Sum Rule Approach to Collective Oscillations of Boson-Fermion Mixed Condensate of Alkali Atoms

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The system is described by the Hamiltonian of in- and out-of-phase oscillations of the boson and fermion condensates.

For the mixed condensate, we introduce a mixing angle of the boson/fermion excitation operators so as to allow the sum rule approach \[3,4\] that has proved to be successful in the studies of collective excitations of Bose condensates.

relevant multipole operator \(E\) useful expression for the average energy of the collective oscillation \[3,7\]. The moments are calculated from formulae.

Studies of collective motions of BEC have been intensively performed. Quite recently the degenerate Fermi gas of phenomena of quantum systems under ideal conditions. Up to now the experimental \[2\] as well as theoretical \[3–5\] realization of the Bose-Einstein condensates (BEC) for trapped Alkali atoms \[1\] offers a possibility to study such static properties \[10–12\], stability conditions \[13,14\], and some dynamical properties \[15,16\] of trapped boson-fermion condensates have been investigated. In the present paper, we study the behavior of collective oscillations of a boson-fermion mixed condensate at \(T = 0\) for both repulsive and attractive boson-fermion interactions. We adopt the sum rule approach \[3,4\] that has proved to be successful in the studies of collective excitations of Bose condensates. For the mixed condensate, we introduce a mixing angle of the boson/fermion excitation operators so as to allow the in- and out-of-phase oscillations of the boson and fermi condensates.

In the sum rule approach we first calculate the energy weighted moments \(m_p = \sum_j (E_j - E_0) \rho_{j}(j|F|0)\) of the relevant multipole operator \(F\), where \(j\)'s represent the complete set of eigenstates of the Hamiltonian with energies \(E_j\), and \(|0\rangle\) denotes the ground state. The excitation energy is expressed as \(\hbar \omega = (m_3/m_1)^{1/2}\) which provides a useful expression for the average energy of the collective oscillation \(\langle F|F\rangle\). The moments are calculated from formulae \(m_1 = \frac{1}{2}(0[F^1, [H, F]] |0\rangle\) and \(m_3 = \frac{1}{2}(0[[F^1, H], [H, [H, F]]]|0\rangle\). We consider three types of multipole operators which are defined by

\[F_{\alpha}^\pm = \sum_{i=1}^{N_b} f_\alpha(\vec{r}_{bi}) \pm \sum_{i=1}^{N_f} f_\alpha(\vec{r}_{fi}), \quad (\alpha = M, D, Q)\]

where the functions \(f_\alpha\) are defined by \(f_M(\vec{r}) = r^2\) for monopole, \(f_D(\vec{r}) = z\) for dipole, and \(f_Q(\vec{r}) = 3z^2 - r^2\) for quadrupole excitations. The indices \(b, f\) denote boson/fermion, \(N_b, N_f\) the numbers of bose/fermi particles, and \pm correspond to the in-phase and out-of-phase oscillation of the two types of particles. We actually take a linear combination of the form

\[F_\alpha(r; \theta) = F_\alpha^+ \cos \theta + F_\alpha^- \sin \theta \quad (-\frac{\pi}{2} < \theta \leq \frac{\pi}{2})\]

parametrized by the mixing angle \(\theta\). We study the value of \(\theta\) that minimizes the calculated frequency \(\omega\) for each \(\alpha\).

We consider the polarized boson-fermion mixed condensate in spherically symmetric harmonic oscillator potential. The system is described by the Hamiltonian

\[H = \sum_{i=1}^{N_b} \left\{ \frac{\vec{p}_{bi}^2}{2m} + \frac{1}{2}m\omega_b^2 r_{bi}^2 + \frac{1}{2} \sum_{j=1}^{N_f} \delta(\vec{r}_{bi} - \vec{r}_{bj}) \right\} + \sum_{i=1}^{N_f} \left\{ \frac{\vec{p}_{fi}^2}{2m} + \frac{1}{2}m\omega_f^2 r_{fi}^2 + \frac{1}{2} \sum_{j=1}^{N_f} \delta(\vec{r}_{fi} - \vec{r}_{fj}) \right\} + \hbar \sum_{i=1}^{N_b} \sum_{j=1}^{N_f} \delta(\vec{r}_{bi} - \vec{r}_{fj})\]
where we assume the same oscillator frequencies and masses for bosons and fermions for simplicity. The coupling constants \( g, h \) are the boson-boson/boson-fermion interaction strengths represented by the s-wave scattering lengths \( a_{bb} \) and \( a_{bf} \) as \( g = 4\pi\hbar^2 a_{bb}/m \) and \( h = 4\pi\hbar^2 a_{bf}/m \). The fermion-fermion interaction has been neglected as the polarized system is considered. Following the standard calculation procedure the excitation frequencies are obtained as:

