Crossover from One to Three Dimensions for a Gas of Hard-Core Bosons

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We develop a variational theory of the crossover from the one-dimensional (1D) regime to the 3D regime for ultracold Bose gases in thin waveguides. Within the 1D regime we map out the parameter space for fermionization, which may span the full 1D regime for suitable transverse confinement.

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It has recently been proved by Lieb and Seiringer [1] that in a suitably defined dilute limit, the many-body ground state of a trapped ultracold gas of bosons in two or three dimensions exhibits Bose-Einstein condensation into that orbital which minimizes the Gross-Pitaevskii (GP) energy functional, and, in fact, that the condensation is *complete* in the sense that the condensed fraction is unity. Their work should be consulted for precise definitions and hypotheses required for the proof; here we reiterate only a few points relevant here. In the 3D case the dilute limit is defined as $a \to 0$ and $N \to \infty$ with both the trap potential and Na fixed where a is the s-wave scattering length and N the number of particles, and in the 2D case it is defined as $a \to 0$ and $N \to \infty$ with the trap potential and $N/|\ln(a^2N)|$ fixed. They point out that in 1D their proof fails, where there is presumably no Bose-Einstein condensate (BEC) even at zero temperature (many-body ground state). In fact, the exact many-body ground state of a *spatially uniform* (untrapped) 1D Bose gas with repulsive zero-range (delta function) interaction was found long ago by Lieb and Liniger (LL) [2] for all values of a 1D coupling constant g_{1D}, and was shown by them to reduce for $g_{1D} \to \infty$ to the exact many-body ground state of the impenetrable point Bose gas ("Tonks gas") found previously by one of us [3], for which Lenard proved rigorously [4] that the occupation of the lowest orbital is bounded above by const $\times \sqrt{N}$, ruling out BEC (occupation proportional to N). In the case of a *trapped* Tonks gas no such rigorous bound is known, but our numerical evaluation of the largest eigenvalue of the reduced single-particle density matrix of our exact many-body ground state [5] suggests strongly that the most highly occupied orbital has occupation behaving like N^p with $0 < p < 1$, again indicating absence of true BEC. In what follows we will use the term 1D condensate to describe the ground state of the trapped gas when the system is still 1D, in that it has the transverse profile of the trap ground state, but the energy has deviated below that for an impenetrable Tonks gas.

It is clear from the above discussion that for real atom waveguides, for which the idealized limits $a \to 0$ and $N \to \infty$ do not strictly apply, a crossover must occur from an effectively 1D system, applicable when the waveguide is so long and narrow (high transverse frequency) that transverse excitations are frozen, to a 3D system with BEC accurately treated by the GP equation (weaker transverse binding), the basis of most theoretical work on trapped BECs. Detailed analysis of this crossover is important for comparison with experiments, since the 1D regime has already been achieved experimentally [6–9] and the Tonks regime (1D *and* sufficiently large g_{1D}) is being approached [9]. The dynamical reduction from 3D to 1D and precise conditions on parameters necessary for achievement of both the 1D limit and the Tonks-gas limit of the 1D regime have been discussed in detail by Olshanii [10] and by Petrov *et al.* [11]. In addition, Dunjko *et al.* [12] have investigated the crossover between the Thomas-Fermi and Tonks-Girardeau regimes in a 1D trap. Here we note only that the 1D regime occurs when the waveguide is so thin (transverse frequency so high) and density and temperature so low that the longitudinal thermal and zero-point energies are both low compared with the lowest transverse excitation energy, resulting in "freezing out" all transverse excitations. The Tonks limit requires, in addition, that the scattering length a is large enough and/or 1D density n low enough that $\hbar^2 n/mg_{1D} \ll 1$ where the effective 1D coupling constant is $g_{1D} = 2\hbar^2 a/m\ell_0^2$ and $\ell_0 = \sqrt{\hbar/m\omega_0}$ is the transverse oscillator length.

