

Matter X waves

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We predict that an ultra-cold Bose gas in an optical lattice can give rise to a new form of condensation, namely matter X waves. These are non-spreading 3D wave-packets which 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 non-interacting atoms. This result has also strong implications for optical propagation in periodic structures.

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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 ultra-cold alkalis [1] has initiated the exploration of many intriguing properties of matter waves, whose macroscopic behavior can be successfully described via mean-field approach in terms of a single complex wave-function with 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 cigar-like or 2D disk-shaped BEC are possible [3]) in which BECs are described by their ground-state wave-function. However, 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 has been observed only in 1D (i.e., soliton waveguides, a trap confining the BEC transversally to the soliton) [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 atom 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 the conditions for which the Bloch state associated with the lattice has a negative effective mass, the natural state of the BEC is a localized *matter X wave* characterized by a peculiar bi-conical shape. 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 into wave-packets traveling undistorted. Remarkably, these matter X waves are not only observ-

able individually, but allow also to describe physically realizable BECs as their superposition, each component maintaining a constant (in time) number of atoms.

The very first step of our derivation is similar to that of matter gap solitons. Starting from the (mean-field) Gross-Pitaevskii (GP) equation [2] with an optical standing wave potential and no additional trap (we set $\eta \equiv \frac{\hbar^2}{2m}$)

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

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

$$\psi = [\psi_f(r, z, t)e^{ikz/2} + \psi_b(r, z, t)e^{-ikz/2}]e^{i\frac{k^2 - 8\Gamma}{4\hbar}t}, \quad (2)$$

which, for $\psi_{f,b}$ slowly varying in z , and dropping rapidly rotating terms, allows us to reduce the GP equation (1) to the coupled equations

$$\begin{aligned} \mathcal{L}_+\psi_f + \Gamma\psi_b - a(|\psi_f|^2 + 2|\psi_b|^2)\psi_f &= 0, \\ \mathcal{L}_-\psi_b + \Gamma\psi_f - a(|\psi_b|^2 + 2|\psi_f|^2)\psi_b &= 0, \end{aligned} \quad (3)$$

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. (3) has two branches $E = E_\pm(\kappa) = \pm\Gamma\sqrt{1+p^2}$ (we set $p \equiv \kappa\eta/\Gamma$), exhibiting an energy gap of width 2Γ . The coupling between ψ_f and ψ_b causes the structure to be strongly dispersive near band-edge and the linear dynamics of atoms to be governed by strong Bragg reflection. Nevertheless, in the 1D limit ($\eta = 0$), where Eqs. (3) 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 [12]. In the attractive case, one might think that the nonlinearity can balance also the kinetic transverse term ∇_\perp leading to bell-shaped 3D atom wave-packets [13]. 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 [15]) approximation [14],

searching for spinor solutions $\vec{\psi} = [\psi_f \ \psi_b]^T$ of the form

$$\vec{\psi} = \epsilon \phi(\epsilon r, \epsilon z, \epsilon t) \vec{\psi}_- \exp(i\kappa z - itE_-/\hbar) + O(\epsilon^2) \quad (4)$$

where ϵ is a small expansion parameter, ϕ is slowly modulating the Bloch state with amplitude $\vec{\psi}_- = [\psi_{f-} \ \psi_{b-}]^T$ (eigenvector of Eqs. (3) with $a = 0$ corresponding to the eigenvalue E_-). At the leading order we find that ϕ obeys the following asymptotic equation

$$i\hbar\partial_t\phi + iE'_-\partial_z\phi + E''_-\partial_z^2\phi + \eta\nabla_\perp^2\phi - \chi|\phi|^2\phi = 0 \quad (5)$$

where $\chi = \frac{a}{2} \frac{3+2p^2}{1+p^2}$, and $E'_- \equiv \frac{dE_-}{d\kappa}$, $E''_- \equiv \frac{d^2E_-}{d\kappa^2}$ account for dispersion. For 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 [16]. In this case Eq. (5) reads explicitly as

$$i\hbar\partial_t\phi + \frac{\hbar^2}{2m} \left(\nabla_\perp^2 - \frac{m}{m_e} \partial_z^2 \right) \phi - \frac{3a}{2} |\phi|^2 \phi = 0, \quad (6)$$

