# Collective Excitation of a Hybrid Atomic/Molecular Bose Einstein Condensate[*]

Chi-Yong. Lin[†], M.S. Hussein[‡], A. F. R. de Toledo Piza

*Instituto de Física, Universidade de São Paulo, CP 66318*

*CEP 05389-970, São Paulo, SP, Brazil*

E. Timmermans

*T-4, Los Alamos National Laboratory*

*Los Alamos, NM 87545, U.S.A.*

## ABSTRACT

The collective excitation of hybrid atomic-molecular condensate are studied using variational method. The dipole response of the system is studied in detail. We found that the out-of-phase dipole oscillation frequency increasing slowly with the detuning parameter and is only few times large than the trap frequency making the experimental observation of this mode of vibration feasible.

The recent realization of Bose-Einstein condensation (BEC) in a dilute gas of alkali atoms has open a new opportunity for the theoretical and experimental investigation in quantum degenerate many-body systems [1, 2]. In contrast to superfluid helium, these weakly interacting gases are much more amenable to the theoretical prediction and quantative analysis. After the observations of such condensates, a new generation of more complex experiments has been done involving the production of multiple species BEC. Such mixture may consist of different hypefine states of same atom or different spin state of same stomic species. In the former case the composition of mixture remains fixed and in the later case the internal conversion leads to important new phenomena. It has been proposed that the interation that bring a binary atom system to an intermediate state molecule in the Feshbach resonance, recently observed in BEC[3, 4], create in the dilute atomic Bose-Eintein condensate (BEC) a second molecular condensate component[5]. The communication between the atomic and molecular condensates ensues through a Josephson-like oscillation of atom pair. It was found that the ground state of this hybrid condensate is a dilute BEC with liquid-like properties of a self-determined density. These findings were obtained using a homogeneous gas approximation (no confining potential). In this work we investigate the collective excitations of the hybrid system of atoms and molecules subjected to an appropriate trap. In particular we derive an appproximate expression for the dipole frequency of the out-of-phase oscillations of the atomic and molecular condensate centers of mass and investigate its dependence on the detuning and Feshbach resonance parameters.

The mean-field hamiltonian density describing the trapped system is

$$\mathcal{H} = \psi_a^* \left[ -\frac{\hbar^2 \nabla^2}{2m} + V_a(\mathbf{r}) + \frac{\lambda_a}{2} \psi_a^* \psi_a \right] \psi_a + \psi_m^* \left[ -\frac{\hbar^2 \nabla^2}{4m} + V_m(\mathbf{r}) + \varepsilon + \frac{\lambda_m}{2} \psi_m^* \psi_m \right] \psi_m$$
$$+ \lambda \psi_a^* \psi_a \psi_m^* \psi_m + \frac{\alpha}{\sqrt{2}} \left[ \psi_m^* \psi_a \psi_a + \psi_m \psi_a^* \psi_a^* \right] , \tag{1}$$

where $\psi_{a(m)}$ denote the macroscopic wavefunction of the atom (molecule) condensate, $\varepsilon$ is the detuning parameter, $\alpha$ is the Feshbach resonance parameter introduced in Ref.[5], and we adopt here a simple form for the atomic (molecular) confining potentials, $V_a = \frac{\omega_a^2}{2m}(\lambda_x^a x^2 + \lambda_y^a y^2 + \lambda_z^a z^2)$, $V_m = \frac{\omega_m^2}{2(2m)}(\lambda_x^m x^2 + \lambda_y^m y^2 + \lambda_z^m z^2)$. As usual, the Gross-Pitaevskii equations of motion for this model can be derived from the action $\Gamma = \int dt \ d^3 r \frac{i}{2} \left[ \psi_a^* \dot{\psi}_a - \dot{\psi}_a^* \psi_a + \psi_m^* \dot{\psi}_m - \dot{\psi}_a^* \psi_a \right] - \int dt \ E[\psi_a, \psi_m]$ , where $E[\psi_a, \psi_m] = \int d^3 r \ \mathcal{H}$ .

