

## *DISSERTATION PROPOSAL FOR THE Ph.D. DEGREE*

### Theory of Atom-Molecule Bose Einstein Condensates

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**Abstract:** A quasi-continuum model of photo-association assumes an atomic Bose Einstein condensate (BEC) coherently coupled to a single mode (diatomic) molecular system in the presence of the laser field. In the “mean-field” formalism the Atom-Molecule Bose Einstein Condensate (AMBEC) is described by a system of two Gross-Pitaevskii equations, one for each BEC. Their interaction captures the coherent photo-associative/photo-dissociative exchange of particles between the condensates: two atoms form a molecule, and a molecule splits into two atoms. We propose to analyze this system of equations numerically and theoretically. We expect our analytical research to reveal the general properties of the coupled AMBEC system, while the numerics should allow detailed analysis of any configuration of interest. It is our goal to find the extent to which the relevant physics is mirrored in our simple mathematical model, in particular, whether the model captures the experimentally observed collapse of a BEC as reported in J. Roberts et al., in Phys. Rev. Lett. 86, 4211 (2001).

### Background

In 1924 and 1925, Bose and Einstein concluded that the ideal gas of identical bosonic particles undergoes phase transition, if cooled to or below a critical temperature. At critical temperature the average particle’s thermal (de Broglie) wavelength becomes comparable to the average interparticle spacing [1,2]. Further lowering of the temperature of the bosonic system causes particles to condense in the system’s ground state, thus creating a macroscopic quantum-mechanical object, a Bose-Einstein Condensate (BEC).

Seventy years later in 1995, the first experimental observations of Bose Einstein condensation in dilute low-temperature atomic vapors were reported [3,4]. These and subsequent experimental results have heightened the interest in the theory of BEC.

### Mean Field Theory of BEC

The two pillars of the theory of BEC are the mean-field approximation by Bogoliubov [5], and the Gross-Pitaevskii equation.

The mean-field approximation is a theoretical approach present in many branches of physics. It allows insight into the behavior of the system in terms of parameters with clear physical meaning, while avoiding heavy numerics associated with the more exact calculations

The mean-field theory of BEC was developed to tackle a many-body problem of a large system of bosonic particles trapped in an external potential at the temperature of absolute zero. Such a system, is ideally described by many-body Hamiltonian  $\hat{H}$ ,

$$\begin{aligned} \hat{H} = & \int d\mathbf{r} \, \hat{\Psi}^\dagger(\mathbf{r}) \left( -\frac{\hbar^2}{2m} \nabla^2 + V_0 \right) \hat{\Psi}(\mathbf{r}) \\ & + \frac{1}{2} \int d\mathbf{r} \, d\mathbf{r}' \, \hat{\Psi}^\dagger(\mathbf{r}) \, \hat{\Psi}^\dagger(\mathbf{r}') \, V(\mathbf{r} - \mathbf{r}') \, \hat{\Psi}(\mathbf{r}') \, \hat{\Psi}(\mathbf{r}), \end{aligned} \quad (1)$$

where  $\hat{\Psi}(\mathbf{r})$  and  $\hat{\Psi}^\dagger(\mathbf{r})$  are the boson annihilation and creation field operators, and  $V(\mathbf{r} - \mathbf{r}')$  is a two-body interatomic potential. Equation (1), as is, is impossible to solve analytically for any physically relevant number of particles ( $10^6$  and higher).

In Eq. (1) let us assume the following: the bosonic system has undergone the Bose-Einstein condensation, meaning that a quantum ground state contains the majority (if not all) of the system particles, and let the system be in thermodynamic limit, that is  $N \rightarrow \infty$  and  $V \rightarrow \infty$  but the limit  $\rho = \frac{N}{V} \rightarrow \rho_0$  exists, where  $N$  is the number of particles and  $V$  volume of the system. These assumptions justify separation of the bosonic field operator  $\hat{\Psi}$  into two components: one pertaining to the ground state, and the other describing the rest of the system. The thermodynamic limit allows the operator corresponding to the ground state to be replaced by a complex number. The general name of this complex number in the language of the “mean-field” theories is “order parameter”, and in the case of BEC it is interpreted as “density amplitude”. The mean-field theory of BEC subsequently allows a development of the “first-order” theory for excitations in gaseous BEC, [6].

