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NONLINEARITY EFFECTS IN WAVE PROPAGATION IN MULTICOMPONENT BOSE–EINSTEIN CONDENSATES

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We consider a spinor Bose–Einstein condensate in its polar ground state. We analyze magnetization waves of a finite amplitude and show that their nonlinear coupling to density waves dramatically changes the dependence of the frequency on the wavenumber. On the contrary, the density wave propagation is much less modified by nonlinearity effects. A similar phenomenon in a miscible two-component condensate is also studied.

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Recent advances in the experimental creation of multicomponent atomic Bose–Einstein condensates (BEC) [1–3] have given rise to the interest in physical properties of such systems. There are numerous works on the properties of degenerate Bose gas mixtures in magnetic traps related to both the ground state [4] and the collective excitations [5]. In Ref. [5], the early work [6] related to a homogeneous Bose gas mixture was generalized to the case of the external harmonic trap potential. Evidently, the number of branches of the dispersion law is equal to the number of different components in the mixed BEC. Because of a nonzero interaction between them, the normal mode oscillations imply a simultaneous mutually coherent motion of the components. In the present paper, however, we first consider a multicomponent BEC of another kind, namely, a spinor BEC. Such a degenerate quantum system can be created in an optical trap, where all the atoms are confined practically independently of m_f, their momentum projection to an arbitrary axis. This independence of the confinement from the spin orientation is a striking feature and a key advantage of optical traps, well justified experimentally [2, 3]. The spin orientation then becomes a new degree of freedom. The differences and similarities between a two-component BEC with fixed values of m_f for both components and a spinor BEC in the context of our study are discussed at the end of this paper.

We note that in all the cited works on collective excitations in multicomponent BECs and in the seminal works on spinor BEC dynamics [7], the oscillation amplitudes were assumed to be sufficiently small to provide linearization of the set of the coupled time-dependent Gross–Pitaevskii equations (GPE). A proper linear transformation then yields equations of the harmonic-oscillator type for the normal modes. But the GPE is essentially nonlinear, and the effects of a finite amplitude of oscillations therefore occur. There are some approaches to taking the nonlinearity into account. The first is to find particular solutions of the GPE in the form of solitons (see, e.g., recent work [8] and references therein). The second approach is to find the oscillating nonlinear solutions that in the case of an infinitesimally small oscillation amplitude coincide with the corresponding eigenfunctions of the linearized version of the GPE or of the equivalent set of quantum hydrodynamical equations. An elegant formalism has been developed for nonlinear oscillations of a scalar BEC in a harmonic trap in the Thomas–Fermi regime [9]. It has been found that nonlinear effects become important if the fraction of mass of the scalar BEC involved in the oscillatory motion is comparable to unity.

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In the present paper, we investigate the validity of the approximation based on the linearization of the GPE by proceeding as follows. We consider plane waves in a spatially homogeneous multicomponent BEC. This can serve as a WKB approximation for excitations in a trapped BEC if the excitation wavelength is much smaller than the atomic cloud size. Moreover, this approach allows us to use, in the most direct and straightforward way, the standard technique of expanding a solution into a series in a small parameter, known as the standard perturbation theory in classical mechanics [10]. The analysis of plane waves in a translationally invariant BEC also provides a possibility of comparing the results with the rigorous analytic formulas in Refs. [6, 7].

The main result of our work is that certain modes in a multicomponent BEC exhibit a strongly nonlinear behavior: the anharmonicity effects become significant even for a relatively small wave amplitude. This effect is absent for the scalar BEC.

