Bose-Einstein Condensation in Geometrically Deformed Tubes

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We show that Bose-Einstein condensate can be created in quasi-one-dimensional systems in a purely geometrical way, namely by bending or other suitable deformation of a tube.

It is well known [1] that there is no Bose-Einstein condensate (BEC) of the continuous free Bose gas in one dimension as well as in tube-shaped domains $D\times\mathbf{R}$ with a compact $D\subset\mathbf{R^2}$. On the other hand, there is an increasing experimental and theoretical interest [2] to the BEC in quasi-one-dimensional systems of trapped boson gases, in particular with the idea to understand properties predicted by the Lieb-Liniger model [3] and the Girardeau-Tonks gas [4].

In this letter we want to draw attention to a way to create BEC in a quasi-one dimensional perfect Bose gas (PBG) based on *geometrical* properties of the recipient [5]. Dealing with a PBG we have naturally to describe first the one-particle spectrum. Consider first a *straight* round-tube-shaped recipient (cylinder) $\mathcal{C}(S_r)=S_r\times\mathbf{R}$ of radius $r>0$ and the associated Dirichlet Laplacian [6]

$$t:=-\Delta_D^{\mathcal{C}(S_r)},\quad \mathrm{Dom}(t)=W_0^{2,2}(S_r\times\mathbf{R})\,. \qquad (1)$$

The spectrum of t equals $\bigcup_{j=1}^{\infty}[E_j,\infty)$, where

$$0<E_1<E_2\le E_3\le\dots \qquad (2)$$

are the eigenvalues of the two-dimensional operator $-(\partial_x^2+\partial_y^2)$ with the Dirichlet boundary conditions on the tube cross section S_r. The lowest one is, of course, non-degenerate; for the circular cross section we have $E_1=\frac{\hbar^2}{2M}\,j_{0,1}^2r^{-2}$, where $j_{0,1}$ is the first zero of $J_0(z)$ and the higher eigenvalues are similarly expressed through other Bessel functions zeros. The integral density of states corresponding to the spectrum of t is given by

$$\mathcal{N}(\varepsilon)=\left[2\sqrt{\pi}\,\Gamma(3/2)\right]^{-1}\sum_{j=1}^{\infty}\theta(\varepsilon-E_j)\sqrt{\varepsilon-E_j}\,, \qquad (3)$$

where θ is Heaviside function. This gives for the PBG in the infinite tube the grand canonical total particle density

$$\rho(\beta,\mu)=\int_0^{\infty}\mathcal{N}(d\varepsilon)\frac{1}{e^{\beta(\varepsilon-\mu)}-1} \qquad (4)$$

for temperature $\beta^{-1}\ge 0$ and chemical potential $\mu<E_1$. Since the critical value $\rho_c(\beta):=\lim_{\mu\nearrow E_1}\rho(\beta,\mu)$ of the density is infinite, there is no BEC of the PBG in this quasi-one-dimensional system.

Several possibilities are known to make the critical density finite, provoking thus a BEC, by changing the one-particle spectrum. One is to replace the Dirichlet boundary condition by a "sticky" one, i.e. by a mixed condition with a positive outside gradient of the one particle wave-function on the boundary [7]. One can also switch in an external local attractive potential producing bound state(s) below the $\inf\sigma(t)=E_1$, the continuum spectrum [8]. A less obvious way is a suppression of the density states at the bottom of the spectrum, leading to convergence of the integral (4) for $\mu=E_1$, by embedding the PBG into a random external potential [9].

In the present note we are going to show that a *geometrical deformation* of the straight tube such as a simple local bending, even a gentle one, may produce the BEC of the PBG with the condensate localized in the vicinity of such a bend. We will also discuss other types of (local) geometrical deformations creating the BEC in these quasi-one dimensional systems as well the conditions under which the effect could be experimentally attainable.

To this aim we have to recall the known results about one-particle spectra in deformed tubes. Consider first a local bending of the infinite cylinder $\mathcal{C}(S_r)$, so that the tube axis is a smooth curve which is straight outside a compact region; we also suppose that the bent tube $\mathcal{C}^*(S_r)$ does not intersect itself. If the deformation is nontrivial, $\mathcal{C}^*(S_r)\neq\mathcal{C}(S_r)$, it generates one or more eigenvalues [10,11] below the continuum threshold E_1.

Their number is finite and the lowest one of them is simple; the form of this discrete spectrum is determined the geometry of the deformed tube. Properties of such bound states in bent tubes are well understood:

(a1) If the tube is only slightly bent there is only bound state with energy ϵ_1^* and the gap $E_1-\epsilon_1^*$ is proportional to φ^4, where φ is the bending angle of $\mathcal{C}^*$, see [11].