(i) Monopole

\[
\frac{\omega_M(\theta)}{\omega_0} = \sqrt{\frac{2}{1 + \frac{E_{\text{kin}}^+ + \frac{3}{2}E_{bb} + \frac{3}{2}E_{bf} + 2(E_{\text{kin}}^- + \frac{3}{2}E_{bb} + \frac{3}{2}E_{bf} - \Delta') \cos \theta \sin \theta - \Delta \sin^2 \theta}{E_{ho}^+ + 2E_{ho}^- \cos \theta \sin \theta}} \tag{4}
\]

(ii) Quadrupole

\[
\frac{\omega_Q(\theta)}{\omega_0} = \sqrt{\frac{2}{1 + \frac{E_{\text{kin}}^+ + 2E_{\text{kin}}^- \cos \theta \sin \theta - \frac{3}{2}\Delta \cos \theta \sin \theta}{E_{ho}^+ + 2E_{ho}^- \cos \theta \sin \theta}} \tag{5}
\]

(iii) Dipole

\[
\frac{\omega_D(\theta)}{\omega_0} = \sqrt{\frac{1 - \frac{4}{3\hbar\omega_0} \Omega \sin^2 \theta}{N^+ + 2N^- \cos \theta \sin \theta}} \tag{6}
\]

Here we defined \( E_{\text{kin}}^\pm = E_{bb}^\pm \pm E_{bf}^\pm, E_{ho}^\pm = E_{bb}^\pm \pm E_{ho}^\pm, \) and \( N^\pm = N_b \pm N_f, \) where \( E_{bb}^{(b,f)} \) and \( E_{ho}^{(b,f)} \) are respectively the expectation values of the kinetic and oscillator potential energies for boson/fermion in the ground state. Boson-boson and boson-fermion interaction energies have been denoted by \( E_{bb} \) and \( E_{bf} \). The quantities \( \Delta, \Delta' \) and \( \Omega \) are given in terms of the boson/fermion densities \( n_b(r), n_f(r) \) in the ground state by

\[
\Delta = \hbar \int d^3r r^2 \frac{dn_b(r)}{dr} \frac{dn_b(r)}{dr}, \quad \Delta' = \hbar \int d^3r \left[ n_f(r) \frac{dn_b(r)}{dr} - \frac{dn_f(r)}{dr} n_b(r) \right], \quad \Omega = \hbar \xi^2 \int d^3r \frac{dn_f(r)}{dr} \frac{dn_b(r)}{dr}, \tag{7}
\]

where \( \xi = \hbar/m\omega_0. \) One may use the stationary condition of the ground state,

\[
2E_{\text{kin}}^+ - 2E_{ho} + 3E_{bb} + 3E_{bf} = 0, \quad 2E_{\text{kin}}^- - 2E_{ho} - 3E_{bb} + \Delta' = 0 \tag{8}
\]

in order to eliminate in eq.\((8)\) the dependences on \( E_{bb}, E_{bf} \) and \( \Delta'. \) The monopole frequency is then rewritten as

\[
\frac{\omega_M(\theta)}{\omega_0} = \sqrt{\frac{5 - E_{\text{kin}}^+ + 2E_{\text{kin}}^- \cos \theta \sin \theta + 2\Delta \sin^2 \theta}{E_{ho}^+ + 2E_{ho}^- \cos \theta \sin \theta}} \tag{9}
\]

We have checked that the Thomas-Fermi calculation of the ground state adopted below gives rise to a negligible difference if one evaluates either the expression \((4)\) or \((5)\).

