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Dimensional Reduction and Localization of a Bose–Einstein Condensate in a Quasi-1D Bichromatic Optical Lattice

L. SALASNICH^{a,b} AND S.K. ADHIKARI^c

^aDipartimento di Fisica “Galileo Galilei” and CNISM, Università di Padova, Via Marzolo 8, 35131 Padova, Italy

^bIstituto Nazionale di Ottica (INO) del Consiglio Nazionale delle Ricerche (CNR), Sezione di Sesto Fiorentino, Via Nello Carrara, 1 - 50019 Sesto Fiorentino, Italy

³Instituto de Física Teórica, Universidade Estadual Paulista, UNESP 01.140-070 Sao Paulo, Sao Paulo, Brazil

We analyze the localization of a Bose–Einstein condensate in a one-dimensional bichromatic quasi-periodic optical-lattice potential by numerically solving the 1D Gross–Pitaevskii equation (1D GPE). We first derive the 1D Gross–Pitaevskii equation from the dimensional reduction of the 3D quantum field theory of interacting bosons obtaining two coupled differential equations (for axial wave function and space-time dependent transverse width) which reduce to the 1D Gross–Pitaevskii equation under strict conditions. Then, by using the 1D Gross–Pitaevskii equation we report the suppression of localization in the interacting Bose–Einstein condensate when the repulsive scattering length between bosonic atoms is sufficiently large.

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1. Introduction

Many years ago Anderson [1] predicted the localization of the electronic wave function in a disordered potential. In the last twenty years the phenomenon of localization due to disorder was experimentally observed in electromagnetic waves [2, 3], in sound waves [4], and also in quantum matter waves [5–8].

In the case of quantum matter waves, Roati et al. [6] observed localization of a non-interacting Bose–Einstein condensate (BEC) of ³⁹K atoms in a 1D potential created by two optical-lattice potentials with different amplitudes and wavelengths. The non-interacting BEC of ³⁹K atoms was created [6] by tuning the inter-atomic scattering length to zero near a Feshbach resonance [9]. The 1D quasi-periodic potentials have a spatial ordering that is intermediate between periodicity and disorder [10–12]. In particular, the 1D discrete Aubry–Andre model of quasi-periodic confinement [11, 12] displays a transition from extended to localized states which resembles the Anderson localization of random systems [13, 14]. Modugno [15] has recently shown that the linear 1D Schrödinger equation with a bichromatic periodic potential can be mapped in the Aubry–Andre model and he studied the transition to localization as a function of the parameters of the periodic potential. To investigate the interplay between the bichromatic potential and the inter-atomic interaction in the localization of a BEC, we use the 1D Gross–Pitaevskii equation (1D GPE) [16]. We first show that the 1D GPE can be derived from the dimensional reduction of the 3D quantum field theory of interacting bosons [17], obtaining a nonpolynomial Schrödinger equation [18, 19] which reduces to the 1D GPE only under strict conditions. Then we numerically solve the 1D GPE by using a Crank–Nicolson predictor-corrector method. We find that the cubic nonlinearity of the 1D GPE, which accurately models the

binary inter-atomic interaction of atoms, has a strong effect on localization: a reasonably weak repulsive nonlinear term is capable of destroying the localization [20]. Our results on the effect of nonlinearity in the localization are in qualitative agreement with similar predictions based both 1D continuous [21] and discrete nonlinear Schrödinger equation with random on-site energies [22].

We stress that, in addition to the results discussed here on a pure BEC in a bichromatic lattice (see also [20]), in the last few years there have been studies of localization of a BEC vortex [23], of a dipolar BEC [24], of a spin-orbit coupled BEC [25], of a Bose–Fermi mixture [26], of a BEC on a random potential [27], among other possibilities of localization of matter wave.

2. 1D Gross–Pitaevskii equation with a quasi-periodic bichromatic potential

In the experiment of Roati et al. [6] the 1D quasi-periodic bichromatic optical-lattice potential was produced by superposing two optical-lattice potentials generated by two standing-wave polarized laser beams of slightly different wavelengths and amplitudes. With a single periodic potential the linear Schrödinger equation permits only delocalized states in the form of the Bloch waves. Localization is possible in the linear Schrödinger equation due to the “disorder” introduced through a second periodic component.