Consider further simplifications of the mean-field equations for the ground state, that is, let us in Eq.(1) replace the interaction potential  $V(\mathbf{r} - \mathbf{r}')$  by  $U_0 \delta(\mathbf{r} - \mathbf{r}')$ . This yields a “zeroth-order” (or semiclassical) equation for the order parameter  $\Phi$ , a BEC density amplitude,

$$i\hbar \frac{\partial \Phi(\mathbf{r}, t)}{\partial t} = \left( -\frac{\hbar^2}{2m} \nabla^2 + V_0(\mathbf{r}, t) \right) \Phi(\mathbf{r}, t) + NU_0 |\Phi(\mathbf{r}, t)|^2 \Phi(\mathbf{r}, t), \quad (2)$$

where  $m$  is the mass of a single particle while  $N$  is the number of them. This is known as

the Gross-Pitaevskii (GP) equation [7–9]. It is valid providing that the  $s$ -wave scattering length  $a_0$ , related to  $U_0$  via

$$U_0 = \frac{4\pi\hbar^2 a_0}{m} \quad (3)$$

is much larger than the average distance between the atoms, and the number of atoms in the condensate is much larger than one [6,10]. This condition is fulfilled in the dilute low-temperature atomic vapors.

If the atom-atom interaction in the above model is assumed repulsive,  $U_0 > 0$ , the ground state and its properties can be calculated, (e.g., particle distribution and chemical potential), see [11] and the references therein. In the opposite case, when the atom-atom interactions are attractive,  $U_0 < 0$ , it is known that for most of the confining geometries there exists a critical number of particles that may be held in a metastable state. If the number of particles is larger than the critical value, a collapse of the BEC distribution to the trap center is predicted.

### Recent Results

Recent experiments [12–14] have achieved a high accuracy in tuning of the  $s$ -wave scattering length in trapped  $^{85}\text{Rb}$  BECs. In all the experiments the control over the scattering length was obtained using Feshbach resonances, [15,16], in an external magnetic field. In particular, Ref. [13] reports on the existence of (*i*) a critical magnetic field at which a  $s$ -wave scattering length reaches a critical negative value, and (*ii*) a phenomenon the authors termed “collapse” that occurs upon decreasing the magnetic field below the threshold. As a result of the collapse the number of atoms in BEC decreases substantially, while the ratio of axial to radial width varies erratically from the initial ratio. The authors concluded that as a result of the collapse, the condensate oscillates in a highly excited state, while losing an undetermined number of the most energetic particles.

Apparently, the properties of the collapse obtained by solving a simple Gross-Pitaevskii equation differ from those observed experimentally. This inadequacy of GPE is emphasized further by the results of Ref. [17]. There it was shown that a quantum many-body system of

particles described by GPE (2) with the attractive atom-atom interaction,  $U_0 < 0$ , undergoes a gas-liquid phase transition. This intuitively plausible result claims, in plain words, that the collapse of a BEC, according to GPE, produces a droplet of liquid.

### Proposed Research

All experimental realizations of BEC in atomic vapors were done with atoms of group *IA* in the periodic table. A pair of these atoms may form a molecule, and the theory of formation of such diatomic molecules has been extensively studied. More recently, a production of the molecules in ultracold atomic collisions became the focus of theoretical research, [18,19]. Typically, such a molecule creation process is analyzed in terms of Feshbach resonances, i.e., the bound motion in one degree of freedom (molecule) is coupled weakly to and can decay into unbound motion in another degree of freedom (pair of atoms) [20]. The mechanism of Feshbach resonances has been suggested to be applicable for the case of atomic BEC in an external magnetic field, where it produces molecules which are both Bose condensed and in coherence with the atomic BEC. This conjecture allows the GPE to be written for the combined system of atom-molecule BEC (AMBEC) [21].

As an alternative to Feshbach resonances, the quasi-continuum photo-association based on quantum field theory (QCPA) was suggested, [22]. In this approach, one considers a quasi-continuum (QC) of free states coupled to a single bound state in the presence of a detuned laser field. In Feshbach resonances molecules are Bose condensed in the trap's ground state, while in QCPA the phase of the molecules is modulated by a factor  $e^{i\mathbf{q}\mathbf{x}}$ , as a result of the recoil of PA photon with momentum  $\mathbf{q}$ . The phase modulation is not all that important, because the nature of molecular BEC does not change, i.e., a single quantum state (with momentum  $\mathbf{q}$ ) is macroscopically occupied. Finally, the QCPA, unlike Feshbach resonances, allows easier identification of the relevant physical parameters in a simple model of AMBEC:  $K$ , the atom-molecule coupling strength and  $\delta$ , the laser energy mismatch from resonance.

