Bose-Fermi variational theory of the BEC-Tonks crossover

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A number-conserving hybrid Bose-Fermi variational theory is developed and applied to investigation of the BEC-Tonks gas crossover in toroidal and long cylindrical traps of high aspect ratio, where strong many-body correlations and condensate depletion occur.

The many-body ground state of a trapped atomic vapor Bose-Einstein condensate (BEC) is described in first approximation by Gross-Pitaevskii (GP) theory and in the next approximation by Bogoliubov theory or time-dependent GP theory. These fail if the condensate is appreciably depleted, as is the case near the BEC condensation temperature, or even at $T = 0$ for sufficiently thin wave guides, low densities, and large scattering lengths. An extreme limiting case of this, the “Tonks gas” where transverse excitations are frozen, the dynamics reduces to one-dimensional (1D) motion, BEC disappears, and the occupation $N_0$ of the lowest orbital behaves like $N^p$ with $p < 1$, can be treated exactly by the Fermi-Bose mapping method. The behavior of the BEC-Tonks crossover is of considerable interest since experiments are now approaching the Tonks regime.

An approximate theory in a strictly 1D model, the Lieb-Liniger (LL) delta-function Bose gas in a harmonic trap, has been given recently by Dunjko, Lorent, and Olshanii. It is unclear how to extend their approach to 3D as it is rooted in the 1D LL model. The condensed fraction $N_0/N$ is expected to be small for narrow waveguides due to the above-described $N^p$ behavior of $N_0$. Variational approaches such as Hartree-Fock-Bogoliubov (HFB) theory or its forerunner, the variational pair theory or Girardeau-Arnovitt (GA) theory of many-boson systems, suggest themselves here. Here we generalize the GA theory so as to treat the gradual onset of “fermionization” as the Tonks limit is approached and apply it to the theory of the BEC-Tonks crossover. We also illustrate how the theory can be extended to 3D by allowing for variable transverse confinement.

Number-conserving pair theory: The most general Bose pairing state involves excitation of pairs to arbitrary excited (uncondensed) states $(n,m)$ by repeated application of pair excitation operators $\hat{a}^\dagger_n \hat{a}^\dagger_m \hat{a}_0^2$ to the completely condensed $N$-particle state $|N\rangle = (N!)^{-1/2} (\hat{a}^\dagger_0)^N |0\rangle$. Here we employ a number-conserving formulation and define unitary condensate annihilation and creation operators $\hat{\beta}_0 = (\hat{N}_0 + 1)^{-1/2} \hat{a}_0$ and $\hat{\beta}_0^\dagger = \hat{a}_0^\dagger (\hat{N}_0 + 1)^{-1/2}$ which commute with each other and with all annihilation and creation operators $\hat{a}_n$ and $\hat{a}_n^\dagger$ for noncondensed atoms ($n \neq 0$); here $\hat{N}_0 = \hat{a}_0^\dagger \hat{a}_0$. Then the number-conserving generalized pair creation operator is $\hat{a}_n^\dagger \hat{a}_m^\dagger \hat{\beta}_0^2$. In the case of a sufficiently symmetrical trap the general pairing state can be reduced to a $\pm k$ pairing form

$$|\Phi_0\rangle = \text{const.} e^{-\hat{F} |N\rangle} , \quad \hat{F} = \frac{1}{2} \sum_{k \neq 0} \Delta_k \hat{a}_k^\dagger \hat{a}^\dagger_{-k} \hat{\beta}_0^2 .$$

by a suitable choice of orbitals $u_k$ where $u_{-k}$ denotes the time reversal conjugate of $u_k$ and $\Delta_k$ is real and even. This state is the vacuum of number-conserving Bose and Fermi quasiparticle annihilation operators.

$$\hat{\xi}_k = (1 - \Delta_k^2)^{-1/2} \hat{\beta}_0 \hat{a}_k + \Delta_k \hat{a}^\dagger_{-k} \hat{\beta}_0^\dagger , \quad k \neq 0 ,$$

and the general pairing state can be written as $|\Phi_0\rangle = \hat{U} |N\rangle$ where $\hat{U}^{-1} \hat{\xi}_k \hat{U} = \hat{a}_k$.