We model the dynamics of a trapped BEC of N atoms in a transverse harmonic potential of frequency ω_{\perp} plus the axial quasi-periodic optical-lattice potential by using the following adimensional 1D GPE [16, 20]:

$$i \frac{\partial}{\partial t} \phi(z, t) = \left[-\frac{1}{2} \partial_z^2 + V(z) + g |\phi(z, t)|^2 \right] \phi(z, t), \quad (1)$$

where

$$V(z) = \frac{4\pi^2 s_1}{\lambda_1^2} \cos^2\left(\frac{2\pi}{\lambda_1} z\right) + \frac{4\pi^2 s_2}{\lambda_2^2} \cos^2\left(\frac{2\pi}{\lambda_2} z\right) \quad (2)$$

is the quasi-periodic bichromatic axial potential, with $\phi(z, t)$ the axial wave function of the Bose condensate normalized to one, i.e.

$$\int_{-\infty}^{\infty} dz |\phi(z, t)|^2 = 1. \quad (3)$$

Here $g = 2Na_s/a_\perp$ is the dimensionless interaction strength with a_s the inter-atomic scattering length and $a_\perp = \sqrt{\hbar/(m\omega_\perp)}$ the characteristic harmonic length of the transverse harmonic confinement [20]. Moreover, $2s_i, i = 1, 2$, are the amplitudes of the optical-lattice potentials in units of respective recoil energies $E_i = 2\pi^2\hbar^2/(m\lambda_i^2)$, and $k_i = 2\pi/\lambda_i, i = 1, 2$ are the respective wave numbers, \hbar is the reduced Planck constant, and m the mass of an atom [6, 20]. The optical potential of wavelength λ_1 is used to create a primary lattice that is weakly perturbed by a secondary lattice of wavelength λ_2 [6, 15]. Moreover, to obtain ‘‘quasi-disorder’’ the ratio λ_2/λ_1 should not be commensurable [15]. In practice we use $\lambda_2/\lambda_1 = 0.86$ that is close to the experimental value $\lambda_2/\lambda_1 = 0.835$ [6, 20].

3. Derivation of the 1D Gross-Pitaevskii equation

Before solving the 1D GPE, let us analyze its derivation from the quantum theory of many-body systems [16, 28]. The quantum many-body Hamiltonian of interacting identical bosons is given by

$$\hat{H} = \int d^3\mathbf{r} \hat{\psi}^\dagger(\mathbf{r}) \left[-\frac{1}{2}\nabla^2 + U(\mathbf{r}) \right] \hat{\psi}(\mathbf{r}) + \int d^3\mathbf{r} d^3\mathbf{r}' \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') W(\mathbf{r}, \mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}), \quad (4)$$

where $\hat{\psi}(\mathbf{r}, t)$ is the bosonic field operator. In our case the external trapping potential reads

$$U(\mathbf{r}) = \frac{1}{2}(x^2 + y^2) + V(z), \quad (5)$$

corresponding to a harmonic transverse confinement of frequency ω_\perp with characteristic length $a_\perp = \sqrt{\hbar/(m\omega_\perp)}$ and the axial optical lattice $V(z)$ of Eq. (2).

In addition, due to the fact that the system is made of dilute and ultracold atoms, we consider a contact interaction between bosons, i.e.

$$W(\mathbf{r} - \mathbf{r}') = \gamma \delta^{(3)}(\mathbf{r} - \mathbf{r}') \quad (6)$$

with $\delta^{(3)}(\mathbf{r})$ the Dirac delta function and

$$\gamma = 2 \frac{a_s}{a_\perp} \quad (7)$$

the adimensional strength of the boson–boson interaction, proportional to the s -wave scattering length a_s of the inter-atomic potential $W(\mathbf{r}, \mathbf{r}')$.

