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Instabilities in a two-component, species-conserving condensate

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We consider a system of two species of bosons of equal mass, with interactions $U^a(|\mathbf{x}|)$ and $U^x(|\mathbf{x}|)$ for bosons of the same and different species, respectively. We present a rigorous proof valid when the Hamiltonian does not include a species-switching term showing that, when $U^x(|\mathbf{x}|)>U^a(|\mathbf{x}|)$, the ground state is fully "polarized" (consists of atoms of one kind only). In the unpolarized phase the low-energy excitation spectrum corresponds to two linearly dispersing modes that are even and odd under species exchange. The polarization instability is signaled by the vanishing of the velocity of the odd modes.

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The experimental observation of Bose-Einstein condensation (BEC) in dilute atomic systems [1] has triggered a very intense theoretical activity [2]. Attention has broadened to include condensates with internal degrees of freedom, or multispecies BEC, which were realized for trapped rubidium [3] and sodium [4]. Early theoretical analysis of m-species condensates focuses on the large m limit for Hamiltonians invariant under $U(m)$ transformations [5], superfluid-helim mixtures [6], and spin-polarized hydrogen [7]. In the context of BEC much of the theoretical attention concentrates on spinor condensates [8] in which the internal degrees of freedom correspond to the different Zeeman states of a particular hyperfine manifold such as the $f=1$ manifold in sodium. In these cases the two-body interaction is invariant under rotation in species space. On the other hand, for rubidium one has two nondegenerate internal states corresponding to two different manifolds, and the two-body interaction is not invariant under SU(2) rotations in species space [9]. The ground state and excitation spectrum of a two-species (a and b) condensate of this kind was studied in mean field in Ref. [10], where it was shown that the quasiparticle energy can become imaginary, signaling an instability when the interspecies repulsion U^x is larger than the intraspecies repulsion U^a. This kind of treatment follows—as do the majority of theoretical approaches to BEC—the gross-Pitaevskii mean-field equation [11]. On the other hand, rigorous results for BEC (and many-body problems in general) are scarce and at the same time useful in providing control for approximate solutions. With this motivation, in this paper we consider a two-species system of interacting bosons, and show rigorously that the instability mentioned above corresponds to the tendency of the system to "polarize," the true ground state consisting of only one species of bosons when $U^x>U^a$. We also discuss the low-energy excitation spectrum and show that the instability is signaled by a divergence of the "compressibility" associated with exchanging particles from one species to the other at fixed total particle number.

The Hamiltonian for our two-species system (a and b) of bosons of equal mass m is given by ($\hbar=1$)

$$H=K+U_a+U_b+U_{ab}, \tag{1}$$

with

$$K=\sum_{\mathbf{k}}\frac{k^2}{2m}[\psi_a^\dagger(\mathbf{k})\psi_a(\mathbf{k})+\psi_b^\dagger(\mathbf{k})\psi_b(\mathbf{k})], \tag{2}$$

$$U_a+U_b=\frac{1}{2}\int d^3x\, d^3y\, U^a(|\mathbf{x}-\mathbf{y}|)[\rho_a(\mathbf{x})\rho_a(\mathbf{y})+\rho_b(\mathbf{x})\rho_b(\mathbf{y})], \tag{3}$$

$$U_{ab}=\int d^3x d^3y\, U^x(|\mathbf{x}-\mathbf{y}|)\rho_a(\mathbf{x})\rho_b(\mathbf{y}). \tag{4}$$

In the above equations K is the kinetic term and the terms (U_a+U_b) and U_{ab} correspond to the interaction between bosons of the same and different species, respectively. The operators $\psi_i(\mathbf{x})$ destroy a boson of species i ($i=a,b$) at position $\mathbf{x}$, and obey the following commutation relations $[\psi_i^\dagger(\mathbf{x}),\psi_j(\mathbf{x}')]=\delta_{i,j}\delta(\mathbf{x}-\mathbf{x}')$. Also, $\rho_i(\mathbf{x})=\psi_i^\dagger(\mathbf{x})\psi_i(\mathbf{x})$ and $\psi_i(\mathbf{k})=V^{-1/2}\int d^3x \exp(i\mathbf{k}\cdot\mathbf{x})\psi_i(\mathbf{x})$ with V the total volume.

