Do Attractive Bosons Condense?

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Motivated by experiments on Bose atoms in traps which have attractive interactions (e.g., ^{7}Li), we consider two models which may be solved exactly. We construct the ground states subject to the constraint that the system is rotating with angular momentum proportional to the number of atoms. In a conventional system this would lead to quantized vortices; here, for attractive interactions, we find that the angular momentum is absorbed by the center of mass motion. Moreover, the state is *uncondensed* and is an example of a "fragmented" condensate discussed by Nozières and Saint James. The same models with *repulsive* interactions are fully condensed in the thermodynamic limit. [S0031-9007(98)05605-1]

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One of the most novel aspects of the creation of Bose condensates with neutral atoms in traps is the possibility of observing a Bose gas with *attractive* interactions (negative scattering lengths). The case of ^{7}Li has been studied both experimentally [1,2] and theoretically. Condensation has been predicted to be stable for a sufficiently small number of particles or sufficiently weak interactions [3,4]. The instability to collapse when these conditions are not obeyed has also been discussed by several authors [5–9].

In this Letter we show, using two exactly soluble models, that there may be other possibilities for noncondensed states with attractive interactions. The states are the "fragmented" condensates discussed by Nozières and Saint James [10] in the context of excitonic Bose condensates. The possibility of such states emerges from the realization [11] that it is the exchange interaction which causes bosons with *repulsive* interactions to condense into a single one-particle state, if there are several one-particle ground states. Conversely for attractive interactions, the exchange term is negative and may prefer "fragmented" [10] condensation into more than one state if there is a degeneracy (or perhaps if the interactions are sufficiently strong). Kagan *et al.* [4] argue that trapped gases with sufficiently large negative scattering lengths are unstable to the formation of clusters using a somewhat different argument, but with the same physical origin.

The two models we examine are as follows: particles in a harmonic trap with L quanta of angular momenta and attractive contact interactions treated as a degenerate perturbation [12], and rotating particles in a harmonic trap interacting with harmonic interactions [13–16]. [Both of these cases have been of interest for *fermions* [12,14], where rotation is replaced by a magnetic field and the phenomena are related to the fractional quantum Hall effect (FQHE).] Rotation is considered in both cases, partly because the nonrotating ground state, in the thermodynamic limit, is trivial in both cases (for different reasons) and partly because the response to rotation is characteristic of superfluidity in the system [17,18].

First consider the Hamiltonian for the two-dimensional contact interaction model, $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$, where

$$\mathcal{H}_0 = -\frac{1}{2}\nabla^2 + \frac{1}{2}\sum_i \mathbf{r}_i^2$$

$$\text{and} \quad \mathcal{H}_1 = \frac{\eta}{2}\sum_{i>j}^{N}\delta(\mathbf{r}_i - \mathbf{r}_j). \tag{1}$$

We work in the limit where the dimensionless coupling is weak [19], $|\eta| \ll 1$, so that the contact interaction can be treated perturbatively. We will determine the ground state subject to the constraint that the system contains L quanta of angular momentum. We note that the center of mass variables will separate in this Hamiltonian because the trap is harmonic. This will be used below.

The single particle spectrum is usefully expressed [20] in terms of the angular momentum quantum number m and the radial quantum number n_r,

$$E = |m| + 2n_r + 1 \tag{2}$$

in dimensionless units. For the noninteracting case, $\eta = 0$, with N particles, it is clear that to minimize the energy $n_r = 0$ for all particles. The angular momentum may be expressed as $L = \sum_m mN_m$ where N_m is the number of particles in the state m. There is a degeneracy, in general, associated with the choice of the set $\{N_m\}$. If the angular momentum is positive, $L > 0$, then because of the modulus signs in Eq. (2) the energy is minimized if one takes only *positive* integers for m. Then for the interacting problem, $0 < |\eta| \ll 1$, we make the approximation of restricting the Hilbert space to the degenerate ground state manifold of the noninteracting problem: the states $\{N_m\}$, such that $L = \sum_{m=0}^{L} mN_m$. The energy levels and wave functions are found by diagonalizing the interaction potential in this Hilbert space. This is exactly equivalent to the lowest-Landau level (LLL) approximation used very successfully in the theory of the FQHE [21] and electrons in quantum dots [22], and is justified because the spacing between noninteracting energy levels is much greater than the two-body interaction strength. Corrections to this approximation will form a power series in the small parameter η.

