Yrast Spectra of Weakly Interacting Bose-Einstein Condensates

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The low energy quantal spectrum is considered as a function of the total angular momentum for a system of weakly interacting bosonic atoms held together by an external isotropic harmonic potential. It is found that besides the usual condensation into the lowest state of the oscillator the system exhibits two additional kinds of condensate and associated thermodynamic phase transitions. These new phenomena are derived from the degrees of freedom of "partition space" which describe the multitude of different ways in which the angular momentum can be distributed among the atoms while remaining all the time in the lowest state of the oscillator.

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The properties of the nonzero angular momentum states of Bose condensates of atoms in external traps have been addressed in several recent publications [1]. Special interest attaches to the lowest energy quantum states with a given angular momentum. Borrowing from nuclear physics terminology we shall refer to this part of the quantum spectrum as the yrast region [2]. Theoretical work on the yrast region for Bose condensates has, with the exception of [3], been based on the Gross-Pitaevski mean field approximation [4]. In the present Letter the yrast spectra are described in terms of the elementary modes that carry the angular momentum. It is found that this approach reveals structures in the yrast spectra that were not recognized in previous work. The picture of the yrast region described in this Letter draws heavily on ideas developed in collaboration with Bohr [5] in connection with the analysis of the stability of persistent currents in superconductors.

The model considered, which has previously been discussed by Wilkin *et al.* [3], involves N spin zero bosons moving in an isotropic harmonic confining potential and a contact interaction with a strength that is assumed to be weak, in the sense

$$v N \ll \hbar \omega_0, \tag{1}$$

where v is the expectation value of the interaction between two particles both in the ground state of the oscillator, and $\hbar \omega_0$ is the quantum energy of the confining potential. Although the so-far published experiments have mainly studied systems that do not satisfy the condition (1), systems that do satisfy this condition are accessible with current experimental techniques and would be especially interesting since this implies that the coherence length in the atomic cloud becomes larger than the size of the system, bringing into sharpest focus the mesoscopic nature of these systems. The eigenstates of a single particle moving in an harmonic oscillator can be labeled by the quantum numbers (nlm) where n is the radial quantum number, l is the angular momentum, and m is the component of l on the axis of quantization. The energy of such a state is $\epsilon = (2n + l + 3/2)\hbar \omega_0$, and for the yrast states we need only consider occupancy of states with $n = 0$, $m = l \geq 0$.

(Without loss of generality we assume that the total angular momentum is in a state of maximum alignment $L = M$.) Thus the relevant single particle states involve only a single non-negative quantum number, m.

In the yrast state with total angular momentum $\hbar L$, the motion in the oscillator will contribute an excitation energy $L \hbar \omega_0$ with respect to the ground state. However, this configuration is degenerate in the absence of the interactions, since the oscillator energy is the same whether the L quanta are distributed among the particles with one quantum to each of L different particles, or with two quanta on one particle and one quantum on each of $L - 2$ other particles, etc. Since the multiplicity $p(L)$ of the partitions of the integer L into positive integers increases asymptotically as [6]

$$p(L) \sim \frac{1}{\sqrt{48}\, L} \exp\left\{ \pi \sqrt{\frac{2L}{3}} \right\}, \tag{2}$$

the magnitude of the degeneracies becomes quite large, even for moderate values of L. This set of states will be called the partition space of L, and the problem of characterizing the yrast spectra thus amounts to finding the lowest quantum states selected by the contact interaction acting within the partition space of L.

Partition space.—Since the construction of appropriate basis states in partition space and their matrix elements plays the crucial role in the subsequent discussion, it is useful to begin with a brief discussion of some of the most elementary features of this interesting space. The standard notation for a partition of the integer L is

$$(1^{n_1} 2^{n_2} \ldots L^{n_L}), \tag{3}$$

where the n_r are restricted by the condition

$$\sum_{r=1}^{L} r n_r = L. \tag{4}$$

The set of integers $\{n_r\}$ satisfying (4) can thus be thought of as a set of quantum numbers characterizing a basis state in the partition space of L.