(a2) The tube need not be straight outside a bounded region; it is sufficient that it is asymptotically straight in the sense that the tube axis curvature decays faster than $|s|^{-1}$ where s is the arc length of the tube axis.

(a3) The cross section need not be circular. In such a case, however, the shape is restricted by the so-called *Tang condition* imposed on the torsion [11]. It is satisfied, in particular, if $\mathcal{C}^*=\mathcal{S}^*\times[0,d]$, where $\mathcal{S}^*$ is a bent planar strip [12].

(a4) The effect is robust. It also does not require the tube $\mathcal{C}^*$ to be bent smoothly; the geometrically induced bound states exist also in sharply bent tubes [13].

Furthermore, bending is not the only way how to produce geometrically a nonempty discrete spectrum:

(b1) Another mechanism is a local change of the cross section. Protrusions and other deformations which do not reduce the volume also give rise to an effective attractive interaction [14].

(b2) Similar effect comes from a tube branching. A cross-form tube is known to support a single bound state [15], numerous isolated eigenvalues arise in a skewed scissor-shaped cross with small enough angle [16].

(b3) One more example are two parallel tubes with a window in the common boundary, where the number of bound states is given by the window length [17].

The geometrically induced discrete spectrum is finite in asymptotically straight ducts. In the bent-tube case, for instance, it follows from the fact that the effective attractive potential falls off faster that $|s|^{-2}$, see [11]. On the other hand, the actual form of the spectrum depends on tube geometry. In particular, if we deal with two or more well localized, identical, and mutually distant perturbations the eigenvalues cluster around those of a single deformation, with a split exponentially small w.r.t. the distance between the perturbations. This is proved mathematically for a tube with a pair of windows [18], however, various examples worked out numerically [19] suggest that such a behavior is generic.

Consider thus such a geometrically induced discrete spectrum below the continuum threshold [20] in a deformed cylinder which consists consists of one or several bound states with energies $\{\epsilon_s^* < E_1 :\ s = 1, 2, \dots\}$ and eigenfunctions localized in the vicinity of the deformation(s). If one orders the bound-state energies naturally, $\epsilon_1^* < \epsilon_2^* \leq \dots < E_1$, then the domain of the allowed chemical potentials is given by the inequality $\mu \leq \epsilon_1^*$. This implies that the critical particle density is bounded,

$$\rho_c^*(\beta) := \lim_{\mu \nearrow \varepsilon_1^*} \int_{E_1}^{\infty} \mathcal{N}^*(d\varepsilon) \frac{1}{e^{\beta(\varepsilon-\mu)} - 1} < \infty ; \qquad (5)$$

here $\mathcal{N}^*(\varepsilon)$ is the integrated density of states for the deformed cylinder. This opens a way to create the BEC.

To make this effect transparent consider first a finite segment of the deformed cylinder $\mathcal{C}_L^*$ of length L. Then the Dirichlet Laplacian which plays here the role of the one-particle Hamiltonian,

$$t_*(L) := -\Delta_D^{\mathcal{C}_L^*} , \quad \mathrm{Dom}(t_*(L)) = W_0^{2,2}(\mathcal{C}_L^*) , \qquad (6)$$

has a purely discrete spectrum $\sigma(t_*(L))$ accumulating at infinity. Denote by $P_I(t_*(L))$ the spectral projection of $t_*(L)$ for a Borel set $I \subset \mathbf{R}$. It allows us to write the finite-volume integrated density of states corresponding to the operator (6) as

$$\mathcal{N}_L^*(\epsilon) := \frac{1}{|\mathcal{C}_L^*|} \mathrm{Tr} \left\{ P_{(-\infty,\epsilon)}(t_*(L)) \right\} , \qquad (7)$$

where $|\mathcal{C}_L^*|$ is the volume of the segment $\mathcal{C}_L^*$. By (7) the total particle density $\rho_L^*(\beta,\mu)$ in $\mathcal{C}_L^*$ acquires the form

$$\int_{-\infty}^{\infty} \mathcal{N}_L^*(d\varepsilon) \frac{1}{e^{\beta(\varepsilon-\mu)} - 1} = \frac{1}{|\mathcal{C}_L^*|} \sum_{\{\epsilon_s^*(L)\}} \frac{1}{e^{\beta(\epsilon_s^*(L)-\mu)} - 1} + \frac{1}{|\mathcal{C}_L^*|} \sum_{\{\varepsilon_j^*(L)\}} \frac{1}{e^{\beta(\varepsilon_j^*(L)-\mu)} - 1} . \qquad (8)$$