Taking into account Eqs. (5) and (6), the Heisenberg equation of motion of the field operator

$$i \frac{\partial}{\partial t} \hat{\psi} = [\hat{\psi}, \hat{H}] \quad (8)$$

gives

$$i \frac{\partial}{\partial t} \hat{\psi}(\mathbf{r}, t) = \left[-\frac{1}{2}\nabla^2 + \frac{1}{2}(x^2 + y^2) + V(z) + 2\pi\gamma \hat{\psi}^\dagger(\mathbf{r}, t) \hat{\psi}(\mathbf{r}, t) \right] \hat{\psi}(\mathbf{r}, t). \quad (9)$$

In the superfluid regime, where the many-body quantum state $|QS\rangle$ of the system can be approximated by a Glauber coherent state $|CS\rangle$ of $\hat{\phi}(z)$ [17, 28], i.e. such that

$$\hat{\psi}(\mathbf{r}, t)|CS\rangle = \psi(\mathbf{r}, t)|CS\rangle, \quad (10)$$

the Heisenberg equation of motion (9) becomes the familiar 3D Gross-Pitaevskii equation (3D GPE) [16]:

$$i \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = \left[-\frac{1}{2}\nabla^2 + \frac{1}{2}(x^2 + y^2) + V(z) + 2\pi\gamma |\psi(\mathbf{r}, t)|^2 \right] \psi(\mathbf{r}, t), \quad (11)$$

where $\psi(\mathbf{r}, t)$ is a complex wave function normalized to the total number N of bosons, i.e.

$$\int d^3\mathbf{r} |\psi(\mathbf{r}, t)|^2 = N. \quad (12)$$

The time-dependent 3D GPE (11) is the Euler–Lagrange equation of the action functional

$$S = \int dt d^3\mathbf{r} \mathcal{L} \quad (13)$$

with Lagrangian density

$$\mathcal{L} = \psi^* \left(i \frac{\partial}{\partial t} + \frac{1}{2}\nabla^2 \right) \psi - \frac{1}{2}(x^2 + y^2) |\psi|^2 - V(z) |\psi|^2 - \pi\gamma |\psi|^4. \quad (14)$$

To perform the dimensional reduction we suppose that

$$\psi(\mathbf{r}, t) = \frac{N^{1/2}}{\pi^{1/2}\sigma(z, t)} \exp\left(-\frac{x^2 + y^2}{2\sigma(z, t)^2}\right) \phi(z, t), \quad (15)$$

where $\sigma(z, t)$ and $\phi(z, t)$ account respectively for the transverse width and for the axial bosonic wave function. We apply this Gaussian ansatz to the action functional of the 3D GPE [29]. Integrating over x and y and neglecting the derivatives of $\sigma(z, t)$, we obtain the effective 1D action [18]:

$$S_e = \int dt dz \mathcal{L}_e \quad (16)$$

with the effective 1D Lagrangian density [19]:

$$\mathcal{L}_e = \phi^* \left(i \frac{\partial}{\partial t} + \frac{1}{2}\partial_z^2 \right) \phi - V(z) |\phi|^2 - \frac{1}{2} \left(\frac{1}{\sigma^2} + \sigma^2 \right) |\phi|^2 - \frac{(\partial_z \sigma)^2}{2\sigma^2} |\phi|^2 - \frac{g}{2\sigma^2} |\phi|^4, \quad (17)$$

and

$$g = N\gamma = \frac{2Na_s}{a_\perp}. \quad (18)$$

Calculating the Euler–Lagrange equations of both $\phi(z, t)$ and $\sigma(z, t)$ one gets [18, 19]:

$$i \frac{\partial}{\partial t} \phi = \left[-\frac{1}{2}\partial_z^2 + V(z) + \frac{1}{2} \left(\frac{1}{\sigma^2} + \sigma^2 \right) + \frac{g}{\sigma^2} |\phi|^2 \right] \phi, \quad (19)$$

and

$$\sigma^4 = 1 + g|\phi|^2 + (\partial_z \sigma)^2 + \frac{\sigma^3}{|\phi|^2} \partial_z \left(\frac{\partial_z \sigma}{\sigma^2} |\phi|^2 \right). \quad (20)$$