Toroidal and long cylindrical geometries: A convenient geometry for discussing the crossover is a toroidal trap of high aspect ratio $R = L/l_0$ where $L$ is the toroid circumference and $l_0$ the transverse oscillator length $l_0 = \sqrt{\hbar/m \omega_0}$ with $\omega_0$ the frequency of transverse oscillations, assumed to be harmonic. The transverse trap potential is assumed to be symmetric about an axis consisting of a circle on which the trap potential is minimum. The longitudinal (circumferential) motion can be described by a 1D coordinate $x$ in terms of plane-wave orbitals $\phi_k(x) = L^{-1/2} e^{ikx}$ satisfying periodic boundary conditions with periodicity length $L$, with allowed longitudinal quantum numbers $k_j = 2\pi n_j/L$ with $n_j = 0, \pm 1, \pm 2, \ldots$. The corresponding 3D orbitals are taken to be $u_k(x) = \phi_k(x) \phi_{\ell z} (\rho)$ where $\rho$ is a transverse radial coordinate measured from the central circle of the toroid; these are cylindrical coordinates with cylinder axis bent into a circle of circumference $L$. This geometry can equally well be interpreted as an infinitely long, straight cylindrical waveguide with periodic boundary conditions in the longitudinal direction. The creation operators in the variational trial state $|\Phi_0\rangle$ refer to the 3D orbitals $u_k(x)$. Use of a single transverse orbital is justified both in the Tonks limit, where transverse excitations are absent, and in the GP limit, where BEC is almost complete.

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and there is a single orbital determined by the GP equation.

**Intertatomic interaction:** We use the usual Fermi pseudopotential \( v(r_{ij}) = 4\pi a \left( h^2 / m \right) \delta(r_{ij}) \) and assume that the s-wave scattering length \( a \) is positive. This leads to a well-defined problem in 1D, the LL model \[4\]. 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) \[10,24\] found in the 3D case. A gapless theory with more complicated pseudopotential, e.g. \[21\], is not warranted here since we are concerned with the ground state, collective phonon excitations of the GA theory are gapless \[24,22\], and the quasiparticle gap removes an unphysical low-momentum divergence in the 1D Bogoliubov theory.

**Pair Hamiltonian:** The second-quantized many-boson Hamiltonian with units \( \hbar = m = 1 \) is

\[
\hat{H} = \sum_k \epsilon_k \hat{a}_k\hat{a}_k + \frac{g}{2L} \sum_{q,k,k'} \hat{a}_{k+q}^\dagger \hat{a}_{k'}^\dagger \hat{a}_{k'}^\dagger \hat{a}_k,
\]

where with single particle energy \( \epsilon_k = (k^2/2) + \epsilon_{tr} \), transverse mode energy

\[
\epsilon_{tr} = \int_0^\infty \phi_{tr}^* \left( -\frac{1}{2}\frac{\partial}{\partial \rho} \rho \frac{\partial}{\partial \rho} + \omega^2 \right) \phi_{tr} 2\pi\rho d\rho,
\]

where the transverse orbital is normalized according to \( \int_0^\infty \phi_{tr}^* (\rho)^2 2\pi\rho d\rho = 1 \), and interaction matrix element \( g = 4\pi a \int_0^\infty \phi_{tr}^* (\rho)^2 2\pi\rho d\rho \). The only interaction terms with nonzero expectation value in the state \( |\Phi_0\rangle \) are those expressible in terms of momentum occupation number operators \( \hat{N}_k = \hat{a}_k^\dagger \hat{a}_k \) and pair operators \( \hat{a}_{-k} \hat{a}_k \) and \( \hat{a}_k^\dagger \hat{a}_{-k}^\dagger \), and of those the transverse terms and the interaction terms with \( q = 0 \) sum to \( \epsilon_{tr} \hat{N} + (g/2L) \hat{N}(\hat{N} - 1) \) where \( \hat{N} = \sum_k \hat{N}_k \) is the total particle number operator. Replacing this operator by its eigenvalue \( N \), one obtains a pair Hamiltonian \[14\]

\[
\hat{H}_P = \epsilon_{tr} \hat{N} + (g/2L)N(N - 1) + \sum_{k \neq 0} [(k^2/2) + (g/L)\hat{N}_0] \hat{N}_k
+ \frac{g}{2L} \sum_{k \neq 0} \{ |\hat{N}_0(\hat{N}_0 - 1)|^{1/2} \hat{\beta}_0^\dagger \hat{\beta}_0^\dagger \hat{a}_{-k} \hat{a}_k + \mathrm{h.c.} \}
+ \frac{g}{2L} \sum_{k \neq 0} \{ \hat{N}_k \hat{N}_{k'}
+ (1 - \delta_{kk'}) - (\delta_{k,-k}) \hat{a}_k^\dagger \hat{a}_{-k}^\dagger \hat{a}_{-k'} \hat{a}_k',
\]

whose expectation value in the state \( |\Phi_0\rangle \) is identical with that of the full Hamiltonian \( \hat{H} \).

