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Effects of Contact Interactions in Molecular Bose-Einstein Condensates

Devin Crowley, Ryan M. Wilson, Seth T. Rittenhouse, and Brandon M. Peden

November 8, 2017

Abstract

We investigate the ground state and low-lying excitations of a Bose-Einstein condensate (BEC) of dipolar molecules interacting via short-range contact and long-range dipole-dipole interactions (ddi). We find the mean field ground state via the variational principle using a separable bosonic wave function as the variational state. This state can be refined to include small excitations in the form of plane waves, and the results of the variational calculation are a set of dispersion relations for the low-lying excitations. We analyze the polarization and stability of the ground state as a function of the strength of the external polarizing electric field, the strength of the ddi, and the strength of the contact interactions. In a certain parameter regime of strong contact interactions that oppose the dipole-dipole interactions, we identify a possible signature of a first-order phase transition: the polarization of the gas discontinuously flips as the electric field is continuously ramped through zero field. By examining the dispersion relations, we find that the ground state in this parameter regime is unstable.

1 Introduction

Bose-Einstein Condensates (BECs) have been useful in simulating more complex systems from condensed matter physics, but so far only atomic BECs have been realized in the lab. In this paper we expand on a qualitative analysis of a molecular BEC interacting via dipole-dipole interactions. We model the BEC as a molecular gas whose constituent particles share identical wave functions. The molecules can be polarized by an external electric field allowing the molecules to interact with one another via long-range dipole-dipole interactions.

We have expanded the model of a molecular BEC, which previously considered only dipole-dipole interactions between particles, to account for contact interactions. Contact interactions are very short-range interactions between molecules that can be either attractive or repulsive. They are easily and flexibly adjustable and therefore add significantly to the variety of systems that can one day be modeled with molecular BECs.

Our results will be useful when the technology to super-cool molecular gases has been further developed and these systems can be physically created and experimented with. Atomic BEC gases have been in use for some time, but molecular BEC gases are just past the horizon, so we expect our results to become relevant in the near future.

The structure of this paper is as follows. In section 2 we discuss the system we are modeling, our assumptions about it, and our methods. In sections 3 and 4 we present and interpret our results regarding the system's polarization and stability, respectively.

2 System, Model, and Methods

The system we have modeled is a BEC of dipolar molecules confined in a quasi-two-dimensional electromagnetic trap and experiencing an electric field parallel to the trap axis. The molecules have no intrinsic dipole moment, but they are polarizable. The electric field separates their charges, inducing an electric dipole moment. We treat the internal structure of the molecules via a two-state approximation where the molecular dipoles are either aligned or anti-aligned with the electric field.

Electric dipoles have electric fields that allow them to interact with each other at long range. If these dipoles are allowed to move freely, they clump up end-to-end. This arrangement is highly self-attractive, leading to collapse and loss of molecules from the trap. This is a form of instability. To avoid this, we prevent the molecules from lining up end-to-end by constraining them to lie in a plane and applying a field perpendicular to the plane in order to align all the dipoles.

This system is modeled by a Hamiltonian, given by

$$\begin{aligned}
 H = \sum_{i=1}^N & \left[-\frac{\hbar^2}{2m} \nabla_i^2 + \frac{1}{2} m \omega^2 z_i^2 - d_{\uparrow} E_0 |\uparrow\rangle \langle \uparrow| - d_{\downarrow} E_0 |\downarrow\rangle \langle \downarrow| - \frac{\Delta}{2} (|\downarrow\rangle \langle \uparrow| + |\uparrow\rangle \langle \downarrow|) \right] \\
 & + \sum_{i < j} \left[d_{\uparrow}^2 \frac{1 - 3 \cos \theta_{ij}}{r_{ij}^3} |\uparrow\uparrow\rangle \langle \uparrow\uparrow| + d_{\downarrow}^2 \frac{1 - 3 \cos \theta_{ij}}{r_{ij}^3} |\downarrow\downarrow\rangle \langle \downarrow\downarrow| \right. \\
 & \left. + d_{\uparrow} d_{\downarrow} \frac{1 - 3 \cos \theta_{ij}}{r_{ij}^3} (|\downarrow\uparrow\rangle \langle \downarrow\uparrow| + |\uparrow\downarrow\rangle \langle \uparrow\downarrow|) \right],
 \end{aligned}$$

where z_i is the position of particle i along the axis normal to the trap, d_{\uparrow} and d_{\downarrow} are the dipole moments of particles respectively in the up and down states, E_0 is the external electric field strength, Δ is the zero-field splitting energy, r_{ij} is the distance between particles i and j , and θ_{ij} is the angle between the dipole vector of particle i and the relative position vector of particle j with respect to particle i .