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. (6). 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. In the attractive case ($a < 0$), Eq. (6) admits matter X waves solutions of the kind $\phi = \varphi(r, z) \exp(i\mu t)$, where $\varphi(r, z)$ is indeed an X-shaped invariant envelope [17]. Notice that X waves, well known in optics [18], acoustics [19], or microwaves [20], as non-spreading (in space and time) solutions of the *linear* Helmholtz wave equation [21], have been only recently discovered for Schrödinger-type models of the form of Eq. (6), by analyzing the so-called paraxial (linear [22] or nonlinear [17]) propagation in dispersive media. However, we emphasize that, while an optical or acoustic field retains a directly observable spatio-temporal X-shape [17, 18], in the case of a Bose gas, the local density of atoms $|\psi|^2$ has an X-shaped spatial envelope $|\phi|^2$ modulating a term $\cos^2(kz/2)$ (periodic with lattice period), due to the form of Eq. (2).

To assess further the regimes of observability of matter X waves, we discuss two crucial issues. First, by extending the analysis of Ref. [17], we are able to show that X wave solutions of Eq. (6) 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 bi-conically 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 modulate the fast sinusoidal variation of the density $|\psi|^2$.

Second, our aim is to show that non-spreading atom

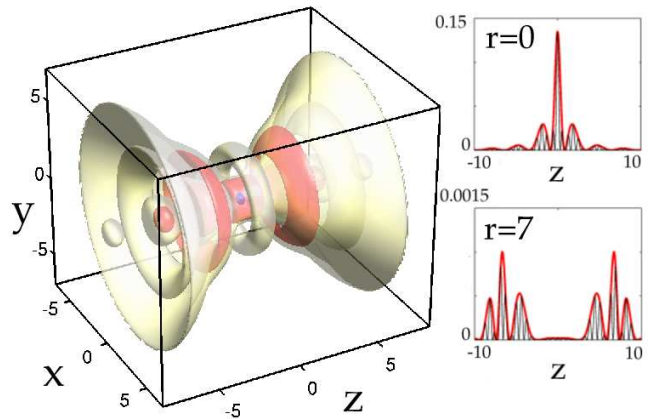


FIG. 1: (Color online) Surfaces of constant (high, intermediate, and low in blue, red, and bronze, respectively) envelope atom density $|\phi|^2$ of a matter envelope X wave solution ($\mu = 0$) of Eq. (6). The insets show on-axis ($r = 0$) and off-axis ($r = 7$) longitudinal profiles of the overall ($|\psi|^2$, black) and envelope ($|\phi|^2$, red) densities. We fix $z_0 = 10/k$ to have dimensionless units.

X-shaped BECs can be formed also in an *ideal noninteracting gas* ($a = 0$), which is realizable by exploiting Feshbach resonance [4]. This is in contrast with other known settings where BEC needs either a confining potential (as in pioneering experiments [1]), or the 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 demonstrate, however, that *linear* matter X waves are observable, we need to address the fundamental issue of their norm finiteness. To this end let us solve Eq. (6) in dimensionless form with $a = 0$

$$(i\partial_t + \nabla_\perp^2 - \partial_z^2) \phi = 0, \quad (7)$$

by seeking for envelopes moving with velocity v

$$\phi(r, z, t) = \varphi(r, \zeta) \exp(-ivz/2 + itv^2/4), \quad (8)$$

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

$$\partial_r^2 \varphi + r^{-1} \partial_r \varphi - \partial_\zeta^2 \varphi = 0. \quad (9)$$