In order to investigate the general properties of the hybrid system described by $\mathcal{H}$, Eq.(1), we employ the time-dependent variational Gaussian ansatz [6]

$$\psi_a(r,t) = \frac{N_a^{1/2}}{\pi^{3/4} q^{3/2}} \prod_{j=x, \, y, \, z} e^{-\left[ \frac{1}{2q_j^2(t)} - i \frac{p_j(t)}{q_j(t)} \right] \left[ r_j - r_j^c(t) \right]^2 + i\pi_j^c(t) \left[ r_j - r_j^c(t) \right] + i\theta_a(t)} \tag{2}$$

$$\psi_m(r,t) = \frac{N_m^{1/2}}{\pi^{3/4} Q^{3/2}} \prod_{j=x, \, y, \, z} e^{-\left[ \frac{1}{2Q_j^2(t)} - i \frac{P_j(t)}{Q_j(t)} \right] \left[ r_j - R_j^c(t) \right]^2 + i\Pi_j^c(t) \left[ r_j - R_j^c(t) \right] + i\theta_m(t)} \tag{3}$$

where $q_j, p_j, r_j^c, \pi_j^c$ $(Q_j, P_j, R_j^c, \Pi_j^c)$ are our variational parameters for the atomic (molecular) condensate wavefunctions and we have introduced the notation $q = (q_x q_y q_z)^{1/3}$ and $Q = (Q_x Q_y Q_z)^{1/3}$. Thus, $\psi_a(\psi_m)$ is a Gaussian centered at $r_j^c$ $(R_j^c)$ with a width $q_j$ $(Q_j)$ and conjugate momenta $\pi_j^c$ $(\Pi_j^c)$ and $p_j$ $(P_j)$ respectively. In addition, we shall use as variational parameters the numbers of the atoms, $\int d^3 r |\psi_a^*|^2 = N_a$, and molecules, $\int d^3 r |\psi_m^*|^2 = N_m$, subject to the constraint $N_a + 2N_m = N$ (fixed).

The action in this approximaion is therefore

$$\Gamma = \int dt \left\{ \theta_a \dot{N}_a + \theta_m \dot{N}_m + \sum_{j=x,\,y,\,z} N_a \pi_j^c \dot{r}_j^c + \frac{N_a}{4}(p_j \dot{q}_j - \dot{p}_j q_j) N_m \Pi_j^c \dot{R}_j^c + \frac{N_m}{4}(P_j \dot{Q}_j - \dot{P}_j Q_j) - E \right\} \tag{4}$$

The total energy has the general form $E = E_a + E_m + E_i + E_{FR}$, where $E_a(E_m)$ are the usual Gaussian Gross-Pitaevskii energy for a single atomic(molecular) condensates [6], $E_a = N_a \sum_{j=x,y,z} [\frac{1}{2m}\pi_j^2 + \frac{1}{4m}p_j^2 + \frac{\hbar^2}{4m}q_j^{-2} + \frac{m}{2}\omega_{a_j}^2(r_j^c)^2 + \frac{m}{4}\omega_{a_j}^2 q_j^2] + \frac{\lambda_a N_a^2}{2(2\pi)^{3/2}}q^{-3}$ ($\pi_j \rightarrow \Pi_j$ and etc for $E_m$). The other two terms are, respectively, the elastic and inelastic collisional contribution between the condensates, $E_i = \frac{\lambda N_a N_m}{\pi^{3/2}}\{\prod_{j=x,\,y,\,z} exp[-\frac{(r_j^c - R_j^c)^2}{q_j^2 + Q_j^2}](q_j^2 + Q_j^2)^{-1/2}\}$, $E_{FR} = \varepsilon N_m + \frac{\alpha N_a N_m^{1/2}}{2^{1/2}\pi^{3/4}q^3 Q^3}\{e^{2i\theta}\prod_{j=x,\,y,\,z} exp[\frac{b_j^2}{4a_j} - c_j]a_j^{-1/2} + \text{c.c.}\}$, where we have used the notations: $a_j = B_j^* + 2\beta_j$, $b_j = -2B_j^* D_j - 4\beta_j r_j^c + i\Pi_j - 2\pi_j$, $c_j = B_j^* D_j^2 + 2\beta_j(r_j^c)^2 - i\Pi_j R_j^c - 2\pi_j r_j^c$, being $a_j = B^* + 2\beta$, $2B = Q^{-2}_j - P_j Q^{-1}$, $2\beta = q^{-2}_j - p_j q_j^{-1}$. The variational equations are then obtained from $\delta\Gamma = 0$ leading a set of first order differential equation of the form

$$\sum_k \mathbf{S}_{ik} \dot{X}_k = \frac{\partial E}{\partial X_i} \,, \tag{5}$$

where $\mathbf{S}$ is an appropriate matrix. These classical equations of motion give a simple picture for the time evolution of the atomic (molecular) condensate wavefunction parametrized by its widths and centers of mass and the dynamics of inter-condensate tunneling driven by the FR interaction. The ground state energy, $E = \int d^3r\, \mathcal{H}$ , on the other hand is determined by the solution of Eq.(5) with $\dot{X}_k = 0$. The small amplitude oscillation dynamics is described by an expansion around the equilibrium solution. Thus, if $X^{(0)}$ is the static equilibrium solution and