While both approaches result in a formally identical coupled two-mode system of GP equations, we choose the formalism and terminology of QCPA for the reasons mentioned

above. This said, the system of equations describing a simple model of AMBEC is:

$$\begin{aligned} i\hbar \frac{\partial \varphi}{\partial t} &= H_{0,a} \varphi - K \varphi^* \psi, \\ i\hbar \frac{\partial \psi}{\partial t} &= (H_{0,m} - \delta) \psi - \frac{K}{2} \varphi^2, \end{aligned} \quad (4)$$

where  $H_{0,a}$  and  $H_{0,m}$  are the Hamiltonians for atomic and molecular harmonic-oscillator like trapping potentials, respectively. The important aspect of Eq. (2) is that the adiabatic expansion with respect to detuning  $\delta$  allows elimination of the molecular field  $\psi$ , yielding the GPE for atomic BEC only,

$$i\hbar \frac{\partial \varphi}{\partial t} \simeq H_{0,a} \varphi - \frac{K^2}{\delta} |\varphi|^2 \varphi. \quad (5)$$

This expression indicates the possibility of changing the effective  $s$ -wave scattering length of the BEC atoms by changing the detuning  $\delta$  and the atom-molecule coupling strength  $K$ . Even the sign change of the  $s$ -wave scattering length is possible by simply changing the sign of detuning. Naturally, the question arises if and how Eq. (4) relates to the problem of collapse: is it in accord with experimentally observed phenomena of Refs. [12–14], or perhaps follows the collapse path of the single GPE (2) discussed earlier?

We propose to examine these questions analytically and numerically.

For the numerical part of the problem, we have developed a novel time-integration method for the nonlinear Hamiltonians [23]. The method, called the *DS-method*, can be modified to calculate the ground state, by integrating in complex instead of the real time. Our intention to explore the  $\{\delta, K\}$  parameter space of the Eq.(4) is motivated by our preliminary results for the one-dimensional problem, where we found a puzzling lack of any collapse whatsoever. We would like to determine whether the same holds for two- and three-dimensional systems, and for different initial configurations of the AMBEC. In parallel, we intend to extend our numerical work, written mainly in combination of RLaB and C/C++, as to allow the detuning  $\delta$  to be time dependent and for PA matrix element  $K$  to depend both on time and the position. The goal we have in mind is to determine whether these results confirm the predictions stemming from adiabatic expansion (5) or not.

While numerical results should provide the details of time evolution of any particular

AMBEC configuration, we surmise that certain general laws can be deduced about the system. We distinguish between the of free and trapped AMBEC.

For the trapped system, our main concern is the structural stability of the system (4), i.e., whether it collapses or not. In order to perform this analysis, we will first determine the equations of motion of the functional  $\eta$  given by

$$\eta(\tau) = \langle \varphi | \mathbf{x}^2 | \varphi \rangle + \langle \psi | \mathbf{x}^2 | \psi \rangle, \quad (6)$$

from (4). This procedure will result in differential equations from which general results might be obtained. Our approach is an extension of the work on the collapse of a single component BEC, [24], that utilizes the Zakharov's collapse analysis method, Refs. [25,26]. In the formalism of this method, a collapse happens when  $\eta \rightarrow 0$ .

In the case of free condensates, we intend to extend the known results from the GP theory of the single component BEC [27]. Primarily, a repulsive atom-atom interaction makes a condensate structurally unstable and prone to modulation instability, while conversely, an attractive atom-atom interaction is instrumental in forming stable soliton-shaped distributions.

## Outlook

Upon successful completion of the work described here, we should be able to answer the following questions: First, to what extent is it possible to manipulate the  $s$ -wave scattering length of the particles in a BEC? Second, to what extent can one control the behavior of the condensates by manipulating the  $s$ -wave scattering length?

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## The Prospectus

Theory of Atom-Molecule Bose Einstein Condensates

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