Neglecting the spatial derivatives of $\sigma(z, t)$ (adiabatic approximation) the last equation becomes [18]:

$$\sigma = (1 + g|\phi|^2)^{1/4}. \quad (21)$$

Equations (19) and (21) give the 1D nonpolynomial Schrödinger equation (NPSE)

$$i \frac{\partial}{\partial t} \phi = \left[-\frac{1}{2} \partial_z^2 + V(z) + \frac{1}{2} \left(\frac{1}{\sqrt{1 + g|\phi|^2}} + \sqrt{1 + g|\phi|^2} \right) + \frac{g|\phi|^2}{\sqrt{1 + g|\phi|^2}} \right] \phi \quad (22)$$

we introduced some years ago [18]. Finally, only under the condition

$$g|\phi(z, t)|^2 \ll 1 \quad (23)$$

one finds $\sigma = 1$ (i.e. $\sigma = a_\perp$ is dimensional units) and Eq. (19) becomes the 1D GPE, Eq. (1). Notice that NPSE, Eq. (22), has been used by many authors to study quasi-1D BECs with a transverse width σ not simply equal to the characteristic length a_\perp of the transverse confinement.

We observe that a generalized Lieb–Liniger action functional, which describes also the Tonks–Girardeau regime [30], where $g|\phi|^2 \ll \gamma^2$, and reduces to the NPSE under the condition $g|\phi|^2 \gg \gamma^2$, was derived in Ref. [31]. Clearly, in the NPSE regime one can distinguish two sub-regimes: the 1D quasi-BEC regime for $\gamma^2 \ll g|\phi|^2 \ll 1$ where $\sigma = 1$ and the 3D BEC regime for $g|\phi|^2 \gg 1$ where $\sigma = (g|\phi|^2)^{1/4}$ [18, 31].

4. Numerical results

We perform the numerical simulation of Eq. (1) with (2) employing real-time propagation with the Crank–Nicholson discretization scheme [32]. Because of the oscillating nature of the optical potential (2) great care is needed to obtain a precisely localized state. The accuracy of the numerical simulation has been tested by varying the space and time steps as well as the total number of space steps. We choose the initial condition

$$\phi(z, 0) = \frac{1}{\pi^{1/4} \eta^{1/2}} e^{-z^2/(2\eta^2)} \quad (24)$$

with $\eta = 1$ and imposing vanishing boundary conditions $\phi(\pm z_B, t) = 0$ with $z_B = 100$. We stop the dynamics when a “stationary” configuration is reached. For $g = 0$ we have numerically verified that a different choice of η in the narrow Gaussian initial wave function does not affect the long-time behavior of the evolving wave function, which is definitely not Gaussian but a multi-peak localized configuration.

We study the effect of interaction in a BEC of ^{39}K atoms with scattering length $a_s = 33a_0 = 1.75 \text{ nm}$ [33] (with $a_0 = 0.5292 \text{ nm}$, the Bohr radius), by solving Eq. (1) with potential (2). In present dimensionless units this will correspond to $a_s/a_\perp = 0.00175$. The inclusion of the repulsive nonlinear potential term in Eq. (1) will reduce the possibility of the appearance of localized bound states.

This is illustrated in Fig. 1 where we plot the density distribution for $\lambda_1 = 4$, $\lambda_2/\lambda_1 = 0.86$, $s_1 = 2$, $s_2/s_1 = 0.2$ for potential (2) and different $g = 2N\hat{a}/a_\perp = (0, 2, 4, 5)$. The figure shows the following remarkable results: (i) for