The single particle states with $n_r = 0$ and $m \geq 0$ are of the form $z^m \exp(-|z|^2/2)$ where $z = x + iy$ and m is the angular momentum quantum number. We have been able to study systems of up to six particles comprehensively. In addition, we can prove that the form of the ground state holds for an arbitrary number of particles.

We find that in all cases the ground state for the attractive interaction ($\eta < 0$) is $\psi_{z_c} = z_c^L \exp[\sum_{i=1}^N -|z_i|^2/2]$ where $z_c = \sum_{i=1}^N z_i/N$ is the center of mass and L is the total angular momentum in the system. The contact interaction energy contribution for the ground state is independent of L, $\epsilon(N,L) \propto \eta N(N-1)/2$. To prove the form of the ground-state wave function we show that ψ_{z_c} is the unique eigenfunction of $V = \sum_{i<j} \delta(\mathbf{r}_i - \mathbf{r}_j)$ corresponding to its largest eigenvalue, $\lambda_{\max}$. First we note that ψ_{z_c} is trivially an eigenfunction of V when $L = 0$ since it is the only state in the $L = 0$ subspace. Since z_c can be separated out in the Hamiltonian, it follows that ψ_{z_c} is an eigenfunction for any L.

Let us now work in the basis

$$|m_1, m_2, \ldots, m_N\rangle = \prod_{i=1}^N z_i^{m_i} e^{-|z_i|^2/2},$$

where $\sum m_i = L$. The matrix elements $\langle m|V|m'\rangle$ are non-negative, and are positive when $m_i + m_j = m_k' + m_l'$ for some i,j,k,l, and $m_p = m_q'$ for the remaining labels. The coefficients $\langle m|\psi_{z_c}\rangle$ are all positive, from which it follows that the eigenvector ψ_{z_c} belongs to the largest eigenvalue $\lambda_{\max}$. To see this note that $\lambda_{\max}$ can be derived from the variational principle

$$\lambda_{\max} = \max\left\{\frac{\langle\psi|V|\psi\rangle}{\langle\psi|\psi\rangle}\right\} = \max\left\{\frac{\sum_{ij} V_{ij}\psi_i\psi_j}{\sum_i \psi_i^2}\right\}. \quad (3)$$

If we take an eigenvector of $\lambda_{\max}$, and replace all its components by their absolute values, the variational functional in Eq. (3) cannot decrease, and so must remain at $\lambda_{\max}$. Therefore there is an eigenvector of $\lambda_{\max}$ whose components are non-negative; ψ_{z_c} has nonzero overlap with this eigenvector, and so must belong to $\lambda_{\max}$.

To prove nondegeneracy of the eigenspace of $\lambda_{\max}$ we note that the matrix V_{ij} is "connected" in the following way: if we take a basis vector $|i\rangle$ and consider all $|j\rangle$ with $V_{ij} > 0$, then consider all $|k\rangle$ with $V_{jk} > 0$ and so on, this includes all basis vectors. If the eigenspace of $\lambda_{\max}$ is degenerate then there must be an eigenvector of $\lambda_{\max}$ whose components are of both signs (since we can choose this eigenvector to be orthogonal to ψ_{z_c}) and all nonzero (if some components are zero, simply add on a very small amount of ψ_{z_c}). The vector made by taking the absolute value of the latter's components will also be an eigenvector. The difference in value of the variational functional for the two vectors can only be zero if the ith and jth components have the same sign when $V_{ij} > 0$. By connectedness we see that this means all components must have the same sign, and thus the eigenspace is nondegenerate. Hence ψ_{z_c} is the nondegenerate ground state of Eq. (1) with an attractive interaction.