Trap geometry.—A convenient geometry for discussing the crossover is a toroidal trap of high aspect ratio $R = L/\ell_0$. The transverse trap potential is symmetric about a circular axis on which the trap potential is minimum, and harmonic with respect to a coordinate ρ measured transversely with respect to this circle. This geometry can equally well be interpreted as an infinitely long, straight cylindrical waveguide with periodic boundary conditions in the longitudinal direction. Such toroidal traps have been experimentally produced and loaded [13,14].

Hamiltonian.—We use a many-body Hamiltonian with harmonic transverse binding and the usual Fermi pseudopotential interaction $v(\mathbf{r}_{ij}) = 4\pi a\delta(\mathbf{r}_{ij})$ with a positive s-wave scattering length a. This leads to a well-defined problem in 1D, the LL model [2]. Our toroidal system is "almost 1D" since the transverse dimensions are confined, and we find that the variational problem with the Fermi pseudopotential does not encounter the difficulties (divergences and poorly posed variational problem) [15,16] found in the 3D case. The Hamiltonian is then

$$\hat{H} = \sum_{j=1}^{N}\left(-\frac{\hbar^2}{2m}\nabla_j^2 + \frac{1}{2}m\omega_0^2\rho_j^2\right) + g_{3D}\sum_{1\le j<\ell\le N}\delta(\mathbf{r}_j - \mathbf{r}_\ell), \quad (1)$$

where $g_{3D} = 4\pi a\hbar^2/m$ is the 3D coupling constant. The Laplacian is to be expressed in cylindrical coordinates $\mathbf{r}_j = (z_j, \rho_j, \theta_j)$ where z_j, with $0 \le z_j \le L$, is a 1D coordinate measured around the torus circumference, and ρ_j is the transverse radial coordinate and θ_j the azimuthal angle measured from the central torus axis.

Variational ground state.—We use a trial variational ground state which assumes factorization of longitudinal and transverse parts, with the transverse part depending on a single orbital ϕ_{tr} independent of azimuthal angle:

$$\Phi_0(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \Phi_{\rm long}(z_1, \ldots, z_N)\prod_{j=1}^{N}\phi_{tr}(\rho_j). \quad (2)$$

The factorization of the coordinate dependencies and use of a single transverse orbital are legitimate variational ansatzes as shown in a recent study [17] of anisotropic BEC where similar trial functions led to results in agreement with experiment in regimes ranging from 3D to effective 1D. Single transverse orbital description is obvious in the two limits: (a) tight transverse confinement, transverse excitations frozen, ϕ_{tr} is the unperturbed transverse oscillator ground state; (b) weak transverse confinement and low density, ϕ_{tr} is the transverse part of GP orbital. More generally, we leave the functional form of ϕ_{tr} free, to be determined as part of the minimization of the variational ground state energy $E_0 = \langle\Phi_0|\hat{H}|\Phi_0\rangle$. Assuming ϕ_{tr} and $\Phi_{\rm long}$ normalized according to

$$\begin{aligned}&\int_0^\infty 2\pi\rho d\rho|\phi_{tr}(\rho)|^2 = 1\\ &\int_0^L dz_1\cdots\int_0^L dz_N|\Phi_{\rm long}(z_1,\ldots,z_N)|^2 = 1\end{aligned} \quad (3)$$

one finds that the energy expectation value of Φ_0 decomposes as $E_0 = N\epsilon_{tr} + E_{\rm long}$ with

$$\begin{aligned}\epsilon_{tr} &= \int_0^\infty 2\pi\rho d\rho\phi_{tr}^*\left(\frac{-\hbar^2}{2m\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} + \frac{1}{2}m\omega_0^2\rho^2\right)\phi_{tr}\\ E_{\rm long} &= \int_0^L dz_1\cdots\int_0^L dz_N\Phi_{\rm long}^*\hat{H}_{\rm long}\Phi_{\rm long}\end{aligned} \quad (4)$$

where $\hat{H}_{\rm long}$ is an effective longitudinal Hamiltonian

$$\hat{H}_{\rm long} = \sum_{j=1}^{N}\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial z_j^2} + g_{1D}\sum_{1\le j<\ell\le N}\delta(z_j - z_\ell) \quad (5)$$

and g_{1D} is an effective 1D coupling constant

$$g_{1D}[\phi_{tr}] = g_{3D}\int_0^\infty 2\pi\rho d\rho|\phi_{tr}(\rho)|^4. \quad (6)$$