The general solution of Eq. (9)

$$\varphi(r, \zeta) = \int_0^\infty f(\alpha) J_0(\alpha r) e^{i\alpha \zeta} d\alpha, \quad (10)$$

represents a class of envelope X waves specified by their spectrum $f(\alpha)$, which generalize to (Schrödinger-type) Eq. (7) the X wave solutions of Helmholtz equation [21]. An exponentially decaying (with arbitrary inverse width Δ) 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. (10), we obtain the full envelope X wave solution of Eq. (7) as

$$\phi(r, z, t) = \int_0^\infty f(\alpha) J_0(\alpha r) e^{i(\alpha - \frac{v}{2})z + i(\frac{v^2}{4} - \alpha v)t} d\alpha, \quad (11)$$

where $|\phi|^2$ clearly travels undistorted along z . However, we have to face the pitfall that these X waves do not represent physical objects since their norm diverges. This follows from the *transverse scalar product* $\langle \phi | \hat{\phi} \rangle_\perp(z, t)$ [25] which yields for any pair of solutions $\phi, \hat{\phi}$ of Eq. (7) with different spectra f, \hat{f} (but equal velocity v)

$$\langle \phi | \hat{\phi} \rangle_\perp = 2\pi \int_0^\infty f(\alpha) \hat{f}^*(\alpha) \alpha^{-1} d\alpha. \quad (12)$$

Since $\langle \phi | \hat{\phi} \rangle_\perp$ does not depend on z and t , the 3D norm $\langle \phi | \phi \rangle$ of any X wave ϕ 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. (12), we can 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 following spectra (and parametrically by their velocity v)

$$f_q^\perp(\alpha) = \frac{\Delta \alpha}{\pi \sqrt{2(q+1)}} L_q^{(1)}(2\Delta \alpha) e^{-\Delta \alpha}. \quad (13)$$

The X waves ϕ_q^\perp satisfy the orthogonality relation $\langle \phi_p^\perp | \phi_q^\perp \rangle_\perp = \delta_{pq}/4\pi$, with δ_{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

$$\langle \phi_p^\perp(r, z, t|v) | \phi_q^\perp(r, z, t|u) \rangle = \delta_{pq} \delta(v - u). \quad (14)$$

From Eq. (14) it is natural to consider the solution $\phi = \phi_\Sigma$ of Eq. (7) given by the superposition of orthogonal X waves $\{\phi_q^\perp\}$ travelling with different velocities v as

$$\phi_\Sigma(r, z, t) = \sum_q \int_{-\infty}^\infty C_q(v) \phi_q^\perp(r, z, t|v) dv. \quad (15)$$

From the orthogonality relation (14), we find that the total number of atoms is

$$\mathcal{N}_\Sigma = \langle \phi_\Sigma | \phi_\Sigma \rangle = \sum_q \mathcal{N}_q, \quad (16)$$

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 ϕ_Σ 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. (15) stems from the fact that ϕ_Σ describes a wide class of physical atom beams. To show this, we start from the integral representation of ϕ_q^\perp in term of its spectrum (13), which yields

$$\phi_\Sigma = \int_{-\infty}^\infty \int_0^\infty F(\alpha, v) J_0(\alpha r) e^{i(\alpha - \frac{v}{2})z - i(\frac{v^2}{4} - \alpha v)t} \alpha d\alpha dv, \quad (17)$$

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. (17) 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. (7), expressed in 3D momentum space (k_t, k_z) , k_t being the momentum transverse to the lattice direction z . 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 α (with $\alpha \in [0, \infty)$), then the atom wave-packet admits the representation (15). The expansion coefficient can be easily calculated as

$$C_q(v) = \frac{\sqrt{2}\Delta}{\pi \sqrt{q+1}} \int_0^\infty U\left(\alpha, \alpha - \frac{v}{2}\right) e^{-2\alpha\Delta} L_q^{(1)}(2\alpha\Delta) \alpha d\alpha,$$

