Low-Dimensional Bose Liquids: Beyond the Gross-Pitaevskii Approximation

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The Gross-Pitaevskii approximation is a long-wavelength theory widely used to describe a variety of properties of dilute Bose condensates, in particular trapped alkali gases. We point out that for short-ranged repulsive interactions this theory fails in dimensions $d \leq 2$, and we propose the appropriate low-dimensional modifications, which have a universal form. For $d = 1$ we analyze density profiles in confining potentials, superfluid properties, solitons, and self-similar solutions.

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Experimental observation of Bose-Einstein condensation (BEC) in trapped alkali vapors [1] has ushered in a new era of superlow temperature physics. The Gross-Pitaevskii (GP) mean-field theory [2] has proven to be an indispensable tool in both analyzing and predicting the outcome of experiments.

With rapid progress in the experimental exploration of BEC systems it is reasonable to anticipate that effectively one- and two-dimensional systems are realistic prospects in the near future [3]. For example, high aspect ratio cigar-shaped traps approximating quasi-one-dimensional BEC systems are already available experimentally [4]. From the theoretical viewpoint low-dimensional systems are rarely well represented by mean-field theories, which leads one to question the validity of the GP theory in one and two dimensions. In this paper we shall show that, indeed, the physics of dilute Bose systems requires a fundamental modification of the GP theory in low dimensions $d \leq 2$.

The GP theory is a quasiclassical (or mean-field) approximation which replaces the bosonic field operator by a classical order parameter field $\Phi(\mathbf{r}, t)$. For short-ranged interactions the interparticle potential $U(\mathbf{r})$ is replaced by $g\delta^d(\mathbf{r})$, where g is the pseudopotential. Then for a system of bosons of mass m in an external potential V one arrives at the energy functional and the equation of motion for Φ of the following form:

$$F_{\mathrm{GP}} = \int d^d r \left[\frac{\hbar^2}{2m} |\nabla\Phi|^2 + V(\mathbf{r})|\Phi|^2 + \frac{g}{2}|\Phi|^4 \right] \quad (1)$$

and

$$i\hbar\partial_t\Phi = \frac{\delta F_{\mathrm{GP}}}{\delta\Phi^*} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) + g|\Phi|^2 \right]\Phi . \quad (2)$$

The GP equations (1) and (2) are widely used to compute a variety of properties of Bose systems [2].

The GP approximation is a long-wavelength theory relying on the concept of the pseudopotential to account for interparticle interactions. However, for repulsive bosons the canonical pseudopotential vanishes in two dimensions [5], implying that an essential modification of the GP theory is necessary for $d \leq 2$. To see how to modify the theory, it is useful to rewrite the last integrand of (1) in terms of the particle density $n = |\Phi|^2$, so that $(g/2)|\Phi|^4 = (g/2)n^2$. This can be recognized [2,6] as the lowest order term of a dilute expansion of the ground-state energy density for $d > 2$. Thus the correct low-dimensional local density theory will instead have the ground-state energy density of the $d \leq 2$ dilute Bose system [5,6], which is not proportional to n^2.

A rigorous derivation of the form of the energy density appropriate to low dimensionality was given in Ref. [6]; it can be understood as follows. Let us write the interparticle interaction in the form $U(\mathbf{r}) = u_0\delta_a^d(\mathbf{r})$ where u_0 is the amplitude of the interparticle repulsion, and the notation $\delta_a^d(\mathbf{r})$ denotes any well-localized function that transforms into the mathematical Dirac δ function when the range of interaction $a \to 0$. Assume the interparticle interaction is so strong that each particle is localized within a cage formed by its neighbors. In the dilute limit $na^d \ll 1$ the size of this cage can be estimated as $R \sim n^{-1/d}$, the ground-state energy per particle follows from the uncertainty principle as $\hbar^2/mR^2 \sim \hbar^2 n^{2/d}/m$, and the ground-state energy density which would go into the energy functional is given by $\hbar^2 n^{(2+d)/d}/m$. The strong interaction assumption is valid if the interaction energy per particle, estimated as u_0/R^d, is much bigger than the ground-state energy per particle due to the zero-point motion, i.e., $u_0/R^d \gg \hbar^2/mR^2$. This can be justified in the dilute limit $R \to \infty$ below two dimensions, and the condition of the strong coupling limit can then be written as $\hbar^2 n^{(2-d)/d}/mu_0 \ll 1$. To conclude, as space dimensionality decreases, it becomes increasingly harder for the repulsive particles to avoid collisions. Thus the correlations dominate, and for $d \leq 2$ the quartic nonlinearity $|\Phi|^4$ in Eq. (1) should be replaced by $|\Phi|^{2(2+d)/d}$. The effect is strongest in one dimension where we will have a $|\Phi|^6$ interaction.