We consider a spinor BEC composed of atoms with the spin $f = 1$ at zero temperature. In the mean-field approximation, the GPE governing the evolution of the complex order parameter (the macroscopic wave function) $\psi(\mathbf{r}, t)$ of the BEC is given by [7]

$$i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2M}\nabla^2\psi - \mu\psi + \hbar c_0(\tilde{\psi}^*\psi)\psi + \\ + \hbar c_2(\tilde{\psi}^*\hat{\mathbf{f}}\psi)\cdot(\hat{\mathbf{f}}\psi), \quad (1)$$

where $\hat{\mathbf{f}}$ is the single-atom angular momentum operator, a vector whose Cartesian components are 3×3 matrices, M is the mass of the atom, and μ is the chemical potential. The coupling constants are defined as

$$\hbar c_0 = \frac{g_0 + 2g_2}{3}, \quad \hbar c_2 = \frac{g_2 - g_0}{3}, \quad g_F = \frac{4\pi\hbar^2 a_F}{M}$$

and a_F is the s-wave scattering length for a pair of slow atoms with the total angular momentum F equal to 0 or 2, respectively. Practically, the magnitudes of these two scattering lengths are close each to other, and hence, $|c_2/c_0| \ll 1$. The order parameter ψ has three components corresponding to the momentum projections to the z axis given by $m_f = 0, \pm 1$,

$$\psi = \begin{pmatrix} \zeta_1 \\ \zeta_0 \\ \zeta_{-1} \end{pmatrix}\sqrt{n},$$

where n is the total equilibrium density of the BEC. We let $\tilde{\psi}$ denote the transposed vector. In other words, the ground state components of the vector ζ are normalized by the condition

$$\sum_{m_f=-1}^{1}\left|\zeta_{m_f}^{(ground)}\right|^2 = 1. \quad (2)$$

We assume that the interaction of atoms in the BEC, is repulsive, i.e., $c_0 > 0$. For definiteness, we also assume that $c_2 > 0$. It follows from the latter condition that the ground state of the system is the so-called polar state [7]. This implies that in the mean-field picture, all the atoms have zero momentum projection on a certain axis. This state is degenerate with respect to the orientation of this axis. We let this axis be the z-axis; in the equilibrium, with the time derivative of ψ in Eq. (1) vanishing, we then have

$$\zeta_{\pm 1}^{(ground)} = 0, \quad \zeta_0^{(ground)} = 1.$$

The chemical potential of the BEC in the polar state is $\mu = c_0 n$.

Before writing Eq. (1) in the explicit form, we introduce the new unknown functions

$$\xi_\pm = \frac{\zeta_1 \pm \zeta_{-1}^*}{\sqrt{2}}, \quad \eta_p = \mathrm{Re}\,\zeta_0 - 1, \quad \eta_i = \mathrm{Im}\,\zeta_0.$$

Equation (1) can then be transformed to the set of equations

$$-\frac{\partial}{\partial t}\xi_- = -\frac{\hbar}{2M}\nabla^2\xi_+ + 2c_2 n\xi_+ + \\ + c_0 n(\xi_+^*\xi_+ + \xi_-^*\xi_- + 2\eta_p + \eta_p^2 + \eta_i^2)\xi_+ + c_2 n\times \\ \times[(\xi_+\xi_-^* - \xi_+^*\xi_- + 2\eta_i + 2\eta_p\eta_i)\xi_- + 2(2\eta_p + \eta_p^2)\xi_+], \quad (3)$$

$$\frac{\partial}{\partial t}\xi_+ = -\frac{\hbar}{2M}\nabla^2\xi_- + c_0 n\times \\ \times(\xi_+^*\xi_+ + \xi_-^*\xi_- + 2\eta_p + \eta_p^2 + \eta_i^2)\xi_- + \\ + c_2 n[(\xi_+\xi_-^* - \xi_+^*\xi_- + 2\eta_i + 2\eta_p\eta_i)\xi_+ + 2\eta_i^2\xi_-], \quad (4)$$

$$-\frac{\partial}{\partial t}\eta_i = -\frac{\hbar}{2M}\nabla^2\eta_p + 2c_0 n\eta_p + c_0 n\times \\ \times[(\xi_+^*\xi_+ + \xi_-^*\xi_- + 3\eta_p + \eta_p^2 + \eta_i^2)\eta_p + \\ + \xi_+^*\xi_+ + \xi_-^*\xi_- + \eta_i^2] + c_2 n\times \\ \times[2\xi_+^*\xi_+\eta_p + 2\xi_+^*\xi_+ + (\xi_+^*\xi_- + \xi_+\xi_-^*)\eta_i], \quad (5)$$