**Bogoliubov theory:** In the case of a untrapped 3D system the Bogoliubov theory is valid at low densities. In the opposite limit of a strictly 1D system with delta-function interaction (LL model), the Bogoliubov theory reproduces the leading terms in the exact ground state energy in the limit of high densities \[4\]. However, the Bogoliubov theory is not fully consistent either in the strictly 1D case or in our geometry: We find a Bogoliubov quasiparticle energy \( \omega_k = |k| \sqrt{n_0g + k^2/4} \) and momentum distribution function behaving like \( |k|^{-1} \sqrt{g_n} \) at low momenta, where \( n_0 \) is the mean value of \( N_0/L \). This leads to a logarithmic divergence of the depletion integral (fractional occupation of orbitals with \( |k| > 0 \)). We therefore proceed directly to the variational theory.

**Variational pair (GA) theory.** The variational ground state energy \( E_{0P} \) is most easily evaluated by recalling that \( |\Phi_0\rangle \) is the vacuum of number-conserving quasiparticle annihilation operators \( \hat{a}_k \), applying Wick’s theorem after rewriting \( H_P \) in terms of quasiparticle annihilation and creation operators via the inverse transformation \( \hat{\beta}_0^\dagger \hat{\beta}_0 = (1 - \Delta_k^2)^{-1/2} \) where \( \Delta_k = \xi_k - \xi_k^\dagger \) is determined by the GP equation \[21,22\]. We use the usual Fermi pseudopotential. Minimizing the energy \( E_{0P} \) with respect to \( \Delta_k \) may be replaced by \( N_0 \) with negligible error and \( N_0 \) eliminated from the second and third lines via the identity \( N_0 = N - \sum_{k \neq 0} \hat{N}_k \) valid for eigenstates of total particle number with eigenvalue \( N \). Applying Wick’s theorem, passing to the thermodynamic limit \( \sum_{k \neq 0} \rightarrow (L/2\pi)^2 \int_0^\infty dk \), and noting that all integrands are even functions of \( k \), one finds eventually

\[
e_{0P} = \epsilon_{tr} + \frac{n_0 g}{2} + \frac{1}{\pi n} \int_0^\infty \frac{dk}{\Delta_k^2 (1 - \Delta_k^2 / L)} \int_0^\infty \frac{dk}{\Delta_k^2 (1 - \Delta_k^2 / L)} \int_0^\infty dk,
\]

where \( e_{0P} = E_{0P} / N \) is the energy per particle, \( n_0 = n_f \) is the condensate number density with condensate fraction \( f = 1 - \sum_{k \neq 0} \hat{N}_k = 1 - \int_0^\infty \frac{dk}{\pi^{1/2}} \hat{N}_k \) the momentum distribution function is \( N_k = \Delta_k^2 (1 - \Delta_k^2 / L) \), and

\[
I_1 = \frac{g}{\pi} \int_0^\infty \frac{\Delta_k}{1 - \Delta_k^2} \hat{N}_k \hat{N}(\hat{N} - 1) \hat{N}_k, \quad I_2 = \frac{g}{\pi} \int_0^\infty \hat{N}_k \hat{N}(\hat{N} - 1) \hat{N}_k dk.
\]