4

$X^{(1)}$ is the perturbation, we have

$$i\omega \, \mathbf{K} \, X^{(1)} = \mathbf{A} \, X^{(1)} \, , \tag{6}$$

where $\mathbf{A}_{ij} = \left.\frac{\partial^2 E}{\partial X_i \partial X_j}\right|_{(0)}$ and $\mathbf{K}$ is an appropriate $26 \times 26$ inertia matrix. The set of 26 coupled equations is diagonalized for the frequencies, which come out in pair of opposite parities. The thirteen physical frequencies can be grouped into three sets: one corresponds to the motion of the centers of mass of atomic/molecular gases; one defines the spatial frontiers of the atomic/molecular condensate and one describes the Josephson tunnelling effects between the two condensates. The frequencies associated with the Josephson tunneling were found in Ref.[5] (no trap) to be $\omega(X_a = \frac{N_a}{N}, n) = \pm n\lambda[4X_a + Xa\sqrt{1 - X_a} + \frac{X_a^2}{1-X_a}]$.

An important new phenomenon in the hybrid condensate physics appears when the system is subjected to the confining trap namely the in-phase and out-of-phase dipole oscillations of the two centers of mass, what results four excitation modes when cylindrically symmetric trap is used. The dipole oscillation of the center of mass of an atomic BEC is entirely determined by the frequency of the trap and does not depend on the interatomic interaction [2]. If, on the other hand, we allow atoms and molecules, with their own confining traps and with Josephson type oscillations, then presumably the dipole mode of oscillation of the respective center of masses will depend on the Feshbach resonance interaction parameter, $\alpha$, and on the detuning parameter $\varepsilon$. If so, then there is an interesting phenomenon to be explored experimentally. An analogous situation is discussed in a homogeneous hybrid condensate (no trap). In that case, the low k-modes are, as experted for superfluids, longitudinal waves, i.e. the oscillating

5

particle current is in the direction of propagation ($\mathbf{k}$). One mode, in which both the atomic and molecular particle current move in the same direction, i.e. a Goldstone mode and its excitation energy vanishes as $k \rightarrow 0$. The other mode has atomic and molecular currents moving in opposite direction like a plasmon mode and it has a gap: it goes to a finite value which depends on the interaction parameters as $k \rightarrow 0$. In our case we would expect two similar modes: one gives an energy $\omega_{trap}$ if atoms and molecules experience the same trap potential as in the case of the single condensate and another mode that has higher energy, which depends mostly on the interaction parameters. In the following we quantify these observations using our model.

For simplicity we consider first the case of isotropic trap, $\lambda_x = \lambda_y = \lambda_z = 1$, for both atoms and molecules. In this case, the following trivial equilibrium solution is found

$$r_c = \pi_c = R_c = \Pi_c = 0 . \tag{7}$$

In addition, it is easy to show that $\frac{\partial^2 E}{\partial X_c \partial X_w} = 0$ where $X^c$ are generic coordinates of the subspaces corresponding the centers of mass and $X^w$ represent the other degrees of freedom of the variational space. Thus, the matrix $A$ reduces to the form $\begin{pmatrix} C & 0 \\ 0 & W \end{pmatrix}$, where $C_{ik} = \frac{\partial^2 E}{\partial X_i^c \partial X_k^c}$ and $W_{ik} = \frac{\partial^2 E}{\partial X_i^w \partial X_k^w}$. As a consequence, $X_c$ decouple from $X_w$ at $X^0$ and the dynamics of the centers of mass system is described by two coupled oscillator equations. Eliminating $\pi_c^{(0)}$ and $\Pi_c^{(0)}$ we find

$$N_a \, \ddot{r}_c = -[N_a \, \omega_a^2 + \Delta\omega^2] \, r_c + \Delta\omega^2 \, R_c \tag{8}$$

$$2N_m \, \ddot{R}_c = -[2N_m \, \omega_a^2 + \Delta\omega^2] \, R_c + \Delta\omega^2 \, r_c \tag{9}$$

where the frequency shift $\Delta\omega$ is produced by the interaction between the atomic and molecular