Note that the separation of transverse and longitudinal energies is only partial, since g_{1D} depends on ϕ_{tr}. We take the value of the g_{1D} corresponding to the transverse ground state, with oscillator length ℓ_0, as a reference

$$g = g_{1D}\left[\frac{1}{\sqrt{\pi}\ell_0}e^{-\rho^2/2\ell_0^2}\right] = \frac{g_{3D}}{2\pi\ell_0^2} \quad (7)$$

and define the fractional 1D coupling constant $\bar{g}_{1D} = g_{1D}/g$. For a 1D system $\bar{g}_{1D} = 1$, whereas it decreases as the system crosses over to 3D. The relevant dimensionless intensive variable of a 1D system $\gamma = mg_{1D}/\hbar^2 n$ [2] suggests a dimensionless measure $\bar{n} = \hbar^2 n/mg$ of the linear density $n = N/L$. We should keep in mind that $g \propto \omega_0$ and will vary as the transverse confinement changes.

The total energy E_0 is to be minimized with respect to variation of both ϕ_{tr} and $\Phi_{\rm long}$ subject to the normalization constraints. We do this in two steps, first holding ϕ_{tr} constant and minimizing $E_{\rm long}$ with respect to $\Phi_{\rm long}(z_1, \ldots, z_N)$, then minimizing the resultant E_0 with respect to $\phi_{tr}(\rho)$. For fixed ϕ_{tr}, hence fixed g_{1D}, the global minimum of $E_{\rm long}$ is realized by the exact ground state of $\hat{H}_{\rm long}$, which is the well-known LL Bethe ansatz solution [2]. One may instead use some simpler variational trial state for $\Phi_{\rm long}$, obtaining an upper bound to the longitudinal energy $E_{\rm long} = N\epsilon_{\rm long}$. This has then to be minimized with respect to variation of ϕ_{tr} subject to the normalization constraint:

$$\frac{\delta\epsilon_{tr}}{\delta\phi_{tr}^*(\rho)} + \frac{\partial\epsilon_{\rm long}}{\partial g_{1D}}\frac{\delta g_{1D}}{\delta\phi_{tr}^*(\rho)} - \mu_{tr}2\pi\rho\phi_{tr}(\rho) = 0, \quad (8)$$

where the transverse chemical potential μ_{tr} is the Lagrange multiplier for the transverse normalization constraint. Evaluation of the functional derivatives leads to the following generalized transverse GP equation:

$$\begin{aligned}\mu_{tr}\phi_{tr} = &-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho}\right)\phi_{tr} + \frac{1}{2}m\omega_0^2\rho^2\phi_{tr}\\ &+ 2g_{3D}\frac{\partial\epsilon_{\rm long}}{\partial g_{1D}}|\phi_{tr}|^2\phi_{tr},\end{aligned} \quad (9)$$

where μ_{tr} is to be adjusted so that ϕ_{tr} satisfies the normalization constraint. The solution depends on g_{1D} which in turn depends on ϕ_{tr}, so the solution has to be determined by a self-consistent iterative procedure, by making an initial guess for g_{1D}, evaluating $\partial\epsilon_{\rm long}/\partial g_{1D}$ at this value of g_{1D}, solving Eq. (8) for ϕ_{tr}, determining a new g_{1D} from Eq. (6), and iterating to convergence.

