STABILITY OF ELECTRIC DIPOLE MOLECULAR CONDENSATE

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Abstract:
A polar molecular gas with a strong dipolar interaction is a system of great interest to both the atomic and molecular physics and condensed-matter physics communities due to the versatile and promising potential applications. With controllable, anisotropic and long range dipole–dipole interactions, they could be used in quantum computation, quantum simulation, precision measurement and controlled cold chemistry. Here we study the stability of trapped NaRb, NaCs and RbCs molecular BECs. For these molecules their electric dipole moments can be polarized by an external electric field. As the applied electric field increases, the dipole moment *d* continuously increases from zero to the permanent dipole moment. We model the dipolar BEC using the mean-field Gross-Pitaevskii equation (GPE). We find that for a particular molecular BEC, the maximum number of molecules for which the condensate will remain stabilized depends on (i) value of dipole moment, (ii) value of contact interaction scattering length. We have also studied the case when the polarizing field is perpendicular to the trap axis.

Keywords: *Molecular condensate; Electric dipolar condensate; Stability of condensate.*

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1. Introduction

A dipolar molecular gas is one of the most widely studied systems in the fields of atomic, molecular, and condensed matter physics because of its broad and promising applications [1,2]. With controllable and anisotropic dipole and dipole interactions over long distances, they can be used for quantum computing [3,4], quantum simulation [5], precision measurement [6, 7] and controlled cold chemistry [8]. STIRAP (Stimulated Raman Adiabatic Passage) is the most recent technique that has been developed to generate almost degenerate gas of KRb molecules in their rovibratory ground state [9, 10]. Unfortunately, the KRb molecules are not stable against two-body decay into K2 and Rb2 molecules [11, 12]. Theoretical calculations suggested that this issue could be overcome by selecting other alkali-metal substituents such as KCs, KNa, NaCs, NaRb, and RbCs [13]. The use of STIRAP on these species is now widely used in many laboratories around the world. Bosonic NaRb molecules, with a constant electric dipole moment of 3.3 debye, have been created by [14,15]. NaCs molecules with dipole moments as large as 4.6 D have been created by [16,17]. Ultracold RbCs molecules have been created by [18]. With these advances, a strong dipolar ground state molecule BEC is now experimentally achievable. While many aspects like rotonic excitation spectra [19-27], anisotropic superfluidity [28,29], droplet formation [30-32], crystallization in one dimension (1D) [33-38], two dimension (2D) [39-43], and into more exotic patterns [43,44] have been extensively discussed for weakly dipolar magnetic atoms, So far, systematic studies on molecules with their large and adjustable electric dipole moment have been rare. Previous theoretical studies have investigated molecular Bose gasses with dipolar interactions in various scenarios from the weakly to the strongly interacting limit in lattices and in bulk systems [45-54]. Purely dipolar systems have also been used to study crystallization [55-57], localization [58] and topological states [59].

2. Objectives

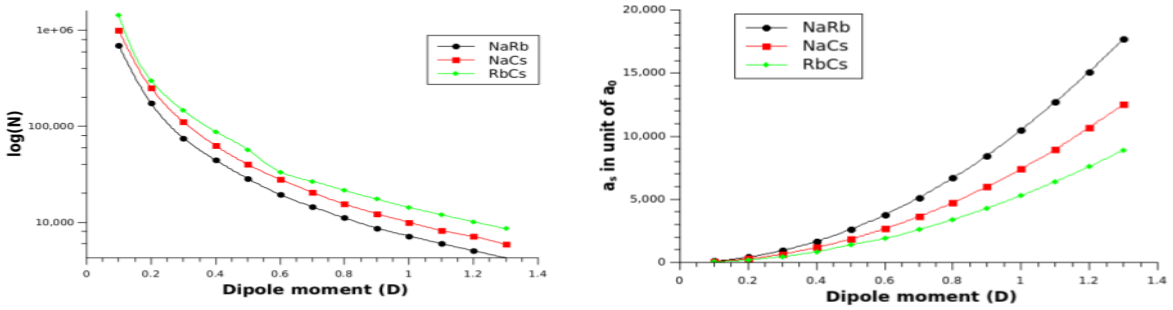
In this work, we leverage the comprehensive toolkit we developed to explore dielectric BECs to investigate the many-body properties that can be predicted with a future molecular BEC. In addition, we explain in detail how to attain collisional stability of the molecules, so that the molecular losses can be disregarded in our simulations. Finally, we show how the desired interaction parameters (contact and dipolar) can be met in experiments. In literature [60], fine-tuned situations have been studied where small repulsive beyond mean field LYH corrections dominate over large attractive mean-field terms, leading to stabilization of systems that are expected to collapse on a pure mean-field level. Here, we study the limit up to which systems can still be stabilized within mean-field approximation.

3. Method

Here we consider dipolar BECs of NaRb, NaCs and RbCs molecules. For these molecules, their electric dipole moments can be polarized by an external electric field (say, along the $\hat{z}$ direction). As the applied electric field increases, the dipole moment d continuously increases from zero to the permanent dipole moment, and different molecules have different values of the permanent dipole moment. From literature we see that the maximum value of dipole moment of NaRb, NaCs and RbCs molecules can be 3.31 D, 4.63 D , and 1.32 D respectively [61]. The two-body dipole-dipole interaction potential studied here can be modeled as $V_D = \frac{d^2(1-3cos^2\theta)}{r^3}$. Now, we take dipolar strength $a_{dd} = \frac{d^2 m}{12\pi\hbar^2\epsilon_0}$ to characterize the strength of the dipolar interaction. For dielectric molecules, a_{dd} can be of the order of $105a_0$ depending on the value of the external electric field. Along with this long range dipolar interaction, we also consider the s-wave contact interaction. The short-range contact interaction between the molecules is characterized by the coupling constant $g = 4\pi\hbar^2 a_s/m$. Where a_s is the s−wave scattering length. As molecules can be lost from two-body processes, as is in general a complex quantity, with the imaginary part related to the losses. We consider here the case with no losses so the imaginary part of a_s is set to zero. We model the dipolar BEC using the mean-field Gross-Pitaevskii equation (GPE) as,