In the present discussion we shall exploit two different ways of associating a basis state with a given partition $\{n_r\}$. The two realizations differ in their identification of the object that carries the r units of angular momentum: (i) $r = m$, the address of a single particle state. In this realization the n_m count the number of different particles, each of which is carrying m units of angular momentum:

$$\Psi_{\{n_m\}} = |(m = 1)^{n_1}(m = 2)^{n_2} \ldots (m = L)^{n_L}\rangle. \quad (5)$$

(ii) $r = \lambda$, the multipole order of a (collective) normal mode of excitation. Assuming that the normal mode is excited by acting on the ground state with the collective operator Q_λ, we have

$$\Psi_{\{n_\lambda\}} \sim \Pi_{\lambda=1}^L (Q_\lambda)^{n_\lambda}|0\rangle. \quad (6)$$

Although these two realizations each provide a complete set of states for describing partition space, these states can be very different when the numbers n_r of excitations is large; thus for a single mode we have the overlap

$$\langle (m = \lambda)^{n_\lambda}| \frac{1}{\sqrt{n_\lambda!}} (Q_\lambda)^{n_\lambda}|0\rangle = \sqrt{\frac{N!}{(N - n_\lambda)! \, N^{n_\lambda}}}$$
$$\sim \exp\left\{-\frac{1}{2N} (n_\lambda)^2\right\}, \quad (7)$$

where we have employed the expression (8) for Q_λ. Thus for states involving condensates in which $n_\lambda \sim \mathcal{O}(L)$ where $L \gg \sqrt{N}$, the two different states derived from the same partition become essentially orthogonal.

In thinking about the structure of the operators Q_λ it is fruitful to take inspiration from Feynman's arguments [7] that identify the long wavelength, low energy excitations of superfluid helium with modes that are excited by acting on the ground state with a sum of single particle operators that impart the conserved quantum numbers (momentum in the case of liquid helium, angular momentum in the present problem) to a single particle of the condensate. Thus we shall assume

$$Q_\lambda = \frac{1}{\sqrt{2N\lambda!}} \sum_{p=1}^N z_p^\lambda, \quad (8)$$

$$z_p = x_p + iy_p, \quad (9)$$

where the spatial coordinates are measured in units of the oscillator length. The operator (8) acting on the $L = 0$ many body ground state of the oscillator creates a symmetrized state with angular momentum $L = \lambda$; the operator (8) raised to the n_λ power creates the many body excitations that appear in (6).

The excitation energies of the normal modes (8) can be evaluated by taking expectation values of the contact interaction in the appropriate harmonic oscillator states:

$$\epsilon_\lambda = \langle 0|Q_\lambda^+ V Q_\lambda|0\rangle - \langle 0|V|0\rangle$$
$$= -vN\left[1 - \left(\frac{1}{2}\right)^{\lambda-1}\right], \quad (10)$$

where the first term in the brackets represents the loss of interaction energy due to the removal of a single particle from the condensate in the ground state ($m = 0$) of the oscillator, and the second term describes the remaining interaction between the condensate particles and the excited single particle moving in an orbit with angular momentum λ. The short range of the interaction is responsible for the rapid decrease of the latter term as the particle with increasing λ moves in orbits with larger and larger radius. It should be emphasized that the energies (10) will be somewhat modified in a many mode excited state as a result of mode-mode interactions, but these interactions contribute terms that are at most of order v and therefore small compared with the leading order term (10). Thus, at least for $L \ll N$, we can consider the Q_λ excitations as a gas of noninteracting particles.

Attractive interactions ($v < 0$).—On the basis of the above, we are now in a position to construct the yrast states and the low energy excitations as a function of the angular momentum L. The phase diagram is somewhat simpler for attractive interaction than for repulsive and so we begin with attraction. The mode energies (10) are seen to be positive for all modes with the exception of $\lambda = 1$ which has $\epsilon_1 = 0$; the vanishing of the mode energy for $\lambda = 1$ can be simply understood from the fact that the operator Q_1 is proportional to the center of mass coordinate and thus does not affect the interactions of the particles which depend only on relative coordinates. Thus, in agreement with [3], we find that the yrast state is described by a wave function

$$\Psi_L \sim (Q_1)^L \Phi_0, \quad (11)$$

in which the excitation energy and angular momentum are entirely associated with the center of mass of the atom cloud moving around in the confining oscillator potential while the relative coordinates and interactions remain exactly as in the $L = 0$ state.