Using a variational argument we will prove that, for potentials satisfying $U^x(|\mathbf{x}|)>U^a(|\mathbf{x}|)$, the ground state of the above Hamiltonian is completely polarized. By "polarized" we mean that either of the two situations is realized: $\langle\hat{N}_a\rangle=0,\langle\hat{N}_b\rangle=N$; or $\langle\hat{N}_a\rangle=N,\langle\hat{N}_b\rangle=0$, with N the total particle number and $\hat{N}_i=\int d^3x\rho_i(\mathbf{x})$.

We note that, since the masses are the same for both species, the kinetic term of Hamiltonian (4) commutes with the "rising" operator defined as

$$\mathcal{O}_R=\int d^3x\, \psi_a^\dagger(\mathbf{x})\psi_b(\mathbf{x})\equiv\sum_{\mathbf{k}}\psi_a^\dagger(\mathbf{k})\psi_b(\mathbf{k}) \tag{5}$$

which conserves the total number of particles but converts particles of type b into particles of type a. More specifically, for the case of different masses for each species we have that $[\mathcal{O}_R,K]=(1/2m_b-1/2m_a)\Sigma_{\mathbf{k}}k^2\psi_a^\dagger(\mathbf{k})\psi_b(\mathbf{k})$.

We have in mind the alkali atoms, which have a hard core interaction, meaning that the exact wave functions vanish when the coordinates of two atoms of either species coincide.

Since the Hamiltonian conserves the particle number for each species, we can start with the normalized ground-state wave function $|\Psi_0(N_a,N_b)\rangle$ in the subspace of $N_a(N_b)$ particles of species $a(b)$. The unpolarized situation corresponds to $N_a=N_b=N/2$. Now let us consider the normalized variational wave function $|\Psi_v(N_a+N_b,0)\rangle$ obtained by the action of the rising operator on $|\Psi_0(N_a,N_b)\rangle$ N_b times,

$$|\Psi_v(N_a+N_b,0)\rangle=\frac{1}{\sqrt{N_b!}}(\mathcal{O}_R)^{N_b}|\Psi_0(N_a,N_b)\rangle. \tag{6}$$

Note that Ψ_v represents a completely polarized wave function, with particles of species a only. Since $[\mathcal{O}_R,K]=0$, we have

$$\begin{aligned}&\langle\Psi_v(N_a+N_b,0)|K|\Psi_v(N_a+N_b,0)\rangle\\&\quad=\langle\Psi_0(N_a,N_b)|K|\Psi_0(N_a,N_b)\rangle,\end{aligned} \tag{7}$$

meaning that the completely polarized variational wave function and the ground state of the subspace (N_a,N_b) have the same expectation value of the kinetic energy. We stress that the function $|\Psi_v(N_a+N_b,0)\rangle$ as defined in Eq. (6) is normalized only because the exact wave function $|\Psi_0(N_a,N_b)\rangle$ vanishes when any two coordinates coincide. Otherwise we would have to worry about permutation factors whenever coordinates coincide.

In order to compute the change in the potential energy we write the expectation values of U^a and U^x as an integral over all the multiparticle configurations $\Gamma\equiv(\Gamma_a,\Gamma_b)$ with coordinates $\{\mathbf{X}\}_\Gamma\equiv\{\mathbf{x}_{1,\Gamma_a},\ldots,\mathbf{x}_{N_a,\Gamma_a};\mathbf{x}_{1,\Gamma_b},\ldots,\mathbf{x}_{N_b,\Gamma_b}\}$. For each configuration Γ let us regard the particle coordinates $\{\mathbf{X}\}_\Gamma$ as nodes of a graph. There are $N_a(N_a-1)/2$ and $N_b(N_b-1)/2$ edges connecting pairs of particles of species a and b, respectively, and N_aN_b edges connecting a particles of different species. The contribution to the expectation value of the potential energy $U_0=\langle U_a\rangle+\langle U_b\rangle+\langle U_{ab}\rangle$ from this configuration is a function of the length of the edges of the graph, which can be classified in three sets: $\{\ell^a_{1,\Gamma_a},\ldots,\ell^a_{N_a(N_a-1)/2,\Gamma_a}\}$, $\{\ell^b_{1,\Gamma_b},\ldots,\ell^b_{N_b(N_b-1)/2,\Gamma_b}\}$, and $\{\ell^{ab}_{1,\Gamma},\ldots,\ell^{ab}_{N_aN_b,\Gamma}\}$, where ℓ^a_{i,Γ_a} is one of the possible lengths $|\mathbf{x}_{k,\Gamma_a}-\mathbf{x}_{l,\Gamma_a}|$, etc. The potential energy is therefore given by