In one dimension the dilute limit $na \ll 1$ and strong coupling condition $\hbar^2 n/mu_0 \ll 1$ are automatically satisfied for a gas of point, impenetrable bosons ($a = 0$ and $u_0 \to \infty$) which are equivalent to a gas of free fermions [7,8] with energy density $\pi^2\hbar^2 n^3/6m$. Therefore, for the

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practically important case of one dimension, the system of Eqs. (1) and (2) is modified to

$$F = \frac{\hbar^2}{2m}\int dx\left[\left|\frac{d\Phi}{dx}\right|^2 + \frac{2m}{\hbar^2}V(x)|\Phi|^2 + \frac{\pi^2}{3}|\Phi|^6\right] \tag{3}$$

and

$$i\hbar\partial_t\Phi = \frac{\hbar^2}{2m}\left[-\partial_x^2 + \frac{2m}{\hbar^2}V(x) + \pi^2|\Phi|^4\right]\Phi\,. \tag{4}$$

Similarly for the marginal two-dimensional case we are led to the conclusion that in the dilute limit [5,6] a theory replacing the GP approximation starts from the energy functional

$$F = \frac{\hbar^2}{2m}\int d^2r\left[|\nabla\Phi|^2 + \frac{2m}{\hbar^2}V(x)|\Phi|^2 + \frac{4\pi^2}{|\ln(|\Phi|^2a^2)|}|\Phi|^4\right]. \tag{5}$$

Ignoring the logarithmic factor will perhaps suffice for many practical purposes; then (5) is precisely of the GP form. A form similar to (5) has appeared previously [9].

As with the GP approximation, the theory based on Eqs. (3)–(5) plays a role similar to that of hydrodynamics in the theory of fluids. For example, going to the amplitude and phase representation of Eq. (4) we recover the equations of hydrodynamics for an ideal liquid with the density dependence of pressure appropriate to that of dilute bosons in one dimension. This justifies the use of the two-component (complex) order parameter field as the hydrodynamical description requires two fields: density and velocity. The fact that BEC does not occur for $d \leq 2$ in uniform systems [2] is an irrelevant issue as the interactions alone lead to the coherence phenomena which we are describing by a single complex order parameter. For example, the coherence phenomena are well known to exist in one-dimensional quantum liquids [10,11] despite the lack of true BEC. For the uniform ground state the description based on (3) also includes the "harmonic liquid" theory [11], but generally goes beyond it. Because of the boson-fermion equivalence in one dimension [7,11], the theory based on Eqs. (3) and (4) is also applicable to a dilute gas of one-dimensional fermions.

A detailed analytical and numerical study of the one- and two-dimensional cases will be given in a longer publication [12]; hereafter we restrict ourselves to only the salient features of one dimension where the deviations from the GP theory are largest.

Density profiles in external potentials.—The stationary solution to Eq. (4) defined via $\Phi(x,t) = \phi(x)e^{-i\mu t/\hbar}$ can be found by solving

$$\frac{d^2\phi}{dx^2} + \frac{2m}{\hbar^2}[\mu - V(x)]\phi - \pi^2\phi^5 = 0\,, \tag{6}$$

subject to the condition of fixed total particle number $N = \int dx\,\phi^2$ which determines the chemical potential μ. For an external potential that varies slowly on the scale of the interparticle spacing the derivative term in (6) can be ignored: this gives the density profile in the Thomas-Fermi (TF) approximation:

$$n_{\rm TF}(x) = \phi_{\rm TF}^2 = \{2m[\mu - V(x)]\}^{1/2}/\pi\hbar\,, \tag{7}$$

with the density being zero in the classically forbidden region $\mu < V(x)$. For the practically important case of a harmonic trap, $V = m\omega^2x^2/2$, and the density profile is elliptical:

$$n_{\rm TF}(x) = [(2m\mu - m^2\omega^2x^2)]^{1/2}/\pi\hbar\,. \tag{8}$$

The chemical potential is given by $\mu_{\rm TF} = \hbar\omega N$, the density in the center of the trap is $n_{\rm TF}(0) = (2m\hbar\omega N)^{1/2}/\pi\hbar$, and the size of the trapped "condensate" is $2(2\hbar N/m\omega)^{1/2}$.