Respectively, these terms represent the center of mass kinetic energy, the potential energy of a molecule in a harmonic trap, the energy stored in the dipoles' orientation with respect to the electric field ($-\vec{d} \cdot \vec{E}$), the internal molecular energy, and the dipole-dipole interactions. We get the ground state energy (GSE) functional by taking the expectation value of the Hamiltonian in a variational wavefunction. This GSE functional approximates the true ground state energy of the system when it is minimized with respect to the proportion of dipoles in the up state, ν .

The ground state energy functional has the following form:

$$\begin{aligned}
 \frac{E}{N} = & \left(\frac{1}{2} \hbar \omega - d_0 E_0 (\nu_{\uparrow} - \nu_{\downarrow}) - \Delta \sqrt{\nu_{\uparrow} \nu_{\downarrow}} \right) + \frac{4}{3} \sqrt{\frac{\pi}{2}} \frac{n d_0^2}{l} \left[\nu_{\uparrow}^2 + \nu_{\downarrow}^2 - 2 \nu_{\uparrow} \nu_{\downarrow} \right] \\
 & + \frac{1}{l \sqrt{2\pi}} \left(g_{\uparrow\uparrow} (n \nu_{\uparrow}^2) + g_{\downarrow\downarrow} (n \nu_{\downarrow}^2) + (g_{\uparrow\downarrow} + g_{\downarrow\uparrow}) (n \nu_{\uparrow} \nu_{\downarrow}) \right),
 \end{aligned}$$

where n is the area-density, $\nu_{\uparrow\downarrow}$ is the proportion of dipoles in the up or down state, d_0 is the inherent strength of the dipoles, E_0 is the strength of the electric field, and Δ is the energy separation between angular momentum states internal to the molecules. The first term is the ground state energy of the harmonic trap. The second term is the dipole

energy associated with the dipoles' orientation in the electric field. Each dipole has energy $-\vec{d}\cdot\vec{E}$. The third term is the zero-field splitting energy associated with the different angular momentum (azimuthal) quantum numbers for these molecules. The next three terms are the energy associated with the dipole-dipole interactions. They are the sum of positive potential energies associated with dipoles of the same orientation, and negative potential energies associated with dipoles of opposite orientations, respectively corresponding to the terms in the factor $[\nu_{\uparrow}^2 + \nu_{\downarrow}^2 - 2\nu_{\uparrow}\nu_{\downarrow}]$.

The last term represents contact interactions. Contact interactions are short range interactions that can be tuned with a great deal of flexibility. They essentially represent interactions between particles that physically overlap, or bump into each other. There are three types of contact interactions between molecules: up-up, down-down, and up-down interactions, referring to the orientations of the interacting dipoles with respect to the upward electric field. Each of these can be independently turned on and adjusted for strength and parity. They are respectively denoted by $g_{\uparrow\uparrow}$, $g_{\downarrow\downarrow}$, and $g_{\uparrow\downarrow}$. Positive values of these parameters represent repulsive interactions while negative values represent attractive interactions.

The system dynamics are governed by the Schrodinger equation with the Hamiltonian given above. To solve this equation, we make a variational ansatz for the ground state. That is, we assume the single particle ground state wavefunction has the form

$$|\Psi(\vec{r})\rangle = \phi_{\uparrow}(\vec{r})|\uparrow\rangle + \phi_{\downarrow}(\vec{r})|\downarrow\rangle = \phi(\vec{r})(\alpha_{\uparrow}|\uparrow\rangle + \alpha_{\downarrow}|\downarrow\rangle),$$

where the first factor $\phi(\vec{r})$ represents the center of mass motion of a single particle and the second factor is the internal state, a linear combination of the two allowed states, $|\uparrow\rangle$ and $|\downarrow\rangle$ (aligned and anti-aligned with the electric field). We further assume that $\phi(\vec{r})$ has the form

$$\phi(\vec{r}) = \frac{1}{\sqrt{l}\sqrt{\pi}}e^{-\frac{z^2}{2l^2}},$$

a plane wave that is uniform across the z -plane but Gaussian along the z -axis, normal to the trap. In the above expression, $l = \sqrt{\frac{\hbar}{m\omega}}$ is effectively the width of the Gaussian in the trap, where ω is the trapping frequency. This guess is sensible; it describes a probability density that is highest in the center of the trap, and uniform across its breadth.