$$\begin{aligned}U_0=\int d^{3N}X_\Gamma|\Psi_0(\mathbf{X}_\Gamma)|^2\Bigg[&\sum_{i=1}^{N_a(N_a-1)/2}U^a(\ell^a_{i,\Gamma_a})\\&+\sum_{i=1}^{N_b(N_b-1)/2}U^a(\ell^b_{i,\Gamma_b})+\sum_{i=1}^{N_aN_b}U^x(\ell^{ab}_{i,\Gamma})\Bigg],\end{aligned} \tag{8}$$

with $\Psi_0(\mathbf{X}_\Gamma)$ the ground-state wave function in first quantization.

In the variational wave function all the edges of type b and ab are both changed to edges of type a. Therefore the contribution to the potential energy of each edge of configuration Γ changes according to $U^a(\ell^b_{i,\Gamma_b})\rightarrow U^a(\ell^b_{i,\Gamma_b})$, $U^x(\ell^{ab}_{i,\Gamma})\rightarrow U^a(\ell^{ab}_{i,\Gamma})$. If we call U_v the expectation value of the potential energy in the variational wave function, and E_v the variational wave function, we obtain that $\Delta E=E_v-E_0=U_v-U_0$ is given by

$$\Delta E=\int d^NX_\Gamma|\Psi_0(\mathbf{X}_\Gamma)|^2\sum_{i=1}^{N_aN_b}[U^a(\ell^{ab}_{i,\Gamma})-U^x(\ell^{ab}_{i,\Gamma})]. \tag{9}$$

We see that when the interactions satisfy $U^x(|\mathbf{x}|)>U^a(|\mathbf{x}|)$ for all values of $\mathbf{x}$, ΔE is a sum of negative terms. In general the potentials have a repulsive short-range term and a long-range attractive tail. The condition for validity of our proof is that there are no "crossings" of the potentials $U^x(|\mathbf{x}|)$ and $U^a(|\mathbf{x}|)$ as a function of the coordinate. The simplest approximation will be to take the attractive components of both potentials as equivalent (of the form $-C_6/R^6$) and differing short-range components. This dependence is consistent with calculations for ultracold Na collisions [12].

Since the completely polarized variational wave function has lower energy than the true ground state of the partially polarized subspace, the gound state will be completely polarized. It is also evident that the proof is also valid in the case with different intraspecies interactions $U^a(\mathbf{x})$ and $U^b(\mathbf{x})$. As long as $U^x>U^a,U^b$, the ground state is polarized with particles of type a $[b]$ when $U^a(|\mathbf{x}|)<U^b(|\mathbf{x}|)$ $[(U^b(|\mathbf{x}|)<U^a(|\mathbf{x}|)]$. This means that the difference $U^b(|\mathbf{x}|)-U^a(|\mathbf{x}|)$ plays the role of a "symmetry-breaking field." Also, note that the above proof is also valid in the presence of an external potential $U_e(\mathbf{x})$ that is equal for both species, meaning that the polarization transition also occurs for trapped atoms.