\( I_2 = n_f (1 - f) \) and need not be evaluated separately. These equations are in one-one correspondence with Eqs. \(21\) and \(22\) of GA \[16\] via the correspondences \( \Delta_k \rightarrow \phi(k), \ n_0g \rightarrow \rho_0 \mu(k), \ I_1 \rightarrow I_1(k), \) and \( I_2 \rightarrow I_2(k) \), but here the integrals \( I_1 \) and \( I_2 \) are independent of \( k \) due to our use of the Fermi pseudopotential. Minimizing the expression \( 6 \) by setting its functional derivative with respect to \( \Delta_k \) equal to zero, taking into account the dependence of \( n_0, I_1, \) and \( I_2 \) on \( \Delta_k \), one finds

\[
(n_0g - I_1)(1 + \Delta_k^2) - 2[(k^2/2) + n_0g + I_1] \Delta_k = 0,
\]

whose solution for \( \Delta_k \) is

\[
\Delta_k = (n_0g - I_1)^{-1/2}[(k^2/2) + n_0g + I_1 - \omega_k],
\]

where \( \omega_k \) is the quasiparticle energy.
Substitution of this expression for $\Delta_k$ back into the definitions of $I_1$ and $I_2$ leads to integrals which can be evaluated in closed form

$$I_1 = \frac{g(n_0g - I_1)}{2\pi} \int_0^\infty \frac{dk}{\omega_k} = \frac{g(n_0g - I_1)}{2\pi} \frac{K}{\sqrt{n_0g}}$$

$$I_2 = ng(1 - f) = \frac{g}{2\pi} \int_0^\infty \frac{dk}{\omega_k} \left(\frac{k^2}{2} + n_0g + I_1 - \omega_k\right) = \frac{g}{2\pi} \sqrt{n_0g} \left(1 + \lambda\right)K - 2E$$

where $\lambda = I_1/n_0g$, and $K = K(\sqrt{1 - \lambda})$ and $E = E(\sqrt{1 - \lambda})$ are complete elliptic integrals [24]. Here we have made use of the fact that $I_1 > 0$, since otherwise $\omega_k$ would become imaginary at small $k$, which further requires that $n_0g > I_1$. The ground state energy per particle is finally found to be

$$e_{0P} = \epsilon_{tr} + \frac{ng}{2} - f(I_1 - I_2 - I_3) + \frac{(I_1^2 + I_2^2)}{2ng}$$

where

$$I_3 = \frac{1}{4\pi n_0} \int_0^\infty k^2 \left[\frac{(k^2/2) + n_0g + I_1}{\omega_k} - 1\right] dk$$

$$= \frac{\sqrt{g/n_0}}{3\pi} \left[(n_0g + I_1)E - 2I_1K\right]$$

The short dash line in Fig. 1 shows a log-log plot of the scaled energy per particle $e_{0P}/g^2$ as a function of scaled linear density $n/g$ calculated using the GA theory in Eqs. (6)-(14) for constant coupling $g$. Fixing $g$ corresponds to the regime where the transverse orbital is frozen as the lowest mode of the harmonic trap, in which case our model coincides with that of Lieb and Liniger [13]. The long dash line in Fig. 1, almost indistinguishable from the solid line, is the scaled energy per particle $e_{LL}(\gamma)/g^2 = (n/g)^2 \epsilon(\gamma)/2$ from the LL theory. There is excellent agreement between the GA theory and LL theory in the high density regime $n/g > 1$, where the LL ground state energy is known to agree with Bogoliubov theory [3,4], but for low densities $n/g < 1$ the predicted energies diverge.

**Hybrid Bose-Fermi variational theory.** The failure of the GA theory for $n/g < 1$ can be traced to “fermionization” in which bosonic atoms become impenetrable at low densities [6]; this is the 1D Tonks gas limit where Bose-Fermi mapping [5] applies. A variational method capable of treating “partial fermionization” is suggested to treat the BEC-Tonks crossover. In the crossover region the system is intermediate between a BEC and a fermionized Tonks gas, so we model it as an interpenetrating mixture of a BEC of $wN$ bosons with pair theory energy functional $e_{0P}$ and $(1 - w)N$ fermions with energy functional $e_{0F}$. Assuming additivity of the Bose and Fermi energies as in the theory of ideal mixtures [23], one obtains an approximate energy functional (total energy per particle)

$$e_{0B}(n) \approx we_{0P}(wn) + (1 - w)e_{0F}(-(1 - w)n)$$

The Fermi energy functional is just that of the ideal Fermi gas, $e_{0F}(n) = \pi^2 n^2/6$, since a contact interaction of spinless fermions is equivalent to no interaction. Then for a fixed linear density $n$ one obtains $e_{0B}(n) \leq we_{0P}(wn) + (1 - w)^2 \pi^2 n^2/6$ and this can be numerically minimized with respect to $w$, using $e_{0P}$ from Eq. (13). The solid line in Fig. 1 shows the resultant scaled ground state energy $e_{0B}/g^2$ versus scaled linear density $n/g$ for constant $g$, and excellent agreement is seen with the LL theory (long dash line) over the full range of densities. In particular, for low densities $n/g$ the energy per particle correctly approaches that of a free Fermi gas [3,5,4]. One notes from Fig. 1 that the variational energy lies above the exact LL energy, providing an a posteriori justification of the minimization with respect to variation of $w$.