6

condensates and thus it contains the $\alpha-$ and $\varepsilon-$ dependence. This is related to the curvature of $E^i$ at $X_0$ by the following simple expression

$$\Delta\omega^2 \; = \; m\omega_a^2\left(\frac{\partial^2 E^i}{\partial\pi_c^2}\right) + \frac{1}{m}\left(\frac{\partial^2 E^i}{\partial r_c^2}\right) + \left(\frac{N}{N_a} + \frac{N}{2N_m}\right)\left(\frac{\partial^2 E^i}{\partial\pi_c^2}\right)\left(\frac{\partial^2 E^i}{\partial r_c^2}\right) \tag{10}$$

The two coupled equations (8) and (9) can be uncoupled in favor of the normal modes, $\eta \equiv N_a r_c + 2N_m R_c$ and $\xi \equiv r_c - R_c$, whose frequencies are, respectively,

$$\Omega_-^2 = \omega_a^2 \,, \qquad \Omega_+^2 = \omega_a^2 + \Delta\omega^2\frac{N}{2N_m(N-2N_m)} \tag{11}$$

The mode $\Omega_-$ is the in-phase solution where the centers of mass of atomic and molecular gases move in the same direction and is independent of the interactions [2]. On the other hand, the out-of-phase dipole oscillation solution $\Omega_+$, depends strongly on the composition of the system, which is self-determined by the equilibrium condition $X_0$. From the previous discussion we have $\frac{\partial^2 E^i}{\partial\pi_c^2} \sim N_a N_m$ and $\frac{\partial^2 E^{FR}}{\partial\pi_c^2} \sim N_a N_m^{1/2}$. Thus, when $N_m << N$, one has $\Omega_+ \to N_m^{-1/2}$. This result is illustrated in Fig.1, where $\Omega_+$ increases dramatically for solutions with small number of molecules.

We turn next to the quadrupole response of the system. In Fig.2 we show the three corresponding frequencies The lowest frequency describes the oscillations $q$, $Q$ and $N_a$ in the same direction. The other two modes describe the out-of-phase solution of $q$ against $Q$, which leads to migration of atomic condensate to molecular condensate (dash-dotted plot) and vice-verse (dotted curves ). This can also be represented by the current $\vec{j}_a = \nabla\rho_a$ ($\vec{j}_m = \nabla\rho_m$) obeying continuity equation $\nabla \cdot (j_a + 2j_m) = 0$. These modes, again, are strongly dependent on the particular equilibrium point of the system.

In conclusion, we have discussed in this paper a variational calculation of the small amplitude dynamics of a hybridatom/molecule Bose Einstein condensate. The out of phase dipole mode of oscillation of center of mass of the two condensed gases is considered in detail. For reasonable values of the physical parameters (the Feshbach resonance strength parameter, densities of gases, etc), we have found that the dipole frequency depends approximatelly quadratically on the detuning parametes, $\varepsilon$, at small value of the latter attaining an almost linear dependence for higher values of $\varepsilon$. This frequency is less than an order of magnitude large than the trap frequencyfor values of $\varepsilon$ of several KHz.

# References

[1] See. W. Ketterle, D.S. Durfee and D.M. Stamper-Kurn, cond-mat/9904034.

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

[3] S. Inouye, M. R. Andrews, J. Stenger, H.-J.Miesner, D. M. Stamper-Kurn and W. Ketterle, Nature **392**, 151 (1998).

[4] J. Stenger, S. Inouye, M. R. Andrews, H.-J.Miesner, D. M. Stamper-Kurn and W. Ketterle, Phys. Rev. Lett. **82**, 2422 (1999), cond-mat/9901056.

[5] P. Tommasini, E. Timmermans, M. S. Hussein and A. K. Kerman, Phys. Rep. **315**, 199 (1999); E. Timmermans, P. Tommasini, R. Côte, M. S. Hussein and A. K. Kerman, To appear in Phys. Rev. Lett.; P. Tommasini, E. Timmermans, M. S. Hussein and A. K.

Kerman, cond-mat/9804015; E. Timmermans, P. Tommasini, R. Côte, M. S. Hussein and A. K. Kerman, cond-mat/9805323;

[6] V. M. Pérez-Garcia, H Michinel, J. I. Cirac, M. Lewenstein and P. Zoller, Phys. Rev. Lett. **77**, 5320 (1996); G. Baym and C.J. Pethick, Phys. Rev. Lett. **76**, 6 (1996).