We note that the bosonic nature of the particles is crucial for establishing our rigorous proof. If the atoms a and b were fermions, the variational argument ceases to be valid: since the Hamiltonian conserves species, atoms belonging to different species can be considered distinguishable, and the wave function does not change sign if we exchange any two atoms a and b following a path P. If we convert an atom a to an atom b, the wave function has to change sign under the particle exchange following the same path P, implying that we have to introduce an additional node in the wave function. Formally this means that $\mathcal{O}_R|\Psi_0(N_a,N_b)\rangle=0$ for fermions.

We now discuss the low-energy excitation spectrum, which in the symmetric case $(U^a=U^b)$ can be computed using longitudinal sum rules [13,14]. In the unpolarized case the excitations correspond to two phonon branches with wave functions $\rho^\pm_{\mathbf{k}}=(\rho^a_{\mathbf{k}}\pm\rho^b_{\mathbf{k}})|0\rangle$. The operators $\rho^i_{\mathbf{k}}=V^{-1/2}\int d^3xe^{i\mathbf{k}\cdot\mathbf{x}}\rho_{\mathbf{x},i}$ are the Fourier transforms of the density operators for each species. In other words, since the Hamiltonian is invariant under exchange of species, the excitations are either even or odd in the species index.

The excitation energies are given by

$$\omega^\pm_{\mathbf{k}}=\frac{\langle0|\rho^\pm_{-\mathbf{k}}H\rho^\pm_{\mathbf{k}}|0\rangle}{\langle0|\rho^\pm_{-\mathbf{k}}\rho^\pm_{\mathbf{k}}|0\rangle}, \tag{10}$$

where we have shifted the origin of energies $(H\rightarrow H-E_0;\ H|0\rangle=0)$. We will first show that $\langle0|\rho^\pm_{-\mathbf{k}}H\rho^\pm_{\mathbf{k}}|0\rangle=nk^2/2m$, with $n=N/V$. Consider

$$\langle 0|\rho^{a}_{-\mathbf{k}}H\rho^{b}_{\mathbf{k}}|0\rangle=\frac{1}{2}\langle 0|\{[\rho^{a}_{-\mathbf{k}},H]\rho^{b}_{\mathbf{k}}+\rho^{a}_{-\mathbf{k}}[\rho^{b}_{\mathbf{k}},H]\}|0\rangle \tag{11}$$

$$=\frac{\hbar^{2}}{2m}\sum_{\mathbf{q},\mathbf{q}'}\mathbf{k}\cdot\mathbf{q}\langle 0|[\psi^{\dagger}_{a}(\mathbf{q}'-\mathbf{k})\times\psi_{a}(\mathbf{q}')\psi^{\dagger}_{b}(\mathbf{q}+\mathbf{k})\psi_{b}(\mathbf{q})-\psi^{\dagger}_{a}(\mathbf{q}+\mathbf{k})\times\psi_{a}(\mathbf{q})\psi^{\dagger}_{b}(\mathbf{q}'-\mathbf{k})\psi_{b}(\mathbf{q}')]|0\rangle, \tag{12}$$

with Eq. (12) following from the direct evaluation of the commutators in Eq. (11). Since the ground state is symmetric under species exchange, and since the operators b and a commute, Eq. (12) implies that $\langle 0|\rho^{a}_{-\mathbf{k}}H\rho^{b}_{\mathbf{k}}|0\rangle=\langle 0|\rho^{b}_{-\mathbf{k}}H\rho^{a}_{\mathbf{k}}|0\rangle=0$. On the other hand, if in Eq. (12) we replace b with a we obtain the usual sum rule $\langle 0|\rho^{a}_{-\mathbf{k}}H\rho^{a}_{\mathbf{k}}|0\rangle=(\hbar^{2}k^{2}/2m)V^{-1}\langle 0|\Sigma_{\mathbf{q}}\psi^{\dagger}_{a}(\mathbf{q})\psi_{a}(\mathbf{q})|0\rangle$, which implies that for the even and odd modes the exact-f sum rule applies [15]: $\langle 0|\rho^{\pm}_{-\mathbf{k}}H\rho^{\pm}_{\mathbf{k}}|0\rangle=nk^{2}/2m$, or, which is equivalent to