The state (11) can be seen to involve two distinct condensates: partly the usual Bose-Einstein condensate that puts all the particles into the lowest state of the oscillator. This condensate is, in the presence of a finite temperature, melted by excitations that move particles to excited states in the oscillator, and this results in a critical transition at the Bose-Einstein condensation temperature [1]

$$T_c \sim N^{1/3}\hbar\omega_0. \quad (12)$$

In addition, the state (11) involves a condensate into a single mode ($\lambda = 1$) out of the many degrees of freedom in partition space. The low energy degrees of freedom of the partition space are described by excitations involving the removal of particles from the $\lambda = 1$ mode and corresponding excitation of the modes with $\lambda = 2, 3, 4, \ldots, L$. Such excitations imply a melting of the partition space condensate and, because of the (near) degeneracy of all the $\lambda \neq 1$ normal modes, the thermal average of their contributions

to the partition function can be easily evaluated and yield a critical temperature

$$T_{pc} = \frac{N\upsilon}{\ln L} \qquad (13)$$

for the partition space phase transition. At this temperature the specific heat has a singularity (decreasing by a factor of 2) and the occupation of the $(\lambda = 1)$ mode decreases from the value $2L(1 + \sqrt{5})^{-1}$ to a value that is of order $\sqrt{L}$. This transition is, of course, in a finite system and therefore the critical region is spread over a finite interval in temperature. However, this interval is

$$\delta T \sim \frac{N\upsilon}{(\ln L)^2} \qquad (14)$$

and thus is small compared to the critical temperature.

Repulsive interactions $(\upsilon > 0)$.—The spectra resulting from repulsive interactions are obtained by inverting those discussed above, and the structure of the yrast region involves an analysis of the configurations that would have been those of highest energy in the earlier discussion. It turns out that there are again two distinct condensates at each value of L and two phase transitions as a function of temperature, and in addition there is a third type of phase structure giving rise to a quantal phase transition (i.e., a transition at $T = 0$) in which the nature of the condensate in partition space changes abruptly as a function of L. These different $T = 0$ phases are distinguished by the different integer number of vortex lines that exist in the ground state.

We can again, for repulsive interaction (and $L \ll N$), consider the spectra constructed from the collective excitations produced by the operators Q_λ, but now the expression (10) yields negative values. The fact that the excitations have a negative energy reflects the fact that for repulsive interactions the interaction energy in the $L = 0$ state is a maximum and all the $Q_\lambda(\lambda \neq 1)$ excitations reduce the energy by putting nodes in the wave function for relative motion and letting the particles get a little further away from each other. The yrast states will therefore be obtained by a condensation into that mode that has the greatest energy gain per unit of angular momentum. As can be seen from Table I, the quadrupole $(\lambda = 2)$ and octupole $(\lambda = 3)$ modes are optimal in this respect; thus, for $L \ll N$, the yrast state will be a condensate involving only

TABLE I. Energies of phonon modes for repulsive interactions. The energies (in units of $N|\upsilon|$) are obtained from (10), and apply to Q_λ excitations in the yrast region for $L \ll N$.

λ	ϵ_λ	ϵ_λ/λ
1	0	0
2	$-1/2$	$-1/4$
3	$-3/4$	$-1/4$
4	$-7/8$	$-7/32$
5	$-15/16$	$-3/16$

these two modes [8]. Excitations of the condensate are obtained by removing quanta from the condensate mode and placing them in other Q_λ modes, always subject to the constraint (4). In the presence of a finite temperature such excitations deplete the condensate and lead to a phase transition at a temperature of order (13).