Two of us have previously developed a variational theory [18] assuming the same toroidal geometry and using a variational trial state for $\Phi_{\rm long}$ based on the variational pair theory of many-boson systems [19]. In that case the transverse GP equation (8) reduces to the previous one, Eq. (16) of [18], after correction of a typo therein [20]. That work was devoted to investigation of the BEC-Tonks crossover in the 1D regime where the transverse orbital is frozen in the unperturbed transverse oscillator state, and no transverse GP equation was solved. Here we are concerned with a different crossover, namely, the 1D-3D crossover, which depends crucially on the solution of the transverse GP equation. In the following two sections we shall separately consider first the case where $\Phi_{\rm long}$ is approximated by the Girardeau-Arnowitt (GA) variational pair theory [19] as in [18], which gives accurate results except in the Tonks-gas regime (1D limit *and* very large scattering length). Then we shall work out the solution using the LL theory [2], the exact ground state of $\hat{H}_{\rm long}$. This latter is accurate even in the Tonks regime, but is more complicated to work out since the LL energy per particle $\epsilon_{\rm LL}$ is known only from numerical solutions of the nonlinear LL integral equation.

Pair theory solution.—Approximating the longitudinal energy by the 1D GA pair theory energy, we will first set $\epsilon_{\rm long} = \epsilon_P$, the expression which we derived in Ref. [18] and can be written as

$$\frac{\hbar^2}{m}\frac{\epsilon_P}{g^2} = \bar{g}_{\rm 1D}^2\Big[\frac{1}{2\gamma} - \frac{1}{3\pi}\sqrt{\frac{f^3}{\gamma}}[(2-\lambda)E - \lambda K] + \frac{f}{8\pi^2}\{(1-\lambda)^2K^2 + [(1+\lambda)K - 2E]^2\}\Big]. \tag{10}$$

Here $K(1-\lambda)$ and $E(1-\lambda)$ are complete elliptic integrals [21] and f is the Bose-condensed fraction related to the dimensionless pair theory parameter λ through the coupled equations

$$\lambda = \sqrt{\frac{\gamma}{f}}\frac{[(1-\lambda)K]}{2\pi}; \qquad \frac{1-f}{f} = \sqrt{\frac{\gamma}{f}}\frac{[(1+\lambda)K - 2E]}{2\pi}. \tag{11}$$

The partial derivative of the pair theory energy has to be taken *before minimization* [18] rather than that of the expression in Eq. (10) which is true only at the minimum

$$\frac{\partial \epsilon_P}{\partial g_{\rm 1D}} = \frac{n}{2}[2 - f^2 - 2\lambda f^2 + \lambda^2 f^2]. \tag{12}$$

LL solution.—Next we shall use the LL energy $\epsilon_{\rm LL}$ [2], which is the global minimum of $\epsilon_{\rm long}$ with respect to unrestricted functional variation of $\Phi_{\rm long}$. It yields, together with Eq. (8), the best possible variational solution obtainable with a trial state of form (2):

$$\frac{\hbar^2}{m}\frac{\epsilon_{\rm LL}}{g^2} = \frac{\bar{g}_{\rm 1D}^2}{2\gamma^2}e(\gamma), \tag{13}$$

where $e(\gamma)$ is obtained by solving the Lieb-Liniger system of integral equations [2]. The partial derivative

$$\frac{\partial \epsilon_{\rm LL}}{\partial g_{\rm 1D}} = \frac{\hbar^2}{2m}n^2 e'(\gamma)\frac{m}{\hbar^2 n} = \frac{n}{2}e'(\gamma) \tag{14}$$

is the same regardless of the order in which the expectation and the derivative are evaluated, unlike in pair theory since the LL solution is an exact eigenstate of $\hat{H}_{\rm long}$ and thus obeys the Hellmann-Feynman theorem.

Numerical results and discussion.—For both pair theory and Lieb-Liniger theory, the transverse GP equation was solved numerically using the method of discrete variable representation [22], a method based on Gauss quadrature with a well-defined discrete normalization. Iterating the solution of the GP equation alternately with the evaluation of the longitudinal energies lead to self-consistent values for $g_{\rm 1D}$ and $\epsilon_{\rm long}$ in both theories. In using LL theory we used the tabulated values of $e(\gamma)$ in [23] for intermediate values of γ and the limiting expressions in [2] for high and low values of γ. For low γ, i.e., for high linear densities, the energies in both pair theory and LL theory coincide with the Bogoliubov energy $ng_{\rm 1D}/2$.