To determine the degree of condensation, if any, the single particle density matrix $\rho(z, z'^*)$ is required for the ground state. Yang [23] showed that off-diagonal long-range order is associated with the largest eigenvalue of the density matrix (the magnitude of the eigenvalue is the fraction condensed) with the "condensate wave function" being the associated eigenvector. The notion of off-diagonal long-range order is not of great use for trapped atoms, but this definition of the *condensate* is useful in an inhomogeneous setting. The single particle density matrix has the form

$$\rho(z, z'^*) = \frac{1}{Q}\int \prod_{i=2}^N dz_i\, dz_i^*\, \psi(z, z_2, \ldots, z_N) \times \psi^*(z', z_2, \ldots, z_N),$$

where Q is the normalization. On integrating we find

$$\rho(z, z'^*) = \frac{e^{-|z|^2/2} e^{-|z'|^2/2}}{\pi} \sum_{m=0}^L z^m z'^{*m} \frac{(N-1)^{L-m} L!}{N^L (L-m)!\, m!^2}.$$

Thus the resulting eigenfunctions and eigenvalues for a given m are

$$\psi_m = e^{-|z|^2/2} z^{*m} \quad \text{and} \quad \rho_m = \frac{(N-1)^{L-m} L!}{N^L (L-m)!\, m!}.$$

If we now consider the case of $L = Nq$ (which in a conventional system, e.g., ^{4}He would correspond to q vortices), then if a condensate exists its eigenvalue will correspond to $m = q$. Simplifying we find

$$\rho_q = (1 - 1/N)^{(qN-q)} \frac{(Nq)!}{N^q (qN-q)!\, q!},$$

which can be rewritten as a Poisson distribution in the limit that $N \to \infty$. On taking the further limit of $q \to \infty$ the maximal eigenvalue becomes $\rho_q \sim 1/\sqrt{2\pi q}$. However, the eigenvalues of significant weight are distributed over $q - \sqrt{q} \lesssim m \lesssim q + \sqrt{q}$. This is clearly not the pronounced peak required for a condensate and is reminiscent of Nozières and Saint James's fragmented condensate [10]. Lest this be thought to be misleading for small q, we note the following results for $q = 1$. We find that the eigenvalue where the putative "condensate" would be, $\rho_1(q=1) = e^{-1}$, that $\rho_0(q=1) = e^{-1}$ as well, and that $\rho_2(q=1) = \frac{1}{2}e^{-1}$. The condensate is not singled out as having a uniquely large eigenvalue.

The first excited state Φ is also of interest, as we find a rudimentary "vortex." The general form is

$$\Phi = z_c^{L-2} \sum_{i>j}^N (z_i - z_j)^2 \quad \text{with } \epsilon_1 \propto N(N-2)/2.$$

Again from symmetry considerations we require a minimum of 2 quanta of angular momentum in order to produce an excited state. For $L = 2$, we find that there are two possible states for all N, and these correspond to the ground state and excited state we have described above. Because of the separation of the center of mass variables mentioned above, this is, in fact, a general result: Φ is an excited state of the system for arbitrary L (although we have not proved that it is always the *first* excited state).

To determine whether the results from the contact interaction model are likely to be generic or are artifacts (for instance, of degenerate perturbation theory), we turn to the second model. The Hamiltonian [15,16] (first discussed in the context of nuclear physics [13]) describes N bosons with attractive harmonic coupling $\tilde{\Lambda} > 0$) (i labels the particles),

$$H = -\frac{\hbar^2}{2m}\sum_i^N \tilde{\nabla}_i^2 + \frac{k}{2}\sum_i^N \mathbf{x}_i^2 + \frac{\tilde{\Lambda}}{4}\sum_{i,j}^N(\mathbf{x}_i - \mathbf{x}_j)^2,$$

where we enforce the symmetry of the wave functions at the end of the calculation. In dimensionless units, $\Lambda = \tilde{\Lambda}/k$, $y = [\hbar^2/(mk)]^{-1/4}x$ and $\nabla = (mk/\hbar^2)^{-1/4}\tilde{\nabla}$

