On Berezinskii-Kosterlitz-Thouless Phase Transition in Quasi-One Dimensional Bose-Einstein Condensate

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(Dated: January 26, 2013)

Abstract

We show that quasi-one dimensional Bose-Einstein condensate under suitable conditions can exhibit a Berezinskii-Kosterlitz-Thouless phase transition. The role played by quantized vortices in the two dimensional case, is played in this case by dark solitons. We find that the critical temperature for this transition lies in nano Kelvin range and below, for a wide range of experimentally accessible parameters. It is seen that the high temperature (disordered) phase differs from the low temperature (ordered) phase in terms of phase coherence, which can be used as an experimental signature for observing this transition.
The continuum version of 2D XY model appears in diverse areas of physics ranging from spin systems to superfluids [1–4], with its Lagrangian being given by
\[ L = -\rho (\vec{\nabla} \theta)^2. \]
It is well known that this model exhibits singular vortex solutions: \( \vec{\nabla} \theta \propto \hat{\phi} r \) (in polar coordinates) [1, 2]. Identifying two dimensional Cartesian plane with complex plane, allows one to write vortex solution in a rather elegant form [5]:
\[ \theta(x, y) = \theta(z = x + iy) = \pm \text{Im} \ln(z - z_0), \quad (1) \]
where \( z_0 \) is the location of vortex. It is evident that the above solution exhibits a discontinuous jump as one traverses along a closed loop enclosing \( z_0 \). This multivaluedness or discontinuity is a characteristic feature of these vortices and distinguishes them from other solutions. It has been shown that the Helmholtz free energy of a system of \( K \) vortices is given by [1, 2],
\[ F = K (2\pi \rho - 2kT) \ln \left( \frac{L}{b} \right), \quad (2) \]
where \( k \) stands for Boltzmann constant, \( L \) represents system size, and \( b \) is vortex core radius. Hence, one finds that below critical temperature \( T_{BKT} = \frac{\pi \rho}{k} \), free energy is minimized by having \( K = 0 \), which means that at temperature low enough vortices are thermodynamically unstable. However, when \( T > T_{BKT} \), free energy minimization requires having \( K \) as large as possible. So the critical temperature \( T_{BKT} \) marks the occurrence of spontaneous proliferation of vortices, which makes condensate inhomogeneous. This is the celebrated Berezinskii-Kosterlitz-Thouless (BKT) phase transition [6, 7]. This phase transition was found to be of infinite order, and unlike second order phase transition, here the ordered (low temperature) phase differs from disordered (high temperature) phase not in terms of symmetry of ground state but rather in terms of topology of the ground state [1, 2]. In the low temperature phase, system exhibits a quasi long range order, where \( \langle e^{i\theta(x)} e^{i\theta(y)} \rangle \approx |x - y|^{-\alpha} \) for some constant \( \alpha \). Above critical temperature the system has vortex excitations, which cause rapid phase variation, and one sees that correlation function \( \langle e^{i\theta(x)} e^{i\theta(y)} \rangle \approx e^{-\beta|x-y|} \) (\( \beta \) is a constant). This means that the quasi long range order present at low temperature is destroyed due to vortices, resulting in rapid decay in correlation.