The accuracy of these predictions can be tested against the exact solution of a dilute system of bosons with repulsive interactions: an ideal candidate being a system of point impenetrable bosons. The boson-fermion equivalence [7] implies that in the many-body system the single-particle energy levels $E_n = \hbar\omega(n + 1/2)$ of the harmonic oscillator are occupied in a fermionic fashion, i.e., with no more than one particle per state. The chemical potential is then given by $\mu = \hbar\omega(N + 1/2)$, which for large N approaches our TF result $\mu_{\rm TF} = \hbar\omega N$. Similarly, the density profile can be computed as a sum of squares of the single-particle wave functions:

$$n(x) = \frac{1}{(\pi l)^{1/2}}\sum_{k=1}^{N-1}\frac{1}{2^k k!}H_k^2(x/l)\exp(-x^2/l^2)\,, \tag{9}$$

where H_k are Hermite polynomials and $l = (\hbar/m\omega)^{1/2}$.

The density distribution (9) is plotted in Fig. 1 where it is compared with (a) the numerical solution of (6) with $V = m\omega^2x^2/2$ and (b) the TF result (8), for different numbers of particles. The main flaw of the theory based on (6) is that it does not reproduce density oscillations due to algebraic ordering of the particles. This is not surprising as (akin to the GP approximation) the discreteness of the particles, which is responsible for the density oscillations, is ignored. Otherwise, the agreement between the approximate and the exact profiles is very good; in the limit of large particle number the differences become imperceptible. These results can be directly tested experimentally; as a comparison we note that the one-dimensional GP theory

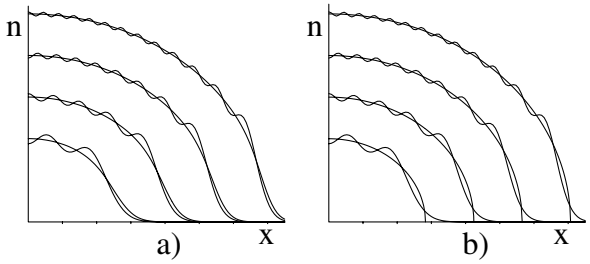

FIG. 1. The density profile (9) plotted for particle numbers $N = 4, 9, 16, 25$ in units $m\omega/\hbar = 1$. The nonoscillating curves correspond to (a) the numerical solution of (6) and (b) the TF result (8).

in the TF approximation predicts [2] $n_{\rm TF} \sim \mu - V(x)$, which is quite distinct from (7), and agrees very poorly with the exact result.

Solitons.—Gray solitons [13] have been recently created and their dynamics was observed in cigar-shaped condensates of ^{87}Rb vapors [14], which makes it important to understand solitonic properties of the system (3) and (4). Let us look for solutions to (4) (with $V = 0$) of the form $\Phi(x,t) = \phi(x,t)e^{-i\mu t/\hbar}$. The function ϕ then obeys the equation

$$i\hbar\partial_t\phi = \frac{\hbar^2}{2m}[-\partial_x^2\phi + \pi^2(|\phi|^4 - \phi_0^4)\phi], \qquad (10)$$

where the chemical potential $\mu = \pi^2\hbar^2\phi_0^4/2m$ is selected so that the particle density $n_0 = \phi_0^2$ is constant at infinity. In dimensionless variables $f = \phi/\phi_0$, $y = \pi n_0 x$, $\tau = \pi^2 n_0^2 \hbar t/m$, Eq. (10) simplifies to