$$\frac{\partial}{\partial t}\eta_p = -\frac{\hbar}{2M}\nabla^2\eta_i + c_0 n\times \\ \times(\xi_+^*\xi_+ + \xi_-^*\xi_- + 2\eta_p + \eta_p^2 + \eta_i^2)\eta_i + c_2 n\times \\ \times[2\xi_-^*\xi_-\eta_i + (\xi_+^*\xi_- + \xi_+\xi_-^*)\eta_p + \xi_+^*\xi_- + \xi_+\xi_-^*]. \quad (6)$$

If we neglect all the nonlinear terms in Eqs. (3)–(6), we immediately obtain solutions in the form of plane monochromatic waves and the corresponding dispersion laws [7]. The first mode is the density wave; in the linear approximation, it corresponds to the periodic oscillations of the $m_f = 0$ component of the order parameter only (i.e., of η_p, η_i), while ξ_+ and ξ_- remain zero. Density waves in a spinor BEC are the same as sound waves in a scalar BEC. The dependence of the frequency ω_{d0} of density waves on the wavenumber k is of the Bogoliubov type,

$$\omega_{d0}^2(k) = \omega_r(k)[\omega_r(k) + 2c_0 n],$$

where

$$\omega_r(k) = \frac{\hbar k^2}{2M}$$

is the recoil frequency associated with the kinetic momentum $\hbar k$. Another branch of the excitation spectrum in a spinor BEC is related to magnetization waves. The left and right circularly polarized magnetization modes are degenerate: in the linear regime, their frequency is given by

$$\omega_{m0}^2(k) = \omega_r(k)[\omega_r(k) + 2c_2 n].$$

The quantum mechanical mean values of the atomic magnetic momentum operator are proportional to ξ_+ and ξ_+^* for the left and right polarization, respectively.

We can now determine the effects of nonlinearity on the magnetization wave propagation using the perturbation theory of classical mechanics [10]. We expand our unknown functions into series as

$$\xi_+ = \sum_{j=0}^{\infty} \xi_+^{(j)},$$

where $\xi_+^{(j)}$ is proportional to the jth power of a certain small parameter ε (in fact, the square of the magnetization amplitude can be naturally regarded as this parameter). Similar expansions hold for the remaining three functions. The zeroth order approximation can also be taken in the form of a plane wave,

$$\xi_+^{(0)} = A_+ \sin(\omega t - \mathbf{k}\cdot\mathbf{r}),$$

but with the frequency ω shifted with respect to the nonperturbed value ω_{m0}. The validity of this method is restricted to the case where the resulting correction to the frequency is small,

$$\left| \frac{\omega - \omega_{m0}}{\omega_{m0}} \right| \ll 1.$$

We also take

$$\xi_-^{(0)} = \omega_r(k)^{-1} \omega A_+ \cos(\omega t - \mathbf{k}\cdot\mathbf{r}),$$

$$\eta_p^{(0)} = 0, \quad \eta_i^{(0)} = 0.$$

The difference between ω and ω_{m0} can also be represented as a series in ε, beginning with the term of the order ε^1.

To find the correction to the frequency of a magnetization wave, we make the following transformation of our set of GPEs. We add to and substract from the right-hand side of Eq. (1) the term $\omega^2\xi_+/\omega_r(k)$. We then note that our zeroth order approximation satisfies the set of equations

$$-\frac{\partial \xi_-}{\partial t} = \frac{\omega^2 \xi_+}{\omega_r(k)}, \quad \frac{\partial \xi_+}{\partial t} = \omega_r(k)\xi_-$$

identically. The remaining terms must be regarded as a perturbation leading to the frequency shift in higher orders of the approximation. Equations (3)–(6) must be satisfied in every order in ε separately, and therefore, all the terms of the order ε^j in the right-hand side must be grouped and set equal to the $O(\varepsilon^j)$ part of the left-hand side of the equation. We restrict our analysis to the linear order in ε, where we obtain