As we go to higher angular momentum quite general arguments [1] suggest that for repulsive interactions and $L \sim N$ the near yrast states will be dominated by a structure involving a unit vortex line

$$\Phi_1 = (\Pi_{p=1}^N z_p)\Phi_0. \qquad (15)$$

In the state (15) all N atoms have been collectively shifted outward in the radial direction of the (x, y) plane effectively expanding the area, reducing the density, and thus reducing the energy associated with the short range repulsive interactions. The state (15) represents a realization of the partition (1^N) in the mode corresponding to (5) and as discussed in connection with Eq. (7) represents a terribly complicated state if expressed in terms of Q_λ excitations. Since there is no efficient way of combining a condensate in the Q_2 mode with a condensation in the $m = 1$ single particle state (unit vortex), the yrast state must undergo a violent rearrangement (many narrowly avoided crossings) at the critical angular momentum that separates these two regimes, i.e., a quantum phase transition.

In the region around $L = N$ the low energy degrees of freedom can be described by the Q_λ operators acting on the vortex state, but now the excitation energies ϵ_λ are different from those given by (10) since the, λ *excitation* now represents a mode in which a particle is removed from the condensate in $(m = 1)$ and excited to a state with $m = \lambda + 1$. There is also an additional mode in these spectra that results from the possibility of removing a particle from the $m = 1$ condensate and exciting it to the $m = 0$ state. This $\lambda = -1$ mode can be excited by the operator

$$Q_{-1} = \frac{1}{\sqrt{2N}} \sum_{p=1}^N \frac{1}{z_p}. \qquad (16)$$

However, the multiple excitations of this mode are not described by powers of the operator (16) since these powers contain terms that go outside the partition space. Rather, the nth excitation of the $\lambda = -1$ mode is created by the operator

$$Q_{-1}^{(n)} \sim \sum_{p_1 < p_2 \ldots < p_n} (z_{p_1} z_{p_2} \ldots z_{p_n})^{-1}. \qquad (17)$$

The degree of freedom associated with the $\lambda = -1$ mode can be seen as a displacement of the vortex line perpendicular to the axis along which the angular momentum is aligned as described by the broken symmetry condensate wave function

$$\Psi \sim [\Pi_{p=1}^N (z_p - a)]\Phi_0. \qquad (18)$$

The main obstacle to the observation of the phenomena discussed in the present paper would seem to be the very low temperatures necessary in order to come below the critical temperature (13). However, since this temperature is only about a factor of 10 below the temperatures that are routinely obtained in current experiments, the observation of these interesting effects would not seem to be an impossible goal.

The many interesting features of rotating Bose condensates that are briefly sketched in the present Letter are the subject of a more systematic report that is under preparation in collaboration with Pethick.

[1] For an extensive review of the present status of theoretical studies in this field, see F. Dalfovo, S. Giorgini, L. P. Pitaevskii, and S. Stringari, Rev. Mod. Phys. **71**, 463 (1999).

[2] The etymology of the term can be traced to the modern Swedish *yr* meaning dizzy; the form *yrast* is the naturally constructed superlative of *yr*. For a review of concepts developed in the context of yrast spectroscopy of atomic nuclei, see the articles "High Angular Momentum Phenomena" by I. Hamamoto, in *Treatise on Heavy-Ion Science,* edited by D. A. Bromley (Plenum Press, New York, 1985), Vol. 3, and "The Shell Model, High Spin, and Deformations" by I. Hamamoto and B. Mottelson, Nucl. Phys. **A507**, 65 (1990).

[3] N. K. Wilkin, J. M. F. Gunn, and R. A. Smith, Phys. Rev. Lett. **80**, 2265 (1998).

[4] See D. A. Butts and D. S. Rokhsar, Nature (London) **397**, 327 (1999) for a contribution that provides an up-to-date picture of the results that have been achieved with this approach.

[5] A. Bohr and B. R. Mottelson, Phys. Rev. **125**, 495 (1962).

[6] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (National Bureau of Standards, Washington, DC, 1964), p. 825.

[7] R. P. Feynman, *Statistical Mechanics* (W. A. Benjamin Inc., Reading, MA, 1972), p. 321ff.

[8] A detailed study, including the effect of mode-mode interactions in the low angular momentum region, has been carried out in collaboration with G. Kavoulakis and C. Pethick. This work establishes the fact that in this region the condensate involves only the quadrupole mode until a critical angular momentum at which both octupole and quadrupole modes become involved.