## Figure Captions

Figure 1. The out-of-phase dipole frequency as function of detuning parameter, $\varepsilon$, for the hybrid condensate in unit of trap frequency. The parameters are: $\lambda_a = \lambda_m = \lambda = 100m\mu^3s^-1$, $N = 10^4$, $V_a = 2\pi * 50Hz$, $\alpha = 200m\mu^{3/2}s$. See text for details.

Figure 2. The three eigenfrequencies for the $q$, $Q$ and $N_a$ degrees of freedom. Same parameters are used as in Fig.1. Lower curve, $\omega(q + Q + N_a)$; middle curve, $\omega(q - Q + N_a)$; upper curve, $\omega(q - Q - N_a)$. See text for details.
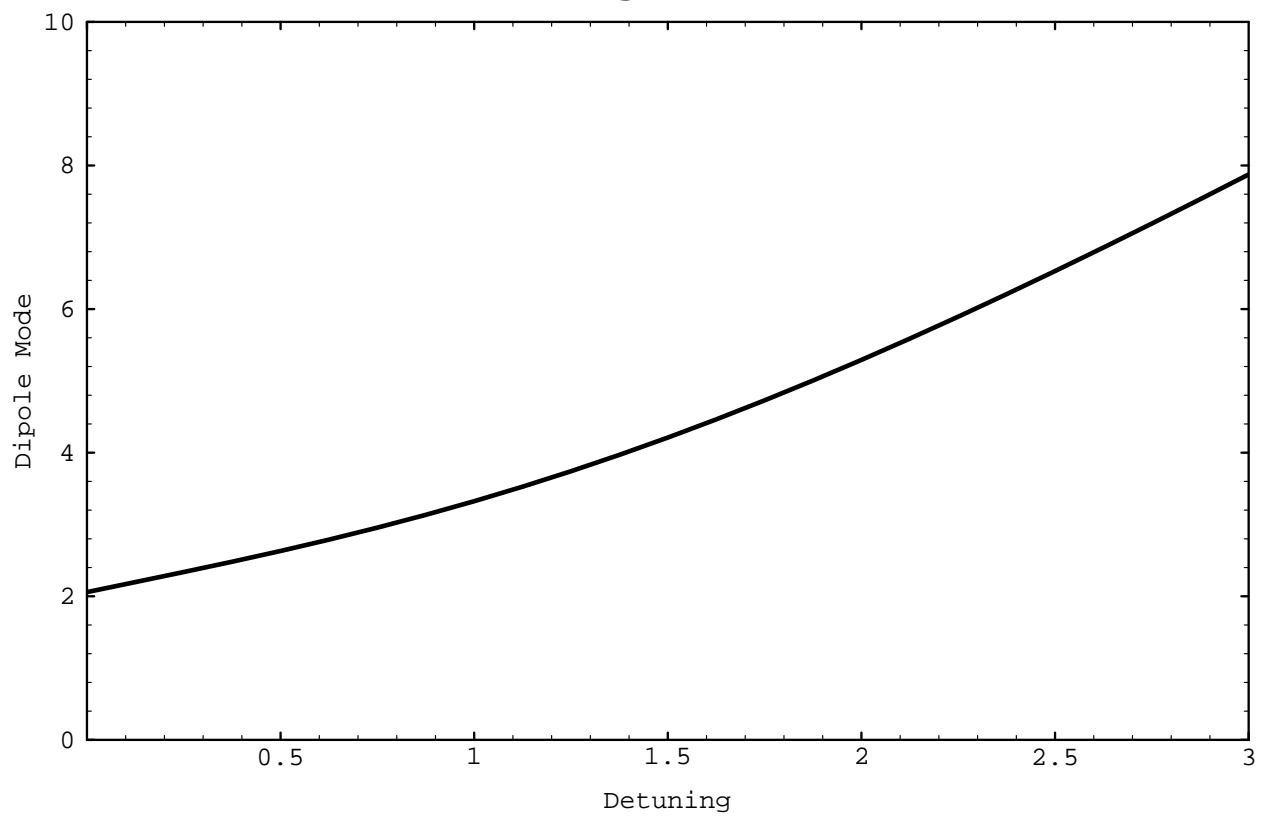
Figure 1

Figure 2