$$\mathcal{H} = -\frac{1}{2}\sum_i^N \nabla_i^2 + \frac{1}{2}\sum_i^N \mathbf{y}_i^2 + \frac{\Lambda}{4}\sum_{i,j}^N(\mathbf{y}_i - \mathbf{y}_j)^2,$$

which upon rearrangement leads to

$$\mathcal{H} = -\frac{1}{2}\sum_i^N \nabla_i^2 + \frac{(1 + N\Lambda)}{2}\sum_i^N \mathbf{y}_i^2 - \frac{\Lambda}{2}\left(\sum_i^N \mathbf{y}_i\right)^2.$$

Here we note that the problem in d dimensions separates into d one-dimensional problems. Hence we will now restrict ourselves to one dimension for clarity.

To determine the degree of condensation we again need to calculate the single particle density matrix. To do this we change variables to the center of mass coordinate, $\zeta_N = 1/\sqrt{N}\sum_i^N y_i$, and ζ_i $(i = 1, \ldots, N - 1)$, which are chosen to form an orthonormal set with ζ_N. The Hamiltonian in these variables is

$$\mathcal{H} = -\frac{1}{2}\nabla_\zeta^2 + \frac{(1 + N\Lambda)}{2}\sum_i^N \zeta_i^2 - \frac{N\Lambda}{2}\zeta_N^2.$$

This leads to the ground-state wave function for zero angular momentum having the form

$$\psi = e^{-(1/2)(1+N\Lambda)^{1/2}\boldsymbol{\zeta}^2} e^{-(1/2)[1-(1+N\Lambda)^{1/2}]\zeta_N^2},$$

where $\boldsymbol{\zeta} = \{\zeta_1, \ldots, \zeta_N\}$. The corresponding frequencies are $\epsilon_i = (1 + N\Lambda)^{1/2}/2$ for $i \neq N$ and $\epsilon_N = 1/2$. We now consider the model in $d \geq 2$ with attractive interactions in the fixed angular momentum subspaces. In the ground state we find that all angular momentum is absorbed by the center of mass variable. This may be seen by noting that the center of mass oscillators (associated with the different components of the center of mass motion) have a lower associated frequency than the other oscillators describing relative motion. The physical interpretation is straightforward: relative motion requires more energy as work must be performed against the attractive interactions. (The converse will hold true for repulsive interactions.) Hence, for two dimensions and L quanta of angular momentum we can immediately write down the ground-state wave function,

$$\psi = z_c^L e^{-(1/2)(1+N\Lambda)^{1/2}|\mathbf{z}|^2} e^{-(1/2)[1-(1+N\Lambda)^{1/2}]|z_c|^2}.$$

In the thermodynamic limit it can be shown that the contribution to the single particle density matrix of the exponential term associated with z_c is negligible. Hence, surprisingly, the density matrix reduces to that of the contact interaction model. The ground-state wave functions will therefore be the same, as will the properties of the single particle density matrix.

We shall now show that these systems are condensed (at least under some conditions) when the interactions are repulsive. Thus the lack of condensation is not due to peculiarities of the models in general, but of the attractive interactions in particular.

First consider the contact interaction model (CIM) when there are N quanta of angular momentum in the system. Conventionally there would then be one vortex, and one might expect that the ground state (subject to the constraint of fixed angular momentum) would be

$$\psi_{L=N}^{\mathrm{mft}} = \prod_{i=1}^N (z_i e^{-|z_i|^2/2}). \tag{4}$$

We conjecture the following form for the CIM:

$$\psi_{L=N}^{\mathrm{exact}} = \prod_{i=1}^N ([z_i - z_c]e^{-|z_i|^2/2}). \tag{5}$$