It is established by now that in the mean field approximation, physics of Bose-Einstein condensate (BEC) is well described by the Gross-Pitaevskii (GP) equation [8]:
\[ \left( -\frac{\hbar^2}{2m} \vec{\nabla}^2 + V(\mathbf{r}) + U_0 |\Psi|^2 \right) \Psi(\mathbf{r}, t) = i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t}. \quad (3) \]
Here \( V(\mathbf{r}) \) is the external trapping potential, and \( U_0 = 4\pi\hbar^2a/m \) is the coupling constant for inter-atomic interaction, where \( m \) and \( a \) are atomic mass and \( s \)-wave scattering length, respectively. The above partial differential equation is an equation of motion describing space-time dependence of BEC, which itself is a ground state of a system of interacting bosons. In case when trapping potential is tightly confining along \( Z \)-direction and absent (or very weak) along the other two spatial dimensions, dynamics of BEC occurs only along the latter two spatial dimensions. The condensate function can then be written as \( \Psi(\mathbf{r},t) = f(z)\phi(x,y,t) \), where \( f(z) \) is a localized Gaussian wave packet along \( Z \)-direction, and \( \phi(x,y,t) \) describes condensate profile in the XY plane. Equation governing dynamics of such quasi-2D BEC can be obtained by integrating out degrees of freedom along \( Z \)-direction. Condensate density, in absence of any potential acting along XY directions, can be expected to be stationary (temporally) and spatially uniform: \( |\phi(x,y,t)|^2 = \rho \), where \( \rho = \text{constant} \), and \( \phi \) field can be written in terms of the polar variables: \( \phi = \sqrt{\rho}e^{i\theta(r,t)} \). It can be shown that in static case, Lagrangian for quasi-2D BEC reads as \( \mathcal{L}_{2D} \propto -\rho(\vec{\nabla}\theta)^2 \), which exactly matches with that of 2D XY model. Hence, one finds that dynamics of quasi-2D BEC is actually captured by XY model, and so one expects to observe BKT transition in this system.

Above discussion is oversimplified, and in reality, bosons are trapped not only in \( Z \)-direction but also in XY directions. Because of this, there appears a confining potential defined over XY plane. This makes the system inhomogeneous, and hence translational invariance is lost. In the last few years, there have been significant activity, on both theoretical and experimental fronts, to gain more understanding about nature of BKT transition in these systems \([9-11]\). A few years back, Hadzibabic et al., reported a direct observation of BKT transition in BEC \([12]\). Further, in recent years study of dynamics of vortices in BEC systems especially, vortex dipoles (vortex-antivortex pairs) has received significant attention \([13-18]\). Vortex dipoles are also produced as the decay products of dark solitons in 2D BECs due to onset of the snake instability \([19]\).

In light of above discussion, it is natural to ask, if a BKT phase transition occurs in BEC in spatial dimensions other than two. The answer is crucially dependent on another question: Do the counterparts of vortices exist in dimensions other than two? Analogues of vortices in three dimension are well known, they are vortex tubes or rings \([20, 21]\). Being spatially extended objects, interaction between them is complicated, which makes the problem rather nontrivial \([22, 23]\). Instead, we ask whether there are any analogues of vortices in one
dimension? If yes, then does one dimensional BEC display BKT type phase transition? Answer to the first question is known. The so called dark soliton solutions are known to be analogues of vortices in one dimension [24, 25]. In what follows, we answer the second question affirmatively. After introducing dark soliton solution of GP equation, we indicate its analogy with two dimensional vortex. Thereafter, we show using exactly similar free energy argument as was originally used by Kosterlitz and Thouless [7] (which is also used in the above discussion) that it is indeed possible to have a finite temperature BKT phase transition in quasi-one dimensional BEC. We estimate the critical temperature for the same and find that it can be tuned over a broad range by changing scattering length and number density. Subsequently, we also show that the long range phase coherence exhibited by the system at low temperature vanishes at the temperatures above critical temperature. We conclude by mentioning that it may be possible to experimentally realize this phase transition.

As mentioned earlier, GP equation (3) governs motion of order parameter \( \Psi(r, t) \), which satisfies normalization condition \( \int |\Psi(r, t)|^2 dr = N \), where \( N \) is the number of the bosons. In present case, we consider trapping potential to be harmonic along the radial direction and infinite square well along the axial direction, i.e.,

\[
V(r, z) = \begin{cases} 
\frac{m}{2} \omega^2 r^2 & \text{if } -\frac{L}{2} < z < \frac{L}{2}, \\
\infty & \text{if } |z| \geq \frac{L}{2},
\end{cases}
\]  

where \( \omega \) is the radial trap frequency and \( L \) is the size of infinite square well potential along axial direction. The infinite square well potential can be created by applying two blue detuned laser beams with narrow beam waist and sufficiently high intensity at \( |z| = L/2 \).