$$i\hbar\partial_t\psi = (\widehat{H}_0 + g|\psi|^2 + V_D)\psi \qquad (1)$$

where the wavefunction $\psi(\vec{r}, t)$ is normalized to the molecule number N and $\widehat{H}_0 = -\frac{\hbar^2\Delta}{2m} + V_{ext}(\vec{r})$. In presence of harmonic trapping potential $V_{ext}(\vec{r}) = \frac{m}{2}(\omega_x{}^2x^2 + \omega_y{}^2y^2 + \omega_z{}^2z^2)$. By



(a) (b)

Figure 1: (a) variation of N_{max} with dipole moment, (b) variation of a_{min} with dipole moment

controlling the electric field, one can make the dipole energy comparable to the Fermi energy.

The dipole-dipole interaction is inherently anisotropic. We may choose the polarizing electric field direction not to coincide with the trap axis. They may make an angle and the stability of the BEC should depend on it. When the electric field makes an angle ϕ with the trap axis, the DDI potential takes form,

$$V_D(\vec{r}) = \frac{d^2(1-3cos^2\theta)}{r^3}\frac{3cos^2\phi - 1}{2} \qquad (2)$$

We have studied two extreme cases, $\phi = 0$, when the polarizing electric field is along the trap axis and $\phi = 90^0$ when the polarizing electric field is perpendicular to the trap axis.

4. Results

We solve the GP equation for NaRb, NaCs and RbCs molecular BEC for different values of N, a_{dd} and a_s and find the limit where systems are stabilized. Our results show, for a particular value of a_{dd} there is a maximum number of molecules N_{max} which can produce stable BEC in a trap. To achieve this BEC with N_{max} number of molecules, a_s has to be set greater than a value called a_{min} . The ratio $\frac{a_{min}}{a_{dd}}$ is fixed for a particular trap and for a quasi-two dimensional trap $\frac{a_{min}}{a_{dd}} = \frac{\omega_x}{\omega_z}$. Figure 1 shows the variation of N_{max} and a_{min} with dipole moment

We find the following results:

- For a particular molecular BEC, N_{max} depends on (i) value of dipole moment, i.e., a_{dd} , (ii) value of contact interaction scattering length, a_s , (iii) trap geometry
- Keeping everything else fixed, if we decrease value of a_s then the number of molecules in the stable condensate, N , decreases. And if we increase a_s then N also increases. But for a fixed value of a_{dd} we cannot increase N beyond N_{max} without making the condensate unstable.
- For same molecule and same value of a_{dd} , N_{max} can be changed by changing the trap geometry
- For the same trap and same dipole moment, N_{max} is inversely proportional to the mass of the molecule.
- For all the three molecules and all dipole moment values, the values of $|\psi(0,0)|^2$ at trap center and $\frac{a_{min}}{a_{dd}}$ are same and depends on trap geometry only.

To determine the stability of the BCE, we have checked whether the wavefunction is still gaussian or not. For $\phi = 90^0$, we find the BEC becomes less stable with an increase in dipole moment and number of molecules. In Table-1 we provide the results.

Table-1. N_{max} for different angles between trap axis and polarizing electric field

Molecule	Dipole moment	N_{max} for $\varphi = 0^0$	N_{max} for $\varphi = 90^0$
NaRb	0.1	1430000	2600
	0.2	300700	600
	0.3	146400	290
	0.4	88300	170
	0.5	57200	100

5. Discussion

In conclusion, we have studied the stability of trapped molecular BECs having electric dipole moments. We have considered BECs of NaRb, NaCs, and RbCs molecules as examples and explored the requirements to create stable BECs of those molecules in a harmonic trap. We have prepared our dipolar BEC using mean-field GPE where we have taken into account both the short-range contact interaction and long-range dipole-

dipole interaction among the molecules. While the contact interaction is isotropic, the dipole-dipole interaction is inherently anisotropic. Initially, we have done the calculations considering the polarizing electric field along the direction of the trap axis. Then, we have also studied the situation considering the polarizing electric field as perpendicular to the trap axis. We solve the GPE to find stable solutions for different values of (i) number of molecules in the Condensate, (ii) electric dipole moments of the molecules, (iii) strength of the contact interaction. We draw the following conclusions: (a) For a particular molecular BEC, the maximum number of molecules present in the stable condensate, N_{max} depends on (i) value of dipole moment , (ii) value of contact interaction scattering length, (iii) trap aspect ratio. (b) Keeping everything else fixed, if we decrease the strength of the contact interaction then the number of molecules in the stable condensate, N decreases. And if we increase the strength of the contact interaction then N also increases. But for a fixed value of the dipole moment we cannot increase N beyond N_{max} without making the condensate unstable. (c) However, for same molecule and same value of the dipole moment, N_{max} can be changed by changing the trap geometry. (d) Again, if we consider different molecules for the same trap and same dipole moment, N_{max} is inversely proportional to the mass of the molecule. (e) for all the three molecules and all dipole moment values, the values of probability density at trap center and the ratio $\frac{a_{min}}{a_{dd}}$ are same and depends on trap aspect ratio only. The potential applications of this study covers broad fields including quantum computation, quantum simulation and controlled cold chemistry. This work opens up path to perform studies like condensate phases and dynamics with dipolar anisotropy [62] and interaction of molecular BEC with optical vortex beams [63].

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