**BEC-Tonks crossover:** Insofar as calculation of the energy via (15) is concerned, the system behaves as if $(1 - w)N$ interacting bosons have been replaced by free fermions. The fermionic contribution dominates when $n/g \ll 1$ where the bosons are impenetrable and the Bose-Fermi mapping theorem [5] applies, whereas the GA theory is accurate in the opposite limit $n/g > 1$. In the crossover region $n/g \sim 1$ we define an effective Bose condensed fraction by $w_f = N_0/N$ where $f = N_0/N_B$ and $N_B = wN$. Figure 2 shows this condensed fraction as a function of the scaled density for constant $g$, and a crossover occurs at $n^*/g = 2.17$ where $w_f = 0.5$: This crossover condition $n^*/g = 2.17$ is very close to

![Log-Log plot of the scaled energy per particle versus the scaled linear number density n/g: Hybrid Bose-Fermi variational theory e_{0B}/g^2 (solid line), exact LL solution e_{LL}/g^2 (long dash line), e_{0P}/g^2 from the GA theory (short dash line).](image)
Olshanii’s prediction \( N^* = L/\pi|a_{1D}| \) for the maximum number of atoms to form a 1D Tonks gas, where we identify \( N^*/L = n^* \) and \( g = 2/\pi|a_{1D}|, a_{1D} \) being the 1D scattering length [3]. Petrov et al. derived the same condition for the crossover from a Tonks gas to a 1D quasicondensate [4].

For an ideal Tonks gas \( w \to 0 \) which requires \( n/g \to 0 \), but as a measure of the density needed to approach a Tonks gas if we require 90% or more of the atoms to be fermionized (\( w=0.1 \)) we need to satisfy \( n/g < 0.026 \). By comparison, for a condensed fraction greater than 90% (\( w_f > 0.9 \)) we require \( n/g > 30 \). By comparison, using hydrostatic equations applied to a trapped LL model [5], Dunjko et al. find that the density profile of the trapped gas is close to the Thomas-Fermi solution for \( n/g = 14 \) (\( \eta = 9 \)) for which \( w_f = 0.85 \), and close to that for a Tonks gas for \( n/g \approx 0.1 (\eta = 0.07) \) for which \( w_f = 0.25 \), where \( \eta = n|a_{1D}| \) in their notation. There is therefore consistency between our results even though we do not consider a gas with longitudinal trapping.

In summary, we have developed a hybrid Bose-Fermi variational theory that accurately describes the BEC-Tonks crossover in 1D. A key virtue of our approach is that it may be extended to 3D: Here we have assumed tight confinement and taken \( g = 4\pi a \int_0^\infty |\phi_{tr}(\rho)|^2 2\pi \rho d\rho \) as a constant whose value for the unperturbed transverse ground orbital is \( g = 2a/\ell_0^2 \) where \( \ell_0 = 1/\sqrt{\omega_0} \) [6]. More generally, minimization of the ground state energy by variation of \( \phi_{tr} \) subject to the normalization constraint leads to the following generalized GP equation:

\[
\mu \phi_{tr} = -\frac{1}{2} \left( \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} \right) \phi_{tr} + \frac{1}{2} \omega_0^2 \rho^2 \phi_{tr} + 4\pi a n (2 - f^2 - 2\lambda f + f^2 \lambda^2) |\phi_{tr}|^2 \phi_{tr},
\]

(16)

where \( \mu \) is the chemical potential. Solving this GP equation for \( \phi_{tr} \) to obtain \( g \), and then solving self-consistently with Eqs. (6)-(14) will allow for the study of the crossover from 1D to 3D and will be the subject of future work.

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\[\text{FIG. 2. Condensed fraction } w_f \text{ versus the logarithm of the scaled linear number density } \log_{10}(n/g).\]