We calculate the ground state energies and densities of the boson-fermion mixed system in the Thomas-Fermi approximation which is valid for \( gN_b \gg 1 \) and \( N_f \gg 1 \) except around the surface region \([10][12][15]\). We take harmonic oscillator length \( \xi \) and energy \( \hbar\omega_0 \) as units, and define scaled dimensionless variables: the radial distance \( x = r/\xi \), boson/fermion densities \( \rho_{b,f}(x) = n_{b,f}(r)\xi^3/N_{b,f}, \) and chemical potentials \( \mu_{b,f} = 2\mu_{b,f}/\hbar\omega_0 \). We solve the coupled Thomas-Fermi equations,

\[
gN_b\rho_b(x) + x^2 + \hbar N_f\rho_f(x) = \mu_b, \quad [6\pi^2 N_f\rho_f(x)]^{2/3} + x^2 + \hbar N_b\rho_b(x) = \mu_f, \tag{10}
\]

where \( g = 2g/\hbar\omega_0\xi^3 \) and \( \hbar = 2h/\hbar\omega_0\xi^3. \)

One of the most promising candidates for the realization of the mixed condensate is the potassium isotope system. Precise values of the scattering lengths are not well known at present and different values have been reported \([17][19]\). We take for the boson-boson interaction the parameters of the \(^{41}\)K-\(^{41}\)K system in \([17]\) and a trapping frequency of 450Hz which gives \( g = 0.2. \) For the boson-fermion interaction we take several values in the range \( h/g = \hbar/g \approx -2.37 \sim 3.2. \) It should be noted that the interaction strength can be controlled using Feshbach resonances \([20]\).

We have performed a numerical calculation for \( N_b = N_f = 10^6. \) In the ground state the fermions have a much broader distribution than bosons because of the Pauli principle. Fermions are further squeezed out of the center for a repulsive boson-fermion interaction \((h > 0)\). They will eventually form a shell-like distribution around the
surface of bosons for $h/g \geq 1$ and will be completely pushed away from the center ($n_f(0) = 0$) at around $h/g \sim 3$.

For an attractive boson-fermion interaction, on the other hand, the central densities of the bosons and fermions increase together. The system becomes unstable against collapse at around $h/g = -2.37$ due to the strong attractive boson-fermion interaction [14].

Figure 1 shows the kinetic energy, the oscillator potential energy, and the interaction energy contributions to the ground state energy against the parameter $h/g$. The figure shows also the quantities $\Delta$ and $\Omega$ which represent the contributions of the boson-fermion interaction to the multipole frequencies (4)-(6) and (7). One may notice that the fermionic kinetic- and potential-energy contributions are a few times larger than the bosonic contribution in the present system. It is noted that $\Delta$ takes large negative values at both large negative and positive regions of $h/g$. In the former region the Bose and fermion density distributions become coherent due to the attractive interaction, and the radial integrals in eqs.(5) takes a large positive value. In the opposite case ($\langle h/g \rangle > 1$), the same integral changes sign because the fermions are pushed away from the center by the repulsive boson-fermion interaction, thus giving a large negative contribution in the bosonic surface region. In the region $0 < h/g < 1$, on the other hand, the integral is slightly positive and $\Delta$ takes a small positive value. The quantity $\Omega$ follows the same trend as $\Delta$, but the absolute value is much smaller than $\Delta$, as the most important contribution to the integral comes from the surface region where $r \gg \xi$.

Once the ground state parameters are obtained the frequencies (4)-(6) are minimized against $\theta$. Usually, the sum rule approach predicts a strength-weighted average energy of eigenstates for a given multipolarity. The calculated energy coincides with the true excitation energy if the relevant strength is concentrated in a single state. By adopting the minimization procedure we simultaneously determine the character of the low-lying collective mode and the corresponding average energy. The character of the mode is given by the value of $\theta$, for instance, $\theta \simeq \pi/4$ for the bosonic- and $-\pi/4$ for the fermionic-modes, $\theta \simeq 0$ for the in-phase oscillation and $\pi/2$ for the out-of-phase oscillation of the two types of particles. As there are two kinds of particles involved in eq.(2), one would expect an emergence of two types of collective oscillations for each multipole. Another collective mode would have a character orthogonal to the low-lying mode as far as the phase relation of the two operators in (2) is concerned. In the present approach we calculate the frequency of the latter mode, the high-lying one, from eqs.(4)-(6), by using the operator $F_\alpha^\dagger \sin \theta_\alpha - F_\alpha^\dagger \cos \theta_\alpha$, for each $\alpha$, where the mixing angle $\theta_\alpha$ is the one determined for the low-lying mode.