$$-\frac{\partial}{\partial t}\xi_-^{(1)} = \frac{\omega^2}{\omega_r(k)}\xi_+^{(1)} + \left\{ \omega_r(k) + 2c_2 n - \frac{\omega^2}{\omega_r(k)} \right\}^{(1)} \times A_+ \sin(\omega t - \mathbf{k}\cdot\mathbf{r}) + c_0 n \left[\sin^2(\omega t - \mathbf{k}\cdot\mathbf{r}) + \frac{\omega^2}{\omega_r^2(k)} \cos^2(\omega t - \mathbf{k}\cdot\mathbf{r}) \right] \times A_+^3 \sin(\omega t - \mathbf{k}\cdot\mathbf{r}), \quad (7)$$

$$\frac{\partial}{\partial t}\xi_+^{(1)} = \omega_r(k)\xi_-^{(1)} + \frac{\omega}{\omega_r(k)} c_0 n \times \left[\sin^2(\omega t - \mathbf{k}\cdot\mathbf{r}) + \frac{\omega^2}{\omega_r^2(k)} \cos^2(\omega t - \mathbf{k}\cdot\mathbf{r}) \right] \times A_+^3 \cos(\omega t - \mathbf{k}\cdot\mathbf{r}). \quad (8)$$

Here, the symbol $\{\ldots\}^{(1)}$ means that only the linear contribution in $\varepsilon \sim A_+^2$ to the expression in the curly brackets is retained. The amplitude A_+ is taken to be real without losing the generality.

Equations (7) and (8) can be easily reduced to the differential equation

$$\frac{\partial^2}{\partial t^2}\xi_+^{(1)} + \omega^2 \xi_+^{(1)} + \left\{ \omega_{m0}^2 - \omega^2 + \frac{c_0 n \omega_r(k)}{4} \times \left[3 + 4\frac{\omega^2}{\omega_r^2(k)} + 3\frac{\omega^4}{\omega_r^4(k)} \right] A_+^2 \right\}^{(1)} \times A_+ \sin(\omega t - \mathbf{k}\cdot\mathbf{r}) + C A_+^3 \sin[3(\omega t - \mathbf{k}\cdot\mathbf{r})] = 0, \quad (9)$$

where C is a certain combination of various frequency parameters of the problem; its calculation is not needed for the determination of the lowest-order correction to the wave frequency.

Equation (9) is inhomogeneous, and the presence of the resonant source term proportional to $\sin(\omega t - \mathbf{k}\cdot\mathbf{r})$ leads to the occurrence of oscillations in the solution for $\xi_+^{(1)}$ with the amplitude growing linearly in time. The essence of the method used here [10] is to avoid these nonphysical (secular) solutions proportional to $t\sin(\omega t - \mathbf{k}\cdot\mathbf{r})$ by setting the prefactor of the resonance term to zero. To the lowest order in the square of the wave amplitude, the magnetization wave frequency is therefore given by

$$\omega^2 = \omega_{m0}^2 + \frac{c_0 n\omega_r(k)}{4}\left[3+4\frac{\omega_{m0}^2}{\omega_r^2(k)}+3\frac{\omega_{m0}^4}{\omega_r^4(k)}\right]A_+^2. \quad (10)$$

In the two limiting cases (of the short and long wavelength), we obtain

$$\omega^2 = \omega_r^2(k) + \frac{5}{4}u_0^2k^2A_+^2, \quad \hbar k \gg Mu_2, \quad (11)$$

and

$$\omega^2 = u_2^2k^2 + 6u_0^2k^2\left(\frac{Mu_2}{\hbar k}\right)^4 A_+^2, \quad \hbar k \ll Mu_2. \quad (12)$$