With this ansatz, we calculate the expectation value of the Hamiltonian and minimize it with respect to ν . $|\Psi(\vec{r})\rangle|_{\nu=\nu_{min}}$ is a good approximation to the true ground state wavefunction for the system. We extend this solution to account for small excitations by layering plane waves $\delta_{\phi_{\uparrow\downarrow}}(\vec{r}, t)$ onto our ground state solution $\Psi(\vec{r})$. That is,

$$\phi_{\uparrow\downarrow}(\vec{r}) \rightarrow \phi_{\uparrow\downarrow}(\vec{r}) + \delta_{\phi_{\uparrow\downarrow}}(\vec{r}, t),$$

where $\delta_{\phi_{\uparrow\downarrow}}(\vec{r}, t)$ has the form

$$\delta_{\phi_{\uparrow\downarrow}}(\vec{r}, t) \propto e^{i(\vec{k}\vec{x}-\omega t)}u_{\vec{k}} + e^{-i(\vec{k}\vec{x}-\omega t)}v_{\vec{k}}^*.$$

The quantities $u_{\vec{k}}$ and $v_{\vec{k}}^*$ are the amplitudes of these plane waves.

Using our wavefunction with these slight excitations in the Schrodinger equation and minimizing our ground state energy functional, we get a set of linear equations for the amplitudes of the $\delta_{\phi_{\uparrow\downarrow}}$ plane waves. This set of equations can be recast in the form of an eigenvalue problem where we diagonalize the fluctuation matrix to get the dispersion relations of the system. These dispersions are the allowable energies of the system. Imaginary

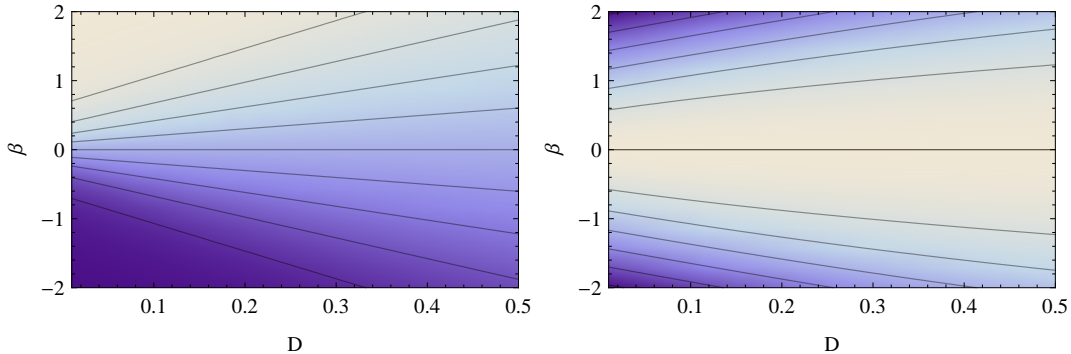


Figure 1: (left) Contour-density plot of the polarization without contact interactions (right) Contour-density plot of the energy without contact interactions

dispersion relations indicate dynamical instability in the system; we cannot have a stable system with a non-real energy.

3 Polarization

In this section we examine the polarization of the gas in various parameter regimes. The polarization

$$p = \sum d = Nd = N(\nu_{\uparrow}d_{\uparrow} + \nu_{\downarrow}d_{\downarrow}) = Nd(\nu_{\uparrow} - \nu_{\downarrow}),$$

where d is the dipole moment per particle, N is the total number of particles, ν_{\uparrow} is the proportion of dipoles in the up state, ν_{\downarrow} is the proportion of dipoles in the down state, and $d_{\uparrow} = -d_{\downarrow} = d$ is the dipole moment of a particle in the up state. So effectively, the polarization is the difference between the proportion of dipoles in the “up” state and the proportion in the down state. For example, a polarization of 1 implies that all the dipoles are spin-up, while a polarization of zero means that half the dipoles are spin-up and the other half are spin-down.

Figure 1 shows the polarization and energy of the gas as functions of the effective interaction strength $D = \frac{nd_0^2}{3l}$ and the electric field strength $\beta = \frac{dE}{\Delta}$ in the absence of contact interactions. This illustrates the behavior of the mean field ground state: the polarization decreases with D and increases with β , while the energy increases with D and decreases with β . The only qualitative effects contact interactions have on the energy diagram is to shift it along the β -axis, so we do not further explore energy diagrams.