Here $\{\epsilon_s^*(L)\}_{s\geq 1}$ and $\{\varepsilon_j^*(L)\}_{j\geq 1}$ are eigenvalues of the operator $t_*(L)$ divided into two groups with $\epsilon_s^* < \varepsilon_j^*$ for any s, j. The first one consists of those which converge to the eigenvalues of the infinite-tube operator t_* as $L \to \infty$; recall that all of them are monotonously decreasing with respect to L. The limit is naturally taken in such a way that the distance of the cut-offs from the deformed part(s) tend to infinity. On the other hand, $\{\varepsilon_j^*(L)\}_{j\geq 1}$ are those eigenvalues which give in this limit the continuous spectrum of t_*. Combining this with the above stated properties of the one-particle spectrum we see that the first group $\{\epsilon_s^*(L)\}_{s\geq 1}$ is finite. Since $|\mathcal{C}_L^*| \to \infty$ as $L \to \infty$, one gets then from (8) for the limiting density of states $\rho^*(\beta,\mu) := \lim_{L\to\infty} \rho_L^*(\beta,\mu)$ the relation

$$\rho^*(\beta,\mu) = \lim_{L\to\infty} \frac{1}{|\mathcal{C}_L^*|} \sum_{\{\varepsilon_j^*(L)\}} \frac{1}{e^{\beta(\varepsilon_j^*(L)-\mu)} - 1} = \int_{E_1}^{\infty} \mathcal{N}^*(d\varepsilon) \frac{1}{e^{\beta(\varepsilon-\mu)} - 1} \qquad (9)$$

provided $\mu \leq \lim_{L\to\infty} \epsilon_1^*(L) = \epsilon_1^* < E_1$, uniformly in μ, where $\mathcal{N}^*(d\varepsilon)$ is the weak limit of the measure family $\{\mathcal{N}_L^*(d\varepsilon)\}_L$. In particular, the limit (9) implies

$$\rho^*(\beta,\mu) < \rho_c^*(\beta) := \rho^*(\beta, \epsilon_1^*) \qquad (10)$$

for $\mu < \epsilon_1^*$ in view of (5).

Now let the total particle density be $\rho > \rho_c^*(\beta)$. To show that this implies the BEC, let us analyze solutions $\{\mu_L(\beta,\rho)\}_L$ of the equation following from (8),

$$\rho = \rho_L^*(\beta,\mu) ; \qquad (11)$$

notice that they always exist and are bounded by $\epsilon_1^*(L)$ from above. Using (8) and (9) one gets for $\rho \leq \rho_c^*(\beta)$

$$\lim_{L\to\infty} \mu_L(\beta,\rho) = \mu(\beta,\rho) \leq \epsilon_1^* . \qquad (12)$$

On the other hand, for $\rho > \rho_c^*(\beta)$ we rewrite eq. (11) as

$$\rho - \frac{1}{|\mathcal{C}_L^*|} \sum_{\{\varepsilon_j^*(L)\}} \frac{1}{e^{\beta(\varepsilon_j^*(L)-\mu_L(\beta,\rho))} - 1} = \frac{1}{|\mathcal{C}_L^*|} \sum_{\{\epsilon_s^*(L)\}} \frac{1}{e^{\beta(\epsilon_s^*(L)-\mu_L(\beta,\rho))} - 1} . \qquad (13)$$

(i) Suppose that the bound-state energies $\{\epsilon_s^*(L)\}_{s\geq 1}$ verify the following conditions as $L \to \infty$,

$$E_1 - \delta > \epsilon_1^*(L) \quad \text{for some } \delta > 0$$

and

$$\epsilon_s^*(L) - \epsilon_1^*(L) \geq a\, |\mathcal{C}_L^*|^{\alpha-1} , \quad a > 0 ,\ \alpha > 0 .$$

This is true, in particular, for a tube with a single bend or protrusion and two cut-offs moving away of it, where in view of the norm-resolvent convergence of $-\Delta_D^{\mathcal{C}_L^*}$ to $-\Delta_D^{\mathcal{C}^*}$ the eigenvalue $\epsilon_1^*(L)$ tends to $\epsilon_1^* < E_1$ and the eigenvalue difference to a nonzero limit.