$$n\int d\omega\,\omega S^{\pm}(k,\omega)=\frac{nk^{2}}{2m}, \tag{13}$$

with

$$S^{\pm}(k,\omega)=n^{-1}\sum_{\nu}|\langle\nu|\rho^{\pm}_{\mathbf{k}}|0\rangle|^{2}\delta(\omega-\omega_{\nu}) \tag{14}$$

the dynamic structure factor of the even and odd modes. The excitation energies are therefore given by

$$\omega^{\pm}_{\mathbf{k}}=\frac{k^{2}}{2mS^{\pm}(k)}, \tag{15}$$

with $S^{\pm}(k)=\int d\omega S^{\pm}(k,\omega)$ the corresponding static-structure factor.

We can establish compressibility sum rules for $S^{\pm}(k,\omega)$ by considering the response of the system to an external perturbation $H'_{\pm}=\lambda/2\Sigma_{\mathbf{k}}(\rho^{\pm}_{\mathbf{k}}+\rho^{\pm}_{-\mathbf{k}})$ that couples to either the even or odd modes. We follow the analysis of Ref. [14] and assume that in the long wave-length limit the perturbed wave function is locally the same as the unperturbed one with a modulated density (even or odd for each mode). We obtain

$$\lim_{k\to 0}\int d\omega\frac{S^{\pm}(k,\omega)}{\omega}=\frac{1}{2mv^{2}_{\pm}}, \tag{16}$$

with

$$v^{2}_{+}=\frac{n}{m}\frac{\partial^{2}\epsilon_{0}(n,n_{-})}{\partial n^{2}},\quad v^{2}_{-}=\frac{n}{m}\frac{\partial^{2}\epsilon_{0}(n,n_{-})}{\partial n^{2}_{-}}, \tag{17}$$

and $\epsilon_{0}(n,n_{-})$ the ground-state energy per unit volume written as a function of the total density $n=n_{a}+n_{b}$ and the density difference $n_{-}=n_{a}-n_{b}$. Since in the long wave-length limit the sum rules are exhausted by the above quasiparticles [15] $[\lim_{k\to 0}S^{\pm}(k,\omega)=S^{\pm}(k)\delta(\omega-\omega^{\pm}_{\mathbf{k}})]$, the sum rules (13) and (16) imply that two branches have energies $\omega^{\pm}_{\mathbf{k}}=v_{\pm}k$, with the corresponding structure factors given by $S^{\pm}(k)=k/2mv_{\pm}$. The low-energy spectrum therefore consists of two linear modes, corresponding to modulations of the density with the two species ‘‘in phase’’(even mode) and ‘‘out of phase’’(odd mode), respectively. The odd mode has total density n constant in all space, and in the spinor language (where the species index is treated as a spin 1/2) corresponds to a spin density wave. We can see qualitatively that the odd modes have lower frequency by perturbing around low values of the interspecies interaction. For $U^{x}=0$ the even and odd modes are degenerate. If we turn on U^{x} the odd mode will have lower expectation value $\langle U^{x}\rangle$ since locally $\langle\rho_{a}(\mathbf{x})\rho_{b}(\mathbf{x})\rangle_{+}>\langle\rho_{a}(\mathbf{x})\rho_{b}(\mathbf{x})\rangle_{-}$. This is reasonable as long as the repulsive component of U^{x} is dominant. If we now increase U^{x} we will reach the instability discussed above: when $U^{x}=U^{a}$ the ground state is multiply degenerate with all the polarized wave functions $|\Psi_{0}[(N-M)/2,(N+M)/2]\rangle$ $(M=-N,\ldots,N)$ having the same energy. This implies that $v_{-}\to 0$, since $\epsilon_{0}(n,n_{-})=\epsilon_{0}(n,0)$. Therefore the instability towards a polarized state is signaled by a vanishing velocity of the odd modes, or, equivalently, by a divergence of the ‘‘compressibility’’ $\kappa_{-}\propto[\partial^{2}\epsilon_{0}(n,n_{-})/\partial n^{2}_{-}]^{-1}$ associated with changes in species polarization at constant particle number.