Here,

$$u_F = \sqrt{\hbar c_F n/M}$$

are the propagation velocities of the density ($F=0$) and magnetization ($F=2$) waves of an infinitely small amplitude in the long wavelength limit. We can therefore conclude that the nonlinearity effects are small until

$$A_+^2 \ll 1, \quad \hbar k \gg Mu_0, \quad (13)$$

$$A_+^2 \ll \left(\frac{\hbar k}{Mu_0}\right)^2, \quad Mu_2 \lesssim \hbar k \lesssim Mu_0, \quad (14)$$

$$A_+^2 \ll \frac{c_2}{c_0}\left(\frac{\hbar k}{Mu_2}\right)^4, \quad \hbar k \ll Mu_2. \quad (15)$$

Interestingly, the condition that the nonlinearity is small coincides with the trivial condition that A_+^2 is small compared to the sum of squares of the absolute values of all the three components $\zeta_{m_f}^{(ground)}$ in the ground state, which is unity in accordance with Eq. (2) only in the short wavelength limit of Eq. (13). In the other cases [Eqs. (14) and (15)], even a small but finite excitation amplitude can result in a significant modification of the wave propagation.

It is easy to show that in the case of magnetization waves, there are no resonance terms in the right-hand sides of Eqs. (5) and (6) in the first order in ε, and these equations do not therefore contribute to the evaluation of the corresponding correction to the wave frequency.

Density waves can be analyzed similarly, and the lowest-order correction results in the formula

$$\omega^2 = \omega_{d0}^2 + \frac{3}{4}c_0 n\omega_r(k)A_p^2, \quad (16)$$

where A_p is the amplitude of the oscillations of η_p. For all momenta k, the correction is small provided that $A_p \ll 1$, i.e., nonlinear effects play a less significant role for waves of this type than for the magnetization waves. Equation (16) also applies to sound waves in a single-component (scalar) BEC.

Because ω_{m0} is independent of c_0 but the latter quantity appears in the right-hand side of Eq. (10), we conclude that the nonlinear coupling to density waves plays a key role in the modification of the magnetization wave frequency. On the contrary, Eq. (16) does not contain c_2, and a travelling density wave is therefore not coupled to magnetization modes.

We now briefly discuss the case of a mixture of two BECs, each of which has a fixed value of m_f, or equivalently, of two scalar BECs. Here, we first must introduce the coupling constants

$$g_{j'j} = 2\pi\hbar a_{j'j}\frac{M_j + M_{j'}}{M_jM_{j'}},$$

where M_j is the mass of an atom of the j-th kind and $a_{j'j}$ is the s-wave scattering length for a pair of atoms of the j-th and j'-th kind, j', $j = 1, 2$. The dispersion laws for the two excitation branches were obtained in the analytic form in Ref. [6] (see also Ref. [5]). If all the three relevant scattering lengths are positive, the criterion of stability of a homogeneous BEC mixture against phase separation is simply $g_{12} < \sqrt{g_{11}g_{22}}$. In this case, the eigenmode frequencies are positive for all values of the momentum k. For simplicity, we here consider the case of equal atomic masses, $M_1 = M_2 \equiv M$. The eigenfrequencies are then simply

$$\omega_\pm^2 = \omega_r(k)[\omega_r(k) + 2\Lambda_\pm],$$

where

$$\Lambda_\pm = [g_{11}n_1 + g_{22}n_2 \pm \sqrt{(g_{11}n_1 - g_{22}n_2)^2 + 4g_{12}^2n_1n_2}\,]/2,$$

n_1, n_2 are the equilibrium number densities of the components, and $\omega_r(k)$ is defined above.

The order parameter perturbation for the j-th component is given by

$$\delta\psi_j = \sqrt{n_1}A_j[\sin(\omega t - \mathbf{k}\cdot\mathbf{r}) + i\omega_r^{-1}(k)\omega\cos(\omega t - \mathbf{k}\cdot\mathbf{r})].$$

After some tedious but straightforward calculations, which are similar to those described above and are valid under the same condition of smallness of the frequency correction, we arrive at the following formula for the wave frequency shifted due to the nonlinearity effects:

$$\omega^2 = \omega_\pm^2 + \frac{\omega_r(k) g_\pm n_1}{2} \left[3 + 4\frac{\omega_\pm^2}{\omega_r^2(k)} + 3\frac{\omega_\pm^4}{\omega_r^4(k)} \right] B_\pm^2. \quad (17)$$