Since $\mu_L(\beta,\rho) < \epsilon_1^*(L)$, we can use the uniform convergence (9) to obtain the asymptotics of the solution of eq. (13) as $L \to \infty$, namely

$$\mu_L(\beta,\rho) = \epsilon_1^*(L) - \frac{1}{\beta(\rho-\rho_c^*(\beta))\,|\mathcal{C}_L^*|} + o\left(|\mathcal{C}_L^*|^{-1}\right). \quad (14)$$

This means that $\lim_{L\to\infty}\mu_L(\beta,\rho) = \epsilon_1^*$, and since $|\mathcal{C}_L^*| = \mathcal{O}(L)$ as $L \to \infty$, the thermodynamic limit in (13) gives rise to BEC at the lowest level ϵ_1^* only,

$$\rho - \rho_c^*(\beta) = \lim_{L\to\infty} \frac{1}{|\mathcal{C}_L^*|} \frac{1}{e^{\beta(\epsilon_1^*(L)-\mu_L(\beta,\rho))} - 1} \quad (15)$$

The same is true for other tube geometries, for instance, for a tube with several well distinguished bends or "bubbles", as long as the limit $L \to \infty$ means that cut-offs move away in the asymptotically straight parts.

(ii) The situation may change when the thermodynamic limit $L \to \infty$ is more complicated and involves a local change of the geometry as well. As a model example, consider again a tube with a finite number $n > 1$ of well distinguished *identical* bends, but suppose now that the distances between them increase also with increasing L. As we have recalled above, the first n eigenvalues $\{\epsilon_s^*(L)\}_{s=1}^n$ then cluster being exponentially close to each other with respect to the separation parameter L,

$$\epsilon_s^*(L) - \epsilon_1^*(L) \le C\, e^{-aL}, \quad 1 \le s \le n, \quad (16)$$

for some positive C, a. By (16) the asymptotics of the solution to eq. (13) is again of the form (14). This means that the limit in (13) gives rise to BEC equally fragmented into the group of n levels $\{\epsilon_s^*(L)\}_{s=1}^n$ which are almost degenerate being exponentially separated,

$$\lim_{L\to\infty} \frac{1}{|\mathcal{C}_L^*|} \frac{1}{e^{\beta(\epsilon_s^*(L)-\mu_L(\beta,\rho))} - 1} = \frac{\rho - \rho_c^*(\beta)}{n} \quad (17)$$

for $1 \le s \le n$. This fragmentation is called a *type-I generalized* BEC , contrasting with the case of the *infinite* fragmentation known as the *type-II generalized* BEC, see [1], [21] and also [22]. What is important is that this condensate is separated from the continuum spectrum by a finite energy gap which makes it more stable than the conventional BEC, see the discussion in [8].

To analyze localization properties of the geometrically induced BEC we employ the PBG *one-body reduced density matrix* with the kernel $\rho_L(\beta,\mu;x,y)$ given by

$$|\mathcal{C}_L^*| \int_{-\infty}^{\infty} \mathcal{N}_L^*(d\varepsilon) \frac{1}{e^{\beta(\varepsilon-\mu)} - 1}\, \overline{\psi_{\varepsilon,L}^*(x)}\psi_{\varepsilon,L}^*(y), \quad (18)$$

where $\{\psi_{\varepsilon,L}^*\}$ are the *normalized eigenfunctions* of the operator (6). The diagonal part of the matrix (18) is the *local* particle density, since by (8)

$$\int_{\mathcal{C}_L^*} dx \rho_L(\beta,\mu;x,x) = |\mathcal{C}_L^*|\, \rho_L(\beta,\mu) \quad (19)$$

is the total number of particles in $\mathcal{C}_L^*$. In fact a relevant quantity for the BEC *space localization* is the *local* particle density *per unit volume* $\tilde\rho_L(\beta,\mu;x)$ given by

$$\int_{-\infty}^{\infty} \mathcal{N}_L^*(d\varepsilon) \frac{1}{e^{\beta(\varepsilon-\mu)} - 1}\, \overline{\psi_{\varepsilon,L}^*(x)}\psi_{\varepsilon,L}^*(x). \quad (20)$$