Finally, we note that our proof is not valid in the presence of a field coupling the two species of the form $\mathcal{R}\int d^{3}x[\psi^{\dagger}_{a}(\mathbf{x})\psi_{b}(\mathbf{x})+\mathrm{H.c.}]$. This term corresponds (in the spinor language) to a magnetic field tilted with respect to the direction of the otherwise fully polarized system. If the system is prepared in the unstable regime with fixed N_{a} and N_{b} and no mechanism of interconversion is allowed, our proof indicates that the system will separate into two phases. This kind of phase separation was discussed within the Bogoliubov model by Nepomnyaschii [16]. An infinitesimal coupling with a heat bath that allows the system to equilibrate will equate the chemical potentials of both species and induce a transition to a state of one species only. The precise kinetics and the time scale to reach equilibrium are beyond the scope of our paper.

When $\mathcal{R}\neq 0$ the solutions will not be completely polarized even in the case where $U^{x}>U^{a}$, but the ground state will be ‘‘rotated’’ with respect to the quantization axis in species space. The detailed mean-field analysis of this problem is the subject of a forthcoming paper [17].

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[1] M.H. Anderson *et al.* Science **269**, 198 (1995); K.B. Davis *et al.*, Phys. Rev. Lett. **75**, 3969 (1995); C.C. Bradley *et al.*, *ibid.* **78**, 985 (1997).

[2] See, for example, F. Dalfovo, S. Giorgini, L.P. Pitaevskii, and S. Stringari, Rev. Mod. Phys. **71**, 463 (1999), and references therein.

[3] C.J. Myatt *et al.*, Phys. Rev. Lett. **78**, 586 (1997).

[4] D.M. Stamper-Kurn *et al.*, Phys. Rev. Lett. **80**, 2027 (1998).

[5] B.I. Halperin, Phys. Rev. B **11**, 178 (1975).

[6] I.M. Khalatinov, Zh. Éksp. Teor. Fiz. **32** 653 (1957) [Sov. Phys. JETP **5**, 542 (1957)].

[7] E.D. Siggia and A.E. Ruckenstein, Phys. Rev. Lett. **44**, 1423 (1980).

[8] T.L. Ho, Phys. Rev. Lett. **81**, 742 (1998); T. Ohmi and K. Machida, J. Phys. Soc. Jpn. **67**, 1822 (1998); M. Koashi and M. Ueda, Phys. Rev. Lett. **84**, 1066 (2000); C. K Law, H. Pu, and N. Bigelow, *ibid.* **81**, 5257 (1998); T.L. Ho and S.K. Yip, *ibid.* **84**, 4031 (2000); M. Ueda, e-print cond-mat/0008189.

[9] For a detailed mean field treatment of the experiments of Ref. [3], see B.D. Esry *et al.*, Phys. Rev. Lett. **78**, 3594 (1997).

[10] E.V. Goldstein and P. Meystre, Phys. Rev. A **55**, 2935 (1997).

[11] E. M. Lifshitz and L. P. Pitaevskii, *Statistical Physics* (Pergamon, New York, 1980), Part 2.

[12] See P. S. Julienne, in *Ultra-Cold Collisions of Atoms and Molecules*, edited by P. Sabatier and E. R. Pike (Academic Press; New York), Chap. 2.6.3; J. Weiner *et al.*, Rev. Mod. Phys. **71**, 1 (1999).

[13] K. Huang and A. Klein, Ann. Phys. (N.Y.) **30**, 203 (1964).

[14] K. Huang, in *Statistical Mechanics* (Wiley New York, 1987), pp. 325–328 and Appendix A.4.

[15] P. Nozieres and D. Pines, *The Theory of Quantum Liquids* (Addison-Wesley, New York, 1990), Vol. 2 p. 26.

[16] Y.A. Nepomnyaschii, Theor. Mat. Phys. **20**, 904 (1974) [Theor. Math. Phys. **20**, 399 (1974)].

[17] C. P. Search, A. G. Rojo, and P. R. Berman, Phys. Rev. A **64**, 013615 (2001); C.P. Search, A.G. Rojo, and P.R. Berman, e-print cond-mat/0012010.