$$2i\partial_\tau f = -\partial_y^2 f + (|f|^4 - 1)f. \qquad (11)$$

We will be looking for a localized traveling wave solution [15] to (11) of the form $f(y,\tau) = f(y - \beta\tau)$ where the dimensionless velocity β is measured in units of the sound velocity $c = \pi\hbar n_0/m$. This problem can be solved exactly. The results are conveniently described in terms of the amplitude A and phase θ of the dimensionless order parameter $f = Ae^{i\theta}$:

$$A^2 = 1 - \frac{3(1-\beta^2)}{2 + (1+3\beta^2)^{1/2}\cosh[2(1-\beta^2)^{1/2}(y-\beta\tau)]}$$
$$2\theta = \cos^{-1}\left[\frac{(3\beta^2/A^2) - 1}{(1+3\beta^2)^{1/2}}\right]. \qquad (12)$$

The spatial behavior given by (12) is shown in Fig. 2.

The amplitude in (12) describes a moving depression (particle deficit) with the minimal value at the soliton center given by $A^2(0) = (1+3\beta^2)^{1/2} - 1$. The soliton exists only for $\beta < 1$ (i.e., the soliton velocity cannot exceed the speed of sound); for $\beta = 1$ Eq. (12) gives the uniform result $A^2 = 1$. On the other hand, for $\beta = 0$ (i.e., a vortex, or dark soliton [13]) the minimal value of the amplitude at the soliton center drops to zero.

The phase expressed in (12) varies rapidly in the vicinity of the amplitude dip, staying approximately constant far away from it. The total phase shift across the soliton can be found as $\Delta\theta = \cos^{-1}[(3\beta^2 - 1)/(1+3\beta^2)^{1/2}]$. It is a continuous function of the soliton velocity varying between $-\pi$ (when $\beta = 0$) and zero (when $\beta = 1$). Antisolitons may be defined as having opposite signs of $d\theta/dy$, and there are no constraints on $\Delta\theta$ for the open line or ring geometries (provided the number of solitons matches the number of antisolitons). However, if there is an imbalance of solitons and antisolitons in the ring geometry, then the uniqueness of the order parameter $f(y,\tau)$ implies that $\Delta\theta$ is a fraction of 2π for any excess soliton; this will in turn mean that the excess soliton velocity is *quantized.*

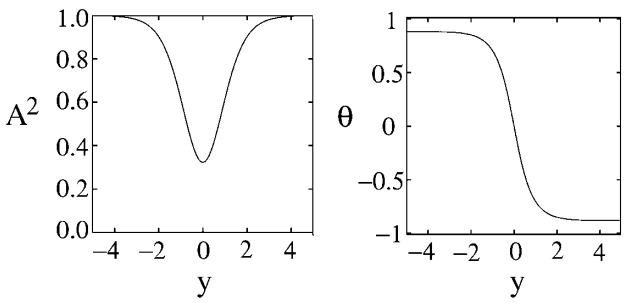

FIG. 2. The density A^2 and the phase θ, for the moving soliton Eq. (12) with $\beta = 1/2$.

The solution (12) bears some similarity with the one-dimensional soliton of the GP theory [13]; the main qualitative difference (seen after recovering the original units) is that in the dilute limit the soliton size is of order $1/(1-\beta^2)^{1/2}n_0$ *independent* of the amplitude of the interparticle repulsion [16].

General methods [13] can be used to compute the soliton energy E and momentum P. For their dimensionless counterparts $\epsilon = 2mE/\pi^2\hbar^2 n_0^2$ and $\mathcal{P} = P/\pi\hbar n_0$ we find

$$\epsilon = \frac{\sqrt{3}}{\pi}(1-\beta^2)\ln\left\{\frac{2 + [3(1-\beta^2)]^{1/2}}{(1+3\beta^2)^{1/2}}\right\},$$
$$\mathcal{P} = -\frac{\beta}{(1-\beta^2)}\epsilon + \frac{1}{\pi}\cos^{-1}\left[\frac{3\beta^2 - 1}{(1+3\beta^2)^{1/2}}\right]. \qquad (13)$$

The dependencies $\epsilon(\beta)$ and $\mathcal{P}(\beta)$ parametrically define the soliton dispersion law $\epsilon(\mathcal{P})$ which should be identified [17] with the "hole" branch of the elementary excitations spectrum [18].