We have demonstrated that this form is correct by explicit calculation on systems of up to 6 bosons. The physical interpretation of this wave function is that the bosons are rotating around the center of mass; this would be a condensate if the center of mass were a c number. We will now show that in the thermodynamic limit the corrections to full condensation are $O(1/N)$. Consider the density matrix constructed from the wave function Eq. (5),

$$\rho(z, z'^*) = e^{-|z|^2/2}e^{-|z'|^2/2}\left(\frac{2}{\pi^N}\right)^{1/2}\int\left\{\prod_{i=2}^N dz_i\,dz_i^*\right\}\left(\omega - \frac{(N-1)}{N}z\right)\left(\omega^* - \frac{(N-1)}{N}z'^*\right)$$
$$\times \prod_{j=2}^N\left\{\left(\omega + \frac{z}{N} - z_j\right)\left(\omega^* + \frac{z'^*}{N} - z_j^*\right)e^{-|z_j|^2}\right\},$$

where $\omega = 1/N\sum_{i=2}^N z_i$. Then to separate the integration over the different z_i we introduce a delta function for the center of mass variable,

$$1 = \int_{-\infty}^{\infty} d\omega_x\,d\omega_y\,\delta\left(\omega_x - \frac{1}{N}\sum_{i=2}^N x_i\right)\delta\left(\omega_y - \frac{1}{N}\sum_{i=2}^N y_i\right),$$

and use the integral representation

$$\delta\left(\boldsymbol{\omega} - \frac{1}{N}\sum_{i=2}^{N}\mathbf{r}_i\right) = \frac{1}{(2\pi)^2}\int d\boldsymbol{\lambda}\, e^{i\boldsymbol{\lambda}\cdot[\boldsymbol{\omega}-(1/N)\sum_{i=2}^{N}\mathbf{r}_i]}.$$

Upon substitution and integration we find that, in the limit that $N \to \infty$, to accuracy $O(1/N^2)$,

$$\begin{aligned}\rho(z, z'^*) &= \sum_n \psi_n(z)\rho_n\psi_n^*(z') \\ &= e^{-|z|^2/2}\left(\frac{1}{N}\frac{1}{\sqrt{\pi}}\frac{1}{\sqrt{\pi}} + \left[1 - \frac{2}{N}\right]\frac{z}{\sqrt{\pi}}\frac{z'^*}{\sqrt{\pi}} \right. \\ &\quad \left. + \frac{1}{N}\frac{z^2}{\sqrt{2\pi}}\frac{z'^{*2}}{\sqrt{2\pi}}\right)e^{-|z'|^2/2}.\end{aligned}$$

Thus there is a condensate with eigenvalue $1 - 2/N$, in the state z, which is fully condensed in the thermodynamic limit. Corrections of size $1/N$ are in the states 1 and z^2. In addition, a Laughlin state is empirically found to be the ground state for $L = N(N - 1)$. This can be proved exactly by a trivial extension of the arguments used in Ref. [12].

Turning to the harmonic interactions model, we note that the center of mass oscillator has a higher frequency than the others when the interaction is repulsive. In that case the other oscillators will be populated in preference when minimizing the energy subject to L (a multiple of N) quanta of angular momentum. Now, the other oscillators are degenerate, and the center of mass factor is not being multiplied by a large multiple of the center of mass coordinate, which it was in the attractive case. The latter implies that the center of mass factor is irrelevant in the thermodynamic limit. Thus the ground state reduces to a single particle form [Eq. (2)], and hence the answer will be a condensate into the state $z^{L/N}$.

In conclusion, we have shown that for a model with degenerate ground states in the absence of interaction, there is no condensate formed when weak interactions are incorporated. Consequently, in this particular case, there is no vortex lattice. In a different model, which does not have degenerate ground states, we have shown that the particles are uncondensed when given an extensive quantity of angular momentum. In both cases the angular momentum of the system resides in the center of mass motion, in contrast to the more familiar case of repulsive interactions. This leads to the general hypothesis: attractive bosons do not condense in the presence of single particle degeneracy, and their angular momentum resides in the center of mass motion. The investigation of *rotating* ^{7}Li might be fruitful in exposing an uncondensed "ground state." Repulsive interactions in the same models lead to condensed ground states, so showing that attractive interactions do indeed lead to different physics.