Since the potential becomes infinitely high at and after \( |z| = L/2 \), condensate density vanishes at \( |z| = L/2 \) and increases smoothly as one moves towards the center. The characteristic length scale over which BEC recovers its bulk density \( n_0 \) is called healing length or coherence length \( \xi = \frac{1}{\sqrt{8\pi n_0 a}} \). The characteristic length of the BEC along radial direction is oscillator length \( a_{osc} = \sqrt{\hbar/(m\omega)} \). When \( a_{osc} \ll \xi, a_{osc} \ll L \), and BEC is in the weakly interacting regime \( 2\pi a N \int r|\Psi(r, z)|^2 dr \ll 1 \), the order parameter can be factorized into radial and axial parts [26]

\[
\Psi(r, z, t) = \chi(r)\psi(z, t),
\]

where \( \chi(r) \) is the normalized ground state of radial trapping potential, which can be considered to be time independent provided, \( kT \ll \hbar \omega \). We consider \( \chi(r) \) to be normalized to
unity \(2\pi \int r|\chi(r)|^2dr = 1\); then from Eq.(3) and Eq.(5), after integrating out the radial order parameter, GP equation reduced to one dimension reads,

\[
\left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + V^a(z) + u|\psi|^2 \right] \psi = i\hbar \frac{\partial \psi}{\partial t},
\]

(6)

where \(u = 2ah\omega\) and \(V^a(z) = \hbar\omega\) for \(-L/2 < z < L/2\) and zero otherwise. The order parameter satisfies normalization condition:

\[
\int_{-L/2}^{L/2} dz |\psi(z)|^2 = N. \]

It is well known, since the pioneering work of Zakharov and Shabat [27], that equation (6) allows for grey solitons solutions. In terms of atoms per unit length along axial direction \(\sigma(z) = |\psi(z)|^2\) and a dynamical phase, solution at \(t = 0\) is given by

\[
\psi(z) = \sqrt{\sigma(z)} e^{i\phi(z)},
\]

where

\[
\sigma(z) = \sigma_0 \left(1 - \frac{\cos^2(\theta)}{\cosh^2(z \cos(\theta)/\zeta)}\right)
\]

and

\[
\phi(z) = \tan^{-1}\left(\frac{c_w}{u} \sqrt{(1 - u^2/c_w^2) \tanh \left(\frac{1 - u^2/c_w^2}{c_w^2}\right) z}\right).
\]

(7)

Here velocity of soliton is given by \(u\) and velocity of sound is \(c_w\). Parameter \(\theta\) is defined as \(\theta = \sin^{-1}(u/c_w)\), whereas \(\zeta\) is defined as \(\zeta = 2\xi(n_0)\), and \(\sigma_0 = n_0\pi a^2_{osc}\) is the linear density far away from the soliton, i.e., in the domain \(v \propto \phi'(z) \to 0\). Notice that above soliton becomes ‘dark’, i.e, condensate density \(\sigma(z)\) vanishes, at \(z = 0\) only when \(u = 0\). Therefore, by construction, a dark soliton in this model is static. Amazingly, in the limit \(u\) approaches zero, from Eq.(7), one sees that the phase of the dark soliton behaves like a Heaviside step function with height \(\pi\) and becomes discontinuous at \(z = 0\), i.e.,

\[
\phi(z) = \begin{cases} 
-\frac{\pi}{2} & \text{if } z < 0, \\
0 & \text{if } z = 0, \\
\frac{\pi}{2} & \text{if } z > 0.
\end{cases}
\]

