha) = \frac{\Delta \alpha}{\pi \sqrt{2(q+1)}} L_q^{(1)}(2\Delta\alpha) e^{-\Delta\alpha}. \quad (12)$$

The  $X$  waves  $\phi_q^\perp$  satisfy the orthogonality relation  $\langle \phi_p^\perp | \phi_q^\perp \rangle_\perp = \delta_{pq}/4\pi$ , with  $\delta_{pq}$  the Kronecker symbol. Importantly, the 3D scalar product shows that such waves are orthogonal also with respect to the velocity, i.e., any pair of waves with velocity  $u$  and  $v$  satisfies the relation

$$\langle \phi_p^\perp(r, z, t|v) | \phi_q^\perp(r, z, t|u) \rangle = \delta_{pq} \delta(v - u). \quad (13)$$

From Eq. (13) it is natural to consider the solution  $\phi = \phi_\Sigma$  of Eq. (6) given by the superposition of orthogonal  $X$  waves  $\{\phi_q^\perp\}$  traveling with different velocities  $v$  as

$$\phi_\Sigma(r, z, t) = \sum_q \int_{-\infty}^\infty C_q(v) \phi_q^\perp(r, z, t|v) dv. \quad (14)$$

From the orthogonality relation (13), we find that the total number of atoms is

$$\mathcal{N}_\Sigma = \langle \phi_\Sigma | \phi_\Sigma \rangle = \sum_q \mathcal{N}_q, \quad (15)$$

where  $\mathcal{N}_q = \int_{-\infty}^\infty |C_q(v)|^2 dv$  represents the atom number of the  $q$ th  $X$  wave component  $\phi_q^\perp(v)$  of the wave

packet. Therefore we obtain the remarkable result that, while the superposition  $\phi_\Sigma$  generally describes atom wave packets which evolve in time, such evolution preserves the distribution of atom number among the  $X$  wave components.

The importance of Eq. (14) stems from the fact that  $\phi_\Sigma$  describes a wide class of physical atom beams. To show this, we start from the integral representation of  $\phi_q^\perp$  in term of its spectrum (12), which yields

$$\phi_\Sigma = \int_{-\infty}^\infty \int_0^\infty F(\alpha, v) J_0(\alpha r) e^{i[\alpha - (v/2)]z - i(v^2/4)t} \alpha d\alpha dv, \quad (16)$$

where  $F(\alpha, v) = \alpha^{-1} \sum_q C_q(v) f_q^\perp(\alpha)$ . By introducing new variables  $k_t, k_z$  such that  $\alpha = k_t$  and  $v = 2(k_t - k_z)$ , and setting  $U(k_t, k_z) = 2F(k_t, 2k_t - 2k_z)$ , Eq. (16) can be cast in the form

$$\phi_\Sigma = \int_{-\infty}^\infty \int_0^\infty U(k_t, k_z) J_0(k_t r) e^{ik_z z} e^{i(k_z^2 - k_t^2)t} k_t dk_t dk_z,$$

which represents the generic axisymmetric solution of Eq. (6), expressed in 3D momentum space  $(k_t, k_z)$ ,  $k_t$  being the transverse (with respect to the lattice) momentum. Here  $U(k_t, k_z)$  is the Fourier-Bessel (or plane-wave) spectrum of the initial atom distribution  $\phi_0(r, z) \equiv \phi(r, z, t=0)$ , and  $U(k_t, k_z) = 2k_t^{-1} \sum_q C_q(2k_t - 2k_z) f_q^\perp(k_t)$  stands for its expansion in terms generalized Laguerre polynomials [any square-integrable  $f(x)$  in  $x \in [0, \infty)$  can be expanded in terms of  $L_q^{(1)}(x)$ ]. This argument can be reversed by stating that, given the initial ( $t=0$ ) distribution of atoms  $U(k_t, k_z)$  in momentum space, if  $F(\alpha, v) = U(\alpha, \alpha - v/2)/2$  is square integrable with respect to  $\alpha$  [with  $\alpha \in [0, \infty)$ ], then the atom wave packet admits the representation (14). The expansion coefficient can be easily calculated as  $C_q(v) = (\sqrt{2}\Delta/\pi\sqrt{q+1}) \int_0^\infty U(\alpha, \alpha - v/2) \exp(-2\alpha\Delta) L_q^{(1)}(2\alpha\Delta) \alpha d\alpha$ . Clearly, most of physically relevant wave packets belong to the class  $\phi_\Sigma$  [25]. For example, a spectrally narrow Gaussian beam can be described by few  $X$  waves (details will be given elsewhere).