Indeed, since in the limit only the eigenfunctions corresponding the eigenfunction family $\{\psi_s^*\}_{s\ge1} \subset L^2(\mathcal{C}^*)$ related to the infinite-tube bound states is preserved, in contrast to all the others which are extended, we get

$$\begin{aligned}\tilde\rho(\beta,\mu;x) &:= \lim_{L\to\infty} \int_{-\infty}^{\infty} \mathcal{N}_L^*(d\varepsilon) \frac{1}{e^{\beta(\varepsilon-\mu)} - 1}\, \overline{\psi_{\varepsilon,L}^*(x)}\psi_{\varepsilon,L}^*(x) \\ &= (\rho - \rho_c^*(\beta))\, \overline{\psi_{\epsilon_1}^*(x)}\psi_{\epsilon_1}^*(x) \quad (21)\end{aligned}$$

for $\rho > \rho_c^*(\beta)$ in the case (15). For the fragmented BEC (17) one gets for $\rho > \rho_c^*(\beta)$ similarly

$$\tilde\rho(\beta,\mu;x) = \frac{\rho - \rho_c^*(\beta)}{n} \sum_{s=1}^{n} \left|\psi_{\epsilon_s}^*(x)\right|^2; \quad (22)$$

it is obvious that $\tilde\rho(\beta,\mu;x) = 0$ holds when $\rho \le \rho_c^*(\beta)$.

Thus in contrast to the BEC in the translation-invariant case, the L^2-localized condensation in the bounded states correspond to an *infinite* accumulation of the local particle density defined by (18). On the other hand, by (15) and (17) in combination with (21), (22), the *total* density of particles condensed in the bounded states,

$$\rho - \rho_c^*(\beta) = \int_{\mathcal{C}^*} dx \tilde\rho(\beta,\mu;x), \quad (23)$$

is *finite*.

After this theoretical analysis let us ask about chances to observe the described type of the BE condensation in an experiment. We are not going to discuss technically the ways in which the Bose gas can be confined in a geometrically deformed tube, generally we have in mind either a modification of the existing elongated traps [23] or using hollow optical fibers [24] as suggested in [25].

The important parameter is the tube radius which for both the elongated traps and hollow fibers can be made as small as $r \approx 5\,\mu m$ which determine the threshold energy by the mentioned expression $E_1 = \frac{\hbar^2}{2M} j_{0,1}^2 r^{-2}$, where M is atom of the mass in question. Let us further introduce the *relative gap* size by $\gamma_{\rm rel} := (E_1 - \epsilon_1^*)/E_1$. This quantity can theoretically reach the value about 0.39 in a smoothly bent tube [26], but a typical value for a bending angle of $90^{\rm o}$ and more is around $\gamma_{\rm rel} \approx 10^{-1}$, see [19].

Two conditions must be satisfied. First of all, the bending-induced gap $\gamma_{\rm rel}E_1$ must be much larger than the effect of the finite length L of the recipient. The latter is characterized by the first longitudinal eigenvalue $\frac{\hbar^2}{2M}(\pi/L)^2$. It is clear that the trap must sufficiently elongated to fulfill the condition, roughly speaking $L/r \gtrsim 20$ is sufficient. This is true in both situations mentioned above, for hollow fibers it can be even much better.

More complicated is the question of thermal stability; the said gap must be larger than the energy $k_{\rm B}T$. This determines a critical temperature above which the bending-induced BEC is likely to be destroyed by thermal fluctuations. Using the value $r \approx 5\,\mu m$ we find that

$$T_{\rm crit} \approx 5.4 \times 10^{-8} \frac{\gamma_{\rm rel}}{Z}\,, \tag{24}$$

where Z is the atomic number in question. Hence lighter nuclei are preferable; there is one order of magnitude difference between Li^7 and Ru^{87}. With above estimate in mind, however, even for the light ones it is difficult to perform the measurement in the available nanokelvin conditions. On the other hand, the effect is not too far from the experimental reach; recall for instance that squeezing the transverse size to a one micron radius would enhance the critical temperature (24) by the factor of 25.

Let us finally mention one more feature of such a geometrically induced BE condensate. The ground-state wave function into which will the atoms of the Bose gas condensate – cf. (21) – is exponentially localized away of the bend; for examples of such wave functions see [19] and the literature mentioned there. This means that, e.g., bending a tube would mean not only the condensation but also that the condensate will squeezed in the bend the more the larger the bending angle is.

In conclusion, we have demonstrated here a purely geometric way to achieve a stable BEC based on local deformations of a tube-shaped recipient and we discussed ways in which the effect could be experimentally observed.

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$$\epsilon_s^*(L) - \epsilon_1^*(L) = a_s\, |\mathcal{C}_L^*|^{-1-\alpha}\ ,\ a > 0\,,\ \alpha \geq 0\,,$$

when the so-called *type-III* ($\alpha = 0$) *and type-III* ($\alpha > 0$) *generalized* BEC can take place [21]. In these situations none of the bound states is macroscopically occupied. This can occur with geometrically deformed tubes only for complicated shapes which are rather mathematical constructs without a relation to a possible experiment.

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