To assess the accuracy of $\epsilon(\mathcal{P})$ given in (13) we compare it with the exact result of Lieb [18] for the system of δ-interacting bosons in the dilute limit $\hbar^2 n/mu_0 \ll 1$: $\epsilon_{\rm exact}(\mathcal{P}) = 2|\mathcal{P}| - \mathcal{P}^2$, for $|\mathcal{P}| \le 1$. Since the velocity β in (13) varies between zero and unity, the momentum (which we choose to be positive) computed from (13) varies between unity and zero in correspondence with the exact result. It is straightforward to show that for $\mathcal{P} \ll 1$ the elimination of β in (13) leads to $\epsilon = 2\mathcal{P}$, which is again in agreement with the exact result. The behavior $\epsilon(\mathcal{P})$ implied by (13) in the vicinity of the end point of the spectrum $\mathcal{P} = 1$ is qualitatively similar, and quantitatively close to the exact dependence. To illustrate these statements we have plotted the dispersion law (13) in Fig. 3 against the exact result.

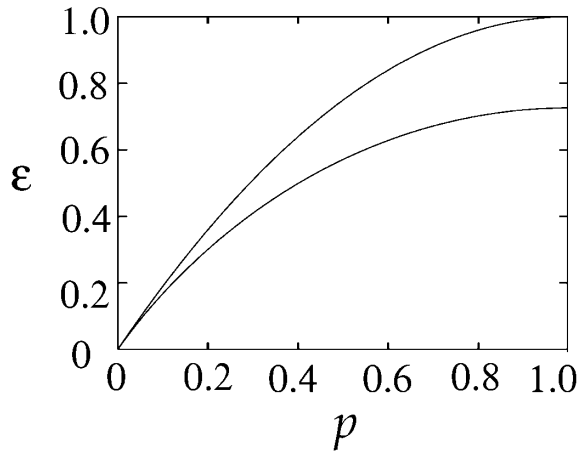

FIG. 3. The spectrum parametrized by (13) (lower curve) compared to the exact result of Lieb (upper curve).

Superflow.—The dimensionless current density is given by $j = A^2\partial_y\theta$, and below we look for solutions with fixed given current j (i.e., the steady state) and $\partial_\tau A = \partial_\tau\theta = 0$. Substituting $f = Ae^{i\theta}$ and $j = A^2 d\theta/dy$ into (11), and imposing fixed chemical potential, we find

$$\frac{d^2A}{dy^2} = \frac{j^2}{A^3} + A^5 - A\,. \tag{14}$$

In the spatially uniform state $\frac{d^2A}{dy^2} = 0$, and one finds the dimensionless amplitude $A_\infty^4 = [1 + (1 - 4j^2)^{1/2}]/2$, which implies that superflow *reduces* the amplitude of the order parameter. The uniform solution and thus superfluidity cease to exist above the critical flow $j_c = 1/2$ when the amplitude drops down to its minimal value $A_\infty^c = 2^{-1/4}$. These results imply that the critical velocity for superfluidity in the original units is $c/\sqrt{2}$.

Equation (14) also has an immobile well-localized solution in the form of a dip of the order parameter; far away from the dip the amplitude recovers to its uniform value. The dip solution is closely related to the soliton previously discussed. Indeed, in the reference frame moving with the flow, the dip solution is moving and thus is identical to a soliton. The functional form of the dip can be deduced from (12) by replacing β by j/A_∞^4, A by A/A_∞, and $(y - \beta\tau)$ by yA_∞^2. The dip solution disappears altogether for $j > j_c$.

Self-similar solutions.—The results derived so far have their counterparts in the context of the one-dimensional GP approximation. However, the theory based on Eqs. (3) and (4) allows self-similar solutions (even in the presence of an external harmonic potential) which do not exist in the one-dimensional GP theory [19]. Unfortunately, we have no space here to enter into details of the analysis.

We have performed direct numerical integration of the nonlinear equation (4), and have confirmed the existence of both the similarity solutions and the moving trains of solitons with quantized velocity, with amplitude and phase as given by (12). More details will be given in a future publication [12].

In conclusion, we have presented a new continuum description of dilute Bose liquids appropriate for low dimensional systems. This description goes beyond the mean-field approximation implicit in the GP theory. It is our hope that the results we have derived from our theory will be testable in BEC experiments in the near future.

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