Once the existence of finite norm linear  $X$  waves is established along with their potential to describe general BECs, the most intriguing question remains whether we expect matter  $X$ -shaped atom distributions to be observable. Such waves correspond to a single fixed value  $q = \bar{q}$  in Eq. (14) and an ideal velocity distribution  $C_{\bar{q}}(v) = \delta(v - \bar{v})$ . However, more generally, we can consider an atomic envelope beam  $\phi_a$  constituted by several replicas of the single  $X$  wave  $\phi_{\bar{q}}^\perp$  traveling with different velocities. Although, strictly speaking, such a beam is not stationary, it can approximate such a state with an arbitrary degree of accuracy. In other words, it is possible to construct solutions that preserve their shape, for an arbitrary long time. Indeed if  $C_{\bar{q}}(v)$  is a narrow function, e.g., peaked around  $v = 0$ , Eq. (14), using also Eq. (7), yields

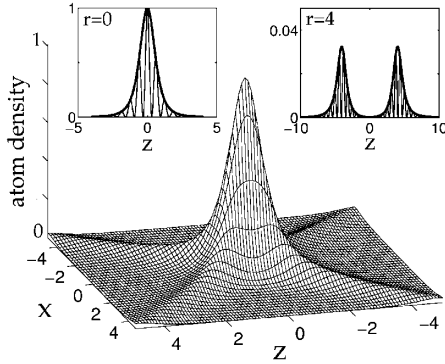


FIG. 2. Atom density of a pure  $X$  wave  $|\phi_q^\perp(r, z)|^2$  with  $q = 0$  and  $\Delta = 1$ , as seen on the  $(x, z)$  plane ( $y = 0$ ). The insets show (same units as in Fig. 1) the overall (thin line) and envelope (bold line) density on axis and off axis, respectively.

the following atom envelope  $\phi_a$ :

$$\begin{aligned} \phi_a(r, z, t) &= \int_{-\infty}^{\infty} \varphi_{\bar{q}}^\perp(r, z - vt) C_{\bar{q}}(v) e^{-i(z/2)z + i(v^2/4)t} dv \\ &\equiv \varphi_{\bar{q}}^\perp(r, z) c(z, t), \end{aligned} \quad (17)$$

where  $c(z, t) = \int_{-\infty}^{\infty} C_{\bar{q}}(v) \exp(-i\frac{v}{2}z + i\frac{v^2}{4}t) dv$  is a solution of the dispersive wave equation  $i\partial_t c - \partial_z^2 c = 0$ . Equation (17) represents an  $X$  wave modulated by a dispersing wave, which gives a sort of *adiabatic* dynamics of the finite norm  $X$  wave. Indeed the atom beam has an invariant spatial shape fixed by  $\varphi_{\bar{q}}^\perp$ , which we display in Fig. 2 as an example for  $\bar{q} = 0$ . It spread on a characteristic time which is longer, the narrower is the velocity distribution function  $C_{\bar{q}}(v)$ . In the linear regime, we expect that such atom states should be somehow prepared. Conversely atom collisions (nonlinear regime) could be envisaged to strongly favor the  $X$  wave formation through instability mechanisms [16,26], when starting from conventionally prepared ball-shaped atom clouds (e.g., after switching off a harmonic 3D trap), an issue that calls for a numerical study of the evolution problem (1).

In summary, we have shown that a lattice supports moving or still localized states of the GP model with envelope  $X$  shape. A matter  $X$  wave entails localization both in momentum and configuration space, thus being a clear signature of a Bose condensed gas, so much as the anisotropy in the distribution function [2] detected in early experiments. Unlike any other form of BEC including solitons, matter  $X$  waves can be observed in free space and in a noninteracting regime, where they are the natural basis to describe the coherent properties of atom wave packets. These results have strong implications in optics where Eqs. (5) and (6) holds for normally dispersive homogeneous media [26], and Eqs. (2) models 3D diffractive propagation in stratified media or along proper directions of 3D photonic crystals.

We thank F. Cataliotti, M. Oberthaler, M. Salerno, and P. Di Trapani for discussions, as well as Fondazione Tronchetti Provera and MIUR for financial support.

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