It is this discontinuity that makes the dark soliton a 1D counterpart of vortex. A cautious reader may ask that the above mentioned solitons are strictly solutions of Eq. (6), when \(\psi(z)\) is defined over whole of real line. In present case, because of particle-in-a-box type potential, it is only defined in domain \(\frac{-L}{2} \leq z \leq \frac{L}{2}\). It was shown by Carr et. al. [24], that dark soliton is indeed a genuine solution in this case too. It can be easily shown that the energy required to create a dark soliton in otherwise homogeneous and uniform condensate is

\[
\varepsilon = \frac{4\sqrt{2}}{3} \sqrt{(\sigma_0 a)\sigma_0 a_{osc}} \hbar\omega.
\]
In terms of $\sigma(z)$, the criterion for applicability of Eq. (6), i.e.,\[2\pi a \int r|\Psi(r,z)|^2dr \ll 1,\]
becomes $\sigma(z)a \ll 1$. The transition between weakly interacting to strongly interacting high density limit occurs for $\sigma(z)a \sim 0.25$. If $N$ is large ($N \to \infty$) such that $\xi/L \to 0$, it can be argued that a dark soliton can be created without disturbing the other soliton. In reality, however, $N$ is finite, and $\xi/L$ is quite small but non-zero. It was shown in Refs. [24, 27], and we have also checked numerically that above argument still holds as long as the distance between two dark solitons is much greater than the healing length. So the energy required to create $K$ solitons is $\varepsilon_K = K\varepsilon$. Entropy associated with $K$ solitons is given by $Kk\ln W$, where $W$ is number of independent states soliton can occupy, and it is easy to see that $W = L/\xi$. Hence, Helmholtz free energy for $K$ solitons is:

$$F = K \left( \frac{4\sqrt{2}}{3} \sqrt{(\sigma_0a)\sigma_0a_{osc}}\hbar\omega - kT \ln \frac{L}{\xi} \right),$$

which changes sign at a characteristic temperature

$$T_{BKT} = \frac{4\sqrt{2}}{3k \ln (L/\xi)} \sqrt{(\sigma_0a)\sigma_0a_{osc}}\hbar\omega.$$

So exactly like in 2D BEC, we see that in 1D BEC also there exists a finite critical temperature $T_{BKT}$, above which a uniform homogeneous condensate becomes thermodynamically unstable and spontaneous proliferation of dark solitons takes place. This indicates that 1D BEC exhibits a non-symmetry breaking BKT phase transition. Note that critical temperature obtained above, depends on various tunable parameters like $a$ and $\sigma_0$. In a typical cold atom experiment, the maximum density in trap ($n_0$) can vary from $10^{11} - 10^{15}$ cm$^{-3}$ [30], whereas typically $\omega$ varies from a few Hertz to kilo Hertz. For $\omega = 130$ Hz, $L = 500\xi$, density around $10^{11}$ cm$^{-3}$, and scattering length around $50a_0$ ($a_0$ is Bohr radius), one finds that $T_{BKT}$ lies in sub nano Kelvin range ($\sim 0.1K$), which is an order of magnitude less than a typical BEC transition temperature. Figure (11) shows dependence of $T_{BKT}$ as a function of scattering length and density, and it is clear that it can be conveniently tuned by varying density and/or scattering length at will.

Dimensionally reduced GP equation (6) can be obtained by extremizing the action $S = \int dx dt \mathcal{L}$, where

$$\mathcal{L} = i\hbar \psi^* \frac{\partial \psi}{\partial t} - \frac{\hbar^2}{2m} \left| \frac{\partial \psi}{\partial z} \right|^2 - \psi^* \left( V^a(z) + u|\psi|^2 \right) \psi.$$
In case when background condensate density is constant, only dynamical degree of freedom left is phase, since \( \psi(x,t) = \sqrt{\sigma_0}e^{i\theta(x,t)} \). Dynamics of \( \theta \) field is governed by Lagrangian

\[
\mathcal{L}_\theta = -\hbar\sigma_0 \frac{\partial \theta}{\partial t} + \frac{\hbar^2\sigma_0}{2m} \frac{\partial^2 \theta}{\partial z^2}.
\]

![FIG. 1. Density plot depicting \( T_{BKT} \) (in nano Kelvins) as a function of bulk density \( n_0 \) and s-wave scattering length \( a \)](image)