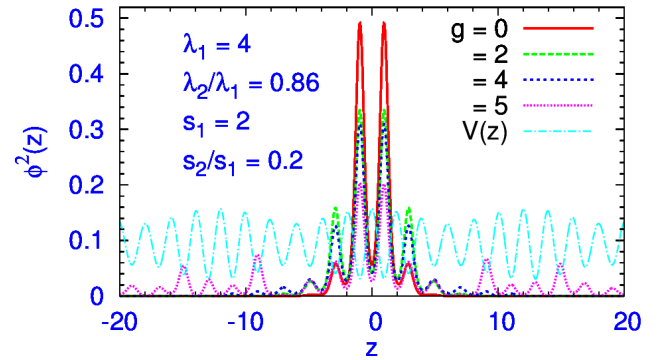


Fig. 1. Typical density distribution $\phi^2(z)$ vs. z for an interacting BEC with different values of the interaction strength $g = 2Na_s/a_\perp$. The quasi-periodic optical-lattice potential $V(z)$, Eq. (2) is plotted in arbitrary units with $\lambda_1 = 4$, $\lambda_2/\lambda_1 = 0.86$, $s_1 = 2$, $s_2/s_1 = 0.2$. Adapted from [20].

$g = 0$ the localized state is confined between $z = \pm 10$; (ii) for $g = 2$ the matter density is reduced in the central peaks and new peaks appear for larger z values; (iii) for $g = 4$ the matter density is further reduced in the central region and new peaks appear in the form of undulating tails near the edges; (iv) with further increase in the value of g , the localized states have larger and larger spatial extension and soon the nonlinear repulsion is so large that no localized states are possible and this happens rapidly as g is increased beyond 5.

The nonlinearity in Eq. (1) is $g = 2a_s N/a_\perp$ and for about 1800 ^{39}K atoms with $a_s = 0.00175$ [33] the nonlinearity has the typical numerical value $g \approx 6$. Such a small nonlinearity has a large effect on localization of a ^{39}K BEC and prohibits the localization. However, the number of K atoms can be increased if the scattering length is reduced by varying an external background magnetic field near a Feshbach resonance [9].

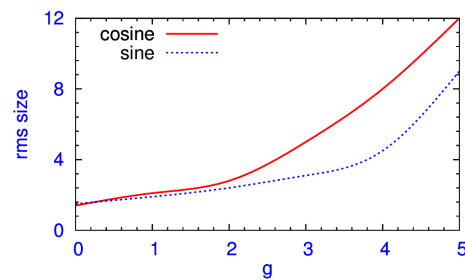


Fig. 2. The root-mean-square (rms) size vs. interaction strength g of the BEC in the quasi-periodic potential of Eq. (2) (cosine), and a similar potential where cosines are substituted by sines (sine), with $\lambda_1 = 4$, $\lambda_2/\lambda_1 = 0.86$, $s_1 = 2$, $s_2/s_1 = 0.2$. All quantities plotted are in dimensionless units. Adapted from [20].

As g value is increased, the root mean square (rms) size of the BEC increases. For values of g larger than 5 the localization is fully suppressed, corresponding to the

destruction of localization. The increase in the rms size of the localized state with the increase in g is illustrated in Fig. 2, where we plot the rms size vs. g for potential (2), and also for a similar potential where cosines are substituted by sines.

It should be noted that in the experiment of Roati et al. [6] the residual scattering length of ^{39}K atoms near the Feshbach resonance was $0.1a_0$ ($= 0.0053$ nm), e.g., they can vary the scattering length in such small steps. Thus it should be possible experimentally to obtain the curves illustrated in Fig. 2 and compare them with the present investigation.

5. Conclusion

By numerically solving the 1D Gross–Pitaevskii equation (here derived from the many-body quantum field theory through a nonpolynomial Schrödinger equation) we have verified the phenomenon of localization for a non-interacting Bose–Einstein condensate in a quasi-periodic 1D optical-lattice potential prepared by two overlapping polarized standing-wave laser beams. However, we have found that a sufficiently large repulsive atomic interaction destroys the localization. In particular, we have investigated this effect by changing the strength $g = 2Na_s/a_{\perp}$ of the nonlinearity in the 1D Gross–Pitaevskii equation: as g is gradually increased, the localization is slowly weakened with the localized state extending over a large space domain. Eventually, for g greater than 5 the localization is substantially suppressed.

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