Figure 2 shows frequencies of the lower (solid lines) and the higher (dashed lines) modes for (a) monopole, (b) quadrupole and (c) dipole cases as functions of $h/g$. The corresponding mixing angles $\theta$ determined by the minimization procedure for the lower mode are plotted in Fig.3 for each multipolarity as a function of $h/g$. Below we discuss the behavior of the frequencies $\omega_\alpha$ by defining three regions of $h/g$: (I) $h/g < 0$, (II) $0 < h/g \lesssim 1$, (III) $1 \lesssim h/g$.

a) monopole:

For a non-interacting boson-fermion system the low-lying monopole mode is the fermionic oscillation with frequency $\omega_M^L = 2\omega_0$, while the higher mode is the bosonic one with $\omega_M^H = \sqrt{5}\omega_0$ in the Thomas-Fermi approximation. Around $h \simeq 0$ one may obtain $\omega_M^L \simeq 2\omega_0 \left(1 + A\hbar N^\dagger\right)$, $\omega_M^H \simeq \sqrt{5}\omega_0 \left(1 - A'\hbar^2 \frac{h}{N} N^\dagger\right)$, where $A = 3 \cdot 6\pi^2/4\sqrt{2\pi}^2$ and $A' = 7\sqrt{3}/20\pi^2 \cdot (8\pi/15)^{\dagger}$. The mixing angle for the lower mode is given as $\theta_M = -\pi/4 - \delta_M$ with $\delta_M = (5\cdot 6\pi/\sqrt{2\pi}^2)\hbar N^\dagger$. This behavior is seen in region (II) where the boson-fermion interaction is weakly repulsive and the lower monopole mode is of a fermionic character, see Fig.3 (solid line). Bosonic oscillation in this region is more rigid than the fermionic one because of the repulsive interaction among bosons. In region (I), the situation is quite different: The low-lying mode becomes a coherent boson-fermion oscillation as represented by the large negative value of $\Delta$, and the excitation energy shows a sharp decrease towards the instability point $h/g \sim -2.37$ of the ground state [14], although $\omega_M$ does not become exactly zero within our approximation. In this region the attractive boson-fermion interaction is much more effective in the excited state than in the ground state and cancels out the increase in the kinetic energy. In region (III), too, we find that the low-lying mode becomes an in-phase oscillation. Here, the boson and the fermion densities in the ground state are somewhat separated, and the in-phase motion which keeps this separation is energetically more favorable than the out-of-phase motion as seen in the value of $\Delta$.

b) quadrupole:

For the quadrupole excitation (Fig.2(b)), the lower (higher) energy mode is almost the pure bosonic (fermionic) oscillation over the broad range of the $h/g$ values studied, Fig.2 (dashed line). To the first order in $\hbar$ the frequencies of the lower and the higher quadrupole modes are given by $\omega_Q^L \simeq \sqrt{2}\omega_0 \left(1 - B\hbar N^\dagger\right)$, $\omega_Q^H \simeq 2\omega_0 \left(1 - B'\hbar^2 \frac{h}{N} N^\dagger\right)$, where $B = 6\pi^2/4\sqrt{2\pi}^2$ and $B' = (15/8\pi)^{\dagger}/(14\cdot 6\pi^2\sqrt{2\pi}^2)$. The corresponding mixing angle for the lower mode is given by $\theta_Q = \pi/4 + \delta_Q$ with $\delta_Q = 2^4 B'\hbar^2 \frac{h}{N} N^\dagger$. For the quadrupole mode similar mechanisms as for the monopole mode are at work concerning the dependence on $|h/g|$. The role of the boson-fermion interaction is however much reduced
compared with the monopole case as seen by the factor 2/5 of eq. [3], which reflects that the quadrupole oscillation has five different components. Thus the quadrupole mode obtains an in-phase character only at large values of $|h/g|$. In the other region of $|h/g|$ the low-lying mode becomes a simple bosonic oscillation. This is because the fermionic mode costs a larger kinetic energy and favors $\theta = \pi/4$ as seen in the term $(E_{\text{kin}}^b - E_{\text{kin}}^f)\sin \theta \cos \theta$ in eq. [3].

c) dipole:

General arguments [1] show that for a harmonic oscillator external potential a uniform shift of the ground state density generates an eigenstate of the system, corresponding to the boson-fermion in-phase dipole oscillation with frequency $\omega_0$. This is evident in Fig. 2c) and also in eq. [3] at $\theta = 0$. In the regions (I) and (III) the out-of-phase oscillation is unfavorable due to the same reason as for the monopole mode: It loses the energy gained in the ground state boson-fermion configuration. For a weakly repulsive $h$ an interesting possibility arises: In the region (II) the out-of-phase mode of the boson-fermion oscillation lies lower than the in-phase mode. Let us first note that at $h = 0$ the out-of-phase oscillation frequency becomes degenerate as the in-phase one because the bosonic and the fermionic dipole modes are independent. One may note that at $h/g \approx 1$ again the degeneracy occurs. Here the potential term for the fermion becomes almost linear to the fermion density itself (see, eq. [10]). This suggests that the fermion density is determined almost entirely by the chemical potentials and becomes nearly constant as far as the boson density is finite. A uniform dipole shift of fermions thus produces almost no effect on bosons, and results in the degeneracy of the frequency. Between $h/g = 0$ and 1, the boson-fermion repulsion is weaker for the out-of-phase oscillation than the in-phase one (and hence the ground state) as reflected in the sign of $\Omega$.

In the present paper, we studied collective oscillations of trapped boson-fermion mixed condensates using sum rule approach. We introduced a mixing angle of bosonic and fermionic multipole operators so as to study if the in- or out-of-phase motion of those particles is favored as a function of the boson-fermion interaction strength. For the monopole and quadrupole cases, the coupling of thebose- and fermi-type oscillation is not large for moderate values of the coupling strength $h$. At large values of $|h/g|$, the low-lying modes become an in-phase oscillation of bosons and fermions. This is especially so for the monopole oscillation at attractive boson-fermion interaction: The excitation energy of this mode almost vanishes at the instability point of the ground state. In the case of the dipole mode, in contrast, the in-phase oscillation remains an exact eigenmode with a fixed energy for harmonic oscillator potentials, while the average energy of the out-of-phase oscillation is strongly dependent on the boson-fermion interaction. We found that at weak repulsive values of the interaction the out-of-phase motion stays lower than the in-phase oscillation. In this paper we calculated also the frequencies of the high-lying modes for each multipole, by adopting the operators orthogonal to the low-lying modes. These modes, too, are collective in character and, in the present framework, their average frequencies showed rather strong dependences on the boson-fermion coupling strength. Deeper insight into the collective modes studied in this paper will require a detailed investigation of the solutions of, e.g., the self-consistent RPA type equations that allow an arbitrary radial dependence of the excitation operators. Studies in this direction are now in progress.

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FIG. 1. (a) Ground state expectation values of the fermion kinetic energy $E^{f}_{\text{kin}}$ (long dashed line), oscillator potential energies $E^{b}_{\text{ho}}$ (short-dash-dotted line) and $E^{f}_{\text{ho}}$ (long-dash-dotted line), boson-boson and boson-fermion interaction energies $E_{bb}$ (dashed line) and $E_{bf}$ (dotted line), and the quantity $\Delta$ (solid line) against the interaction strength ratio $h/g$. The values are given in the unit of $N\hbar\omega_0$ and are dimensionless. (b) The quantity $\Omega$ in the same unit.

FIG. 2. Excitation frequencies of collective oscillations (a) monopole, b) quadrupole, c) dipole) as functions of $h/g = \tilde{h}/\tilde{g}$, calculated based on the eqs.(4)-(6). The mixing angle $\theta$ has been determined so as to minimize $\omega$ for each multipole operator. The ordinates are given in the unit of $\omega_0$ and are dimensionless. The solid (dashed) lines are the lower (higher) energy mode for each oscillation.

FIG. 3. Mixing angles of in/out-of-phase excitation modes which are determined by minimizing excitation energies in Fig.3. The solid line shows the monopole, the dashed line the quadrupole, and the dotted line the dipole oscillations. Shaded areas show mainly in-phase (hatches) and mainly out-of-phase (cross-hatches) regions in $\theta$ Angles for pure bosonic- or fermionic-modes are also indicated.
FIG. 1 Ground state expectation values
FIG. 2 Excitation frequencies
FIG. 3 Mixing angles