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[1] C.C. Bradley, C.A. Sackett, J.J. Tollett, and R.G. Hulet, Phys. Rev. Lett. **75**, 1687 (1995).
[2] C.C. Bradley, C.A. Sackett, and R.G. Hulet, Phys. Rev. Lett. **78**, 985 (1997).
[3] P.A. Ruprecht, M. Edwards, K. Burnett, and C.W. Clark, Phys. Rev. A **54**, 4178 (1996).
[4] Y. Kagan, G.V. Shlyapnikov, and J.T.M. Walraven, Phys. Rev. Lett. **76**, 2670 (1996).
[5] G. Baym and C.J. Pethick, Phys. Rev. Lett. **76**, 6 (1996).
[6] R.J. Dodd, M. Edwards, C.J. Williams, C.W. Clark, M.J. Holland, P.A. Ruprecht, and K. Burnett, Phys. Rev. A **54**, 661 (1996).
[7] E.V. Shuryak, Phys. Rev. A **54**, 3151 (1996).
[8] L.P. Pitaevskii, Phys. Lett. A **221**, 14 (1996).
[9] V.S. Babichenko and A.N. Kozlov, JETP Lett. **64**, 729 (1996).
[10] P. Nozières and D. Saint James, J. Phys. (Paris) **43**, 1133 (1982).
[11] P. Nozières, in *Bose-Einstein Condensation*, edited by A. Griffin, D.W. Snoke, and S. Stringari (Cambridge University Press, Cambridge, 1995), Chap. 2.
[12] S.A. Trugman and S. Kivelson, Phys. Rev. B **31**, 5280 (1985).
[13] S. Gartenhaus and C. Schwartz, Phys. Rev. **108**, 482 (1957).
[14] S.M. Girvin and T. Jach, Phys. Rev. B **28**, 4506 (1983).
[15] N.F. Johnson and M.C. Payne, Phys. Rev. Lett. **67**, 1157 (1991).
[16] F. Brosens, J.T. Devreese, and L.F. Lemmens, Phys. Rev. E **55**, 6795 (1997).
[17] A.J. Leggett, Phys. Fenn. **8**, 125 (1973).
[18] P. Nozières and D. Pines, *The Theory of Quantum Fluids* (Addison-Wesley, Redwood City, CA, 1990), Vol. II.
[19] To be more accurate in the consideration of what constitutes "weak" interaction, we must compare the relative size of matrix elements between states within the lowest Landau level, and between the lowest and the next higher Landau levels. The latter matrix elements can be $O(N^{3/2})$, for example, between $|0\rangle = (c_{00}^\dagger)^N|\text{vac}\rangle$ and $|1\rangle = (c_{00}^\dagger)^{N-1}c_{10}^\dagger|\text{vac}\rangle$, where $c_{nm}^\dagger$ creates the one-particle state with radial quantum number n and angular quantum number m. The former can be $O(N^2)$ for an extensive amount of angular momentum $L = qN$—for example, between the set of states $(c_{02}^\dagger)^{q_1N}(c_{01}^\dagger)^{q_2N}(c_{00}^\dagger)^{q_3N}|\text{vac}\rangle$ with $q_1 + q_2 + q_3 = 1$ and $2q_1 + q_2 = q$. The fact that the matrix elements to states outside the ground state manifold are smaller than those to states within it means that we can work in the ground state manifold for $|\eta| \ll 1$.
[20] S. Flugge, *Practical Quantum Mechanics* (Springer-Verlag, Berlin, 1974), p. 109.
[21] *The Quantum Hall Effect*, edited by R.E. Prange and S.M. Girvin (Springer-Verlag, New York, 1990), Chaps. 7 and 8.
[22] T. Seki, Y. Kuramoto, and T. Nishino, J. Phys. Soc. Jpn. **65**, 3945 (1996), and references therein.
[23] C.N. Yang, Rev. Mod. Phys. **34**, 694 (1962).