Provided that there are no dark solitons, static spatial phase correlation function can be easily found from the above Lagrangian and is

\[
\langle \theta(z)\theta(0) \rangle = \frac{m}{2\hbar^2} |z|,
\]

which clearly indicates that system indeed has phase coherence, a characteristic feature of any BEC. However, situation changes when dark solitons are present. Phase field now can be decomposed into a regular continuous part and a discontinuous part, \( \theta(z,t) = \theta_{\text{reg}}(z,t) + \theta_{\text{dis}}(z) \), respectively. Substituting this in the above Lagrangian, one finds

\[
\mathcal{L}_\theta = -\hbar\sigma_0 \frac{\partial \theta_{\text{reg}}}{\partial t} + \frac{\hbar^2\sigma_0}{2m} \theta_{\text{reg}} \frac{\partial^2 \theta_{\text{reg}}}{\partial z^2}
+ \frac{\hbar^2\sigma_0}{2m} \theta_{\text{dis}} \frac{\partial^2 \theta_{\text{dis}}}{\partial z^2} + \frac{\hbar^2\sigma_0}{m} \theta_{\text{dis}} \frac{\partial^2 \theta_{\text{reg}}}{\partial z^2}.
\]

The effect of dark solitons on phase correlation can be inferred by first integrating out the singular part of field to yield an effective action for regular field. Very interestingly, one finds that integration of \( \theta_{\text{dis}} \) gives rise to a term \( -\frac{\hbar^2\sigma_0}{2m} \theta_{\text{reg}} \frac{\partial^2 \theta_{\text{reg}}}{\partial z^2} \), which exactly cancels the gradient term already present in the action. Hence, phase field in presence of solitons does not propagate, and system losses long range phase correlation. In the absence of solitons, phase
variation along the condensate profile is rather slow, and hence such a condensate would yield a well defined interference pattern, an authentic signature of coherence. However, when solitons are present, phase receives random discontinuous kicks along the profile, as a result phase ultimately gets averaged out. Such a condensate would certainly exhibit poor interference pattern, an indication of loss of coherence. Hence we conclude that high temperature solitonic phase is actually a disordered phase, and transition from uniform condensate to solitonic state is a phase transition.

We have shown that like 2D BEC, 1D BEC can also exhibit a BKT phase transition at finite temperature. The role played by vortices in 2D is, in 1D case, played by dark solitons. It is found that critical temperature for this transition depends on atom number density and scattering length, both of which can be finely controlled in a typical experiment. It is this particular feature that could facilitate and strengthen possibility of an experimental realization of this transition. One may wonder whether above discussed phase transition indicates violation of Coleman-Mermin-Wagner-Hohenberg theorem [1, 2]. This theorem states that a continuous symmetry in given infinite system (not bounded by a finite volume), which is homogeneous and isotropic with short range local interactions, can not be broken at zero temperature in one spatial dimension and at finite temperature in two spatial dimensions. The proof of above theorem is based on the fact that in such a system, breaking of a continuous symmetry results in existence of gapless Goldstone modes which by construction lead to infrared divergence. It was shown that in one spatial dimension, this divergence is so severe that it does not allow ordered phase to exist, and hence a continuous symmetry is not broken even at absolute zero temperature. As is obvious, this theorem does not hold for our system of 1D BEC for several reasons. Firstly, we are dealing with a system which is externally confined into a finite volume by trapping potentials, and hence is neither homogeneous nor isotropic and certainly not of infinite extent. Further, we are actually looking at a quasi 1D BEC, where BEC itself lives in 3D but at sufficiently low energies, degrees of freedom along other dimensions are frozen. Moreover in BKT phase transition, no symmetry of Hamiltonian is spontaneously broken by ground state [1, 2, 5]. So we see that Coleman-Mermin-Wagner-Hohenberg theorem does not hold for our system. Possibility of BKT transition in 1D systems (in thermodynamic limit) have been studied in Refs. [31, 32], and both find transition temperature to be absolute zero. Interestingly, taking $L \rightarrow \infty$ in equation (9), one sees that $T_{BKT}$ goes to zero, which agrees with their
results. Issues pertaining to critical behavior and universality class of this transition are currently being investigated and will be published in due course.

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