In the Tonks limit of completely impenetrable bosons, all of the atoms are "fermionized" and the energy per atom is simply the energy of free fermions,

$$\frac{\hbar^2}{m}\frac{\epsilon_F}{g^2} = \frac{\pi^2\bar{n}^2}{6}. \tag{15}$$

We can get a sense of the degree of "fermionization" of the system by evaluating the ratio $\epsilon_{\rm LL}/\epsilon_F$. In the Tonks limit this would be unity, but as the atoms become penetrable the energy approaches a linear dependence on the density so that the ratio will approach zero. In Fig. 1 we plot this ratio (for LL theory) as a function of the density $\bar{n}$ for different values of the dimensionless quantity $mg^2/\hbar^3\omega_0$ proportional to the transverse trapping frequency ω_0. In the same figure we also plot $\bar{g}_{\rm 1D} = g_{\rm 1D}/g$ as function of $\bar{n}$. While the plot of $\epsilon_{\rm long}/\epsilon_F$ gives a measure of the impenetrability of the atoms, the plot of $\bar{g}_{\rm 1D}$ provides a measure of the dimensionality, since $\bar{g}_{\rm 1D} = 1$ in 1D and decreases as the system crosses over to 3D. Since g depends linearly on ω_0 the actual magnitudes of the densities are different in the three plots shown in Fig. 1. Along the right axis in Fig. 1 we plot the scaled longitudinal energies computed from pair theory and LL theory. We see that the density range where the pair theory energies deviate from the LL energies corresponds closely to the region where $\epsilon_{\rm long}/\epsilon_F$ starts to deviate from unity. This is to be expected since pair theory cannot describe the Tonks regime.

We see that for low values of the transverse trapping potential as in Fig. 1(a) there is a regime of density where the gas is one dimensional but not yet a Tonks gas. Pair theory is valid in this region, and it intrinsically allows for a "Bose-condensed" fraction f which has the more general interpretation as the nontrivial fraction of atoms in the ground state. Thus in this regime we should see a 1D condensate, in the sense defined earlier. However, as we increase the transverse trapping potential we see that the region where such a 1D condensate can exist gets narrower as the curve for $\bar{g}_{\rm 1D}$ approaches the curve for $\epsilon_{\rm long}/\epsilon_F$ until the former is on the left of the latter as we see in Fig. 1(c); this means that for large transverse trapping potentials there will never be a 1D condensate and the system will pass directly from 3D to the impenetrable Tonks-gas regime. This is clearly illustrated in Fig. 2; using $\bar{g}_{\rm 1D} = 0.5$ as the criterion for crossover from 1D to 3D and $\epsilon_{\rm long}/\epsilon_F = 0.5$ as the criterion for crossover to the Tonks gas, we plot the scaled densities at the crossover points as a function of the transverse confinement strength measured by $mg^2/\hbar^3\omega_0$. The triangular region between the two