Clearly, most of physically relevant wave-packets belong to the class ϕ_Σ [26]. 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 together with their potential to describe general BECs, the most intriguing question remains whether we can expect matter X-shaped atom distributions to be observable. Such waves correspond to a single fixed value $q = \bar{q}$ in Eq. (15) and an ideal velocity distribution $C_{\bar{q}}(v) = \delta(v - \bar{v})$. However, more generally, we can consider an atomic envelope beam ϕ_a constituted by several replicas of the single X wave $\phi_{\bar{q}}^\perp$ travelling with different velocities. Although, strictly speaking, such 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. (15), using also Eq. (8), yields the following atom envelope ϕ_a

$$\begin{aligned} \phi_a(r, z, t) &= \int_{-\infty}^\infty \varphi_{\bar{q}}^\perp(r, z - vt) C_{\bar{q}}(v) e^{-i\frac{v}{2}z + i\frac{v^2}{4}t} dv \\ &\cong \varphi_{\bar{q}}^\perp(r, z) c(z, t) \end{aligned} \quad (18)$$

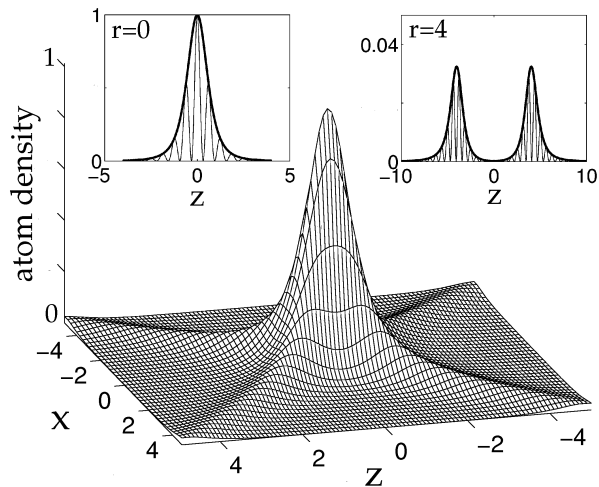


FIG. 2: Atom density of a pure X wave $|\phi_q^\perp(r, z)|^2$ with $q = 0$ and $\Delta = 1$, as seen on the (x, z) plane ($y = 0$). The insets show (same units as in Fig. 1) the overall (thin line) and envelope (bold line) density on-axis and off-axis, respectively.

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 $i\partial_t c - \partial_z^2 c = 0$. Eq. (18) 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 spreads on a characteristic time which is longer, the narrower is the velocity distribution function $C_{\bar{q}}(v)$. Finally, while in the linear regime we expect that such atom states should be somehow prepared, we envisage that atom collisions (nonlinear regime) can strongly favour the formation of X waves from more conventional ball-shaped atom clouds (e.g., obtained by a harmonic 3D trap which is then switched off) through instability mechanisms [17, 23], an issue which will be deepened elsewhere.

In conclusion we have shown that a periodic potential supports moving or still localized states of the GP model with envelope X-shape (strictly or nearly) preserved upon motion. A matter X waves entails localization both in momentum and configuration space and is a clear signature of a Bose condensed gas, so much as the anisotropy in the distribution function [2] detected in early experiments. However, unlike any other form of BEC including solitons, matter X waves can be observed in free-space and in the non-interacting regime, where they constitute a natural basis of expansion to describe the coherent properties of atom wave-packets. These results have strong implications also in optics, where the model (7) holds for normally dispersive bulk media [22], or in nonlinear optics of stratified media where Eqs. (3) describe propagation in a 1D bulk grating in the presence of diffraction, or propagation in a fully 3D photonic

crystal (along proper directions).

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cylindrically symmetric functions ϕ, η as $\langle \phi | \eta \rangle_{\perp} = 2\pi \int_0^{\infty} \phi(r, z, t) \eta^*(r, z, t) r dr$, as well as the 3D (in x, y, z) scalar product $\langle \phi | \eta \rangle = \int_{-\infty}^{\infty} \langle \phi | \eta \rangle_{\perp} dz$.

[26] Exceptions can be found, e.g. if $U(k_t, k_z) = U(k_z - k_t)$,

then $F(\alpha, v)$ does not depend on α and cannot be expanded in terms of $L_q^{(1)}$.