Here, the upper sign corresponds to the case where $B_+ \neq 0$ and $B_- = 0$, and the lower sign corresponds to the opposite case, $B_+ = 0$ and $B_- \neq 0$. The eigenmode amplitudes are defined as

$$\begin{aligned} B_+ &= \cos\theta_g\, A_1 + \sqrt{\frac{n_2}{n_1}} \sin\theta_g\, A_2, \\ B_- &= -\sin\theta_g\, A_1 + \sqrt{\frac{n_2}{n_1}} \cos\theta_g\, A_2. \end{aligned} \quad (18)$$

By definition, we also set

$$g_+ = g_{11}\cos^4\theta_g + 2g_{12}\cos^2\theta_g \sin^2\theta_g + g_{22}\sin^4\theta_g, \quad (19)$$

$$g_- = g_{11}\sin^4\theta_g + g_{22}\cos^4\theta_g, \quad (20)$$

$$\operatorname{tg}\theta_g = \\ = \frac{g_{22}n_2 - g_{11}n_1 + \sqrt{(g_{22}n_2 - g_{11}n_1)^2 + 4g_{12}^2 n_1 n_2}}{2g_{12}\sqrt{n_1 n_2}}. \quad (21)$$

Equation (17) is similar to Eq. (10) and leads to a similar restriction on the wave amplitude. If the two BECs are composed of atoms accumulated on two different magnetic or hyperfine sublevels of the ground internal state, the difference between g_{12} and $\sqrt{g_{11}g_{22}}$ is relatively small, and the lower-frequency mode is extremely sensitive to the effects of nonlinearity in the long wavelength limit. We note that both branches of the excitation spectrum of a two-component BEC in an external magnetic field are sensitive to nonlinear effects for small k, while the spinor BEC collective excitations exhibit a different behavior: the nonlinearity effects are much more important for magnetization waves than for density waves.

In summary, we must note that the nonlinearity effects in the wave propagation in a BEC studied here are related to the Beliaev damping [11] (cf. the closely related recent publication [12] on an efficient damping of the relative motion of two condensates in a trap by a nonlinear interaction). The Beliaev damping is also described by the cubic nonlinear term in the GPE. It is in fact the decay of a collective excitation quantum into two quata of lower energies, provided that the energy and momentum are conserved. This process results in the occurrence of an imaginary part of the wave frequency (the damping constant). In the present paper, we have calculated the real small addend to the wave frequency. While the Beliaev damping becomes less important as k approaches zero, nonlinear corrections to the magnetization mode in the spinor BEC and to each of the modes in the usual two-component BEC become more pronounced.

Finally, we present a numeric example. The ground state of a spinor BEC of sodium atoms with $f = 1$ is simply a polar (antiferromagnetic) state [2]. We take $(a_0 + 2a_2)/3 \approx 5$ nm, $(a_2 - a_0)/3 \approx 0.08$ nm and set $n \approx 10^{14}$ cm^{-3}. We let the excitation wavenumber be about $3.5 \cdot 10^3$ cm^{-1} (the corresponding wavelength is several times smaller than the atomic cloud size in the experiment with a large number of atoms in a trap as in Ref. [2], and therefore, the WKB approximations is still satisfactory). As $A_+ \to 0$, the linear theory [7] gives the magnetization wave frequency $\omega_{m0} \approx 300$ s^{-1}. But if $A_+ \approx 0.044$, in other words, only

$$[1 + \omega_r^{-2}(k)\omega^2] A_+^2/2 \approx 0.005$$

of the total mass of the BEC is involved into the motion, then the frequency rises by one third of its primary value and becomes equal to 400 s^{-1} in accordance with Eq. (10). Similarly, a strongly nonlinear behavior of low-lying magnetization modes of the spinor BEC in a finite-size optical trap can be expected because the trapped BEC spectrum must reveal the most important qualitative features present in the translationally invariant case, as has been shown for two-component BECs in magnetic traps [5].

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