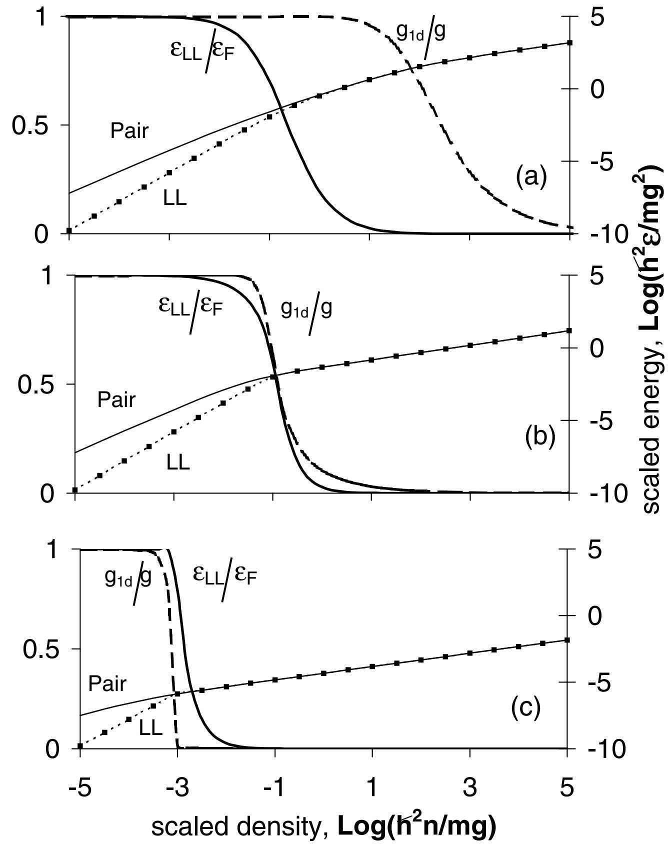

FIG. 1. Left axis: ratios $\epsilon_{\mathrm{LL}}/\epsilon_F$ and $g_{1\mathrm{D}}/g$. Horizontal axis: logarithm of scaled linear density $\bar{n} = \hbar^2 n/mg$. Right axis: logarithms of scaled energies calculated according to pair theory \hbar2ϵP/mg2 and Lieb-Liniger theory $\hbar^2\epsilon_{\mathrm{LL}}/mg^2$. The plots are shown for three different strengths of the transverse trap frequencies ω_0 directly proportional to the value of the dimensionless quantity as follows: (a) $\mathrm{mg}^2/\hbar^3\omega_0 = 10^{-2}$, (b) $\mathrm{mg}^2/\hbar^3\omega_0 = 10^2$, and (c) $\mathrm{mg}^2/\hbar^3\omega_0 = 10^8$. Note that the scale of actual linear densities n differs in the three plots since g is different for each plot.

curves on the left of their point of intersection roughly defines the range of scaled densities and transverse trap frequencies over which a 1D condensate can exist. On the right of the point of intersection the trap strength is too high.

In conclusion, we have used Lieb-Liniger theory as well as pair theory to study the crossover of an axially homogeneous 3D Bose-condensed system to effective 1D and eventually to an impenetrable regime. We have evaluated the densities at which the system crosses over from 3D to 1D and then to a Tonks gas for different transverse trap frequencies. We have demonstrated that for weak transverse confinement there is a physically allowed regime where a 1D axially homogeneous condensate can exist, while for sufficiently high transverse confinement the only possibilities are a 3D condensate or a Tonks gas.

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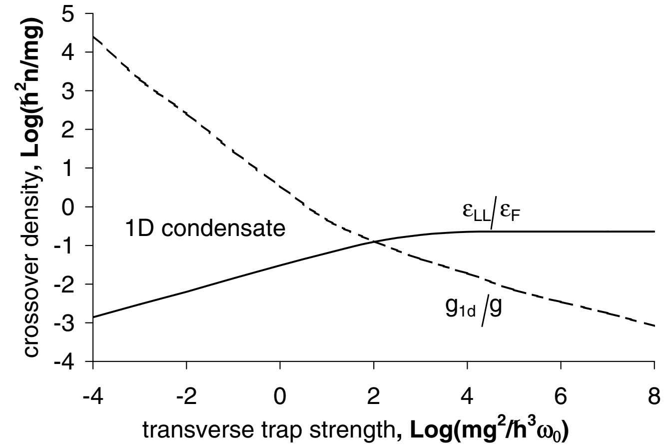

FIG. 2. Log-log plots of scaled linear densities $\hbar^2 n/mg$ versus transverse confinement strength $mg^2/\hbar^3\omega_0$ at the BEC-Tonks crossover points defined by $\epsilon_{\mathrm{long}}/\epsilon_F = 0.5$ and at the 1D-3D crossover points defined by $g_{1\mathrm{D}}/g = 0.5$

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