The ground state’s polarization increases toward 1 (fully polarized) with β because a strong electric field makes the up state more energetically favorable, eventually dominating the repulsive effect of the dipole-dipole interaction when nearby dipoles share the same orientation. The polarization is pushed towards zero (an even mix of up and down dipole orientations) when D is increased because it increases the strength of the repulsive dipole-dipole interactions, thereby making nonzero polarizations less favorable. The polarization is therefore a consequence of competition between the effects of the intermolecular interactions and the external electric field.

This result is consistent with previous work. However, we have extended our investigation of the polarization in Figures 2-4 by including certain contact interactions. When contact

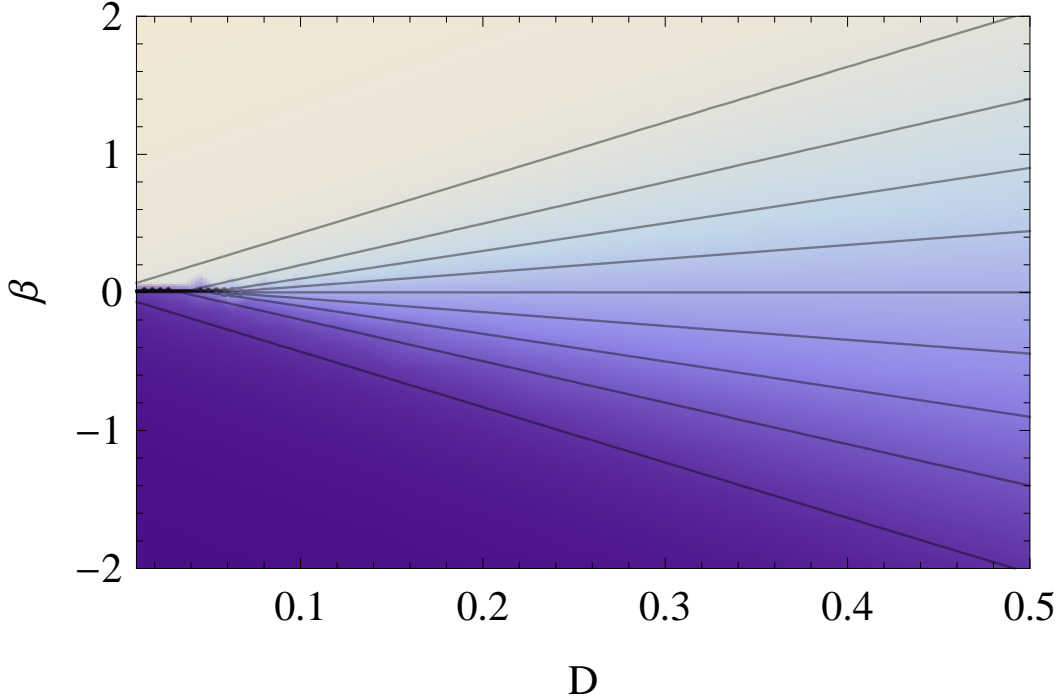


Figure 2: Polarization plot with $g_{\uparrow\uparrow} = 0$, $g_{\downarrow\downarrow} = 0$, $g_{\uparrow\downarrow} = 8$

interactions are turned on in such a way that they act against the tendencies of the dipole-dipole interactions—that is, when the contact interactions make high polarizations more favorable than low ones like the dipole-dipole interactions do—interesting features begin to appear in the polarization diagram.

In Figure 2, we have plotted the polarization with a repulsive contact interaction between dipoles of opposite orientation ($g_{\uparrow\downarrow}$ positive) turned on. This makes a low polarization state less favorable. If we make this contact interaction strong enough to dominate the dipole-dipole interactions for small D as in Figure 2, the polarization contours overlap one another in what appears as a thick horizontal line segment at $\beta = 0$, starting at $D = 0$ and continuing until D is strong enough to not be dominated by the contact interactions.

Immediately above this line the polarization is large and positive, while below it is large and negative. This tells us that even an infinitesimal change in β that crosses zero (i.e. when the electric field switches direction, no matter how small the change), the polarization of the ground state discontinuously changes from large and negative (or positive, depending on the initial sign of β), to large and positive (or negative). This is significant because it shows the quality of the ground state's behavior has changed; without contact interactions, the polarization strictly changes continuously with changes in D and β .

We have found that this feature of the polarization can be created or enhanced by other contact interaction schemes that make high magnitude polarizations more favorable than low ones. In Figure 3 we show the effects of adding both attractive up-up and down-down contact interactions (negative $g_{\uparrow\uparrow}$ and $g_{\downarrow\downarrow}$), with and without repulsive up-down interactions (positive $g_{\uparrow\downarrow}$). We note that it is more efficient to produce this feature by increasing up $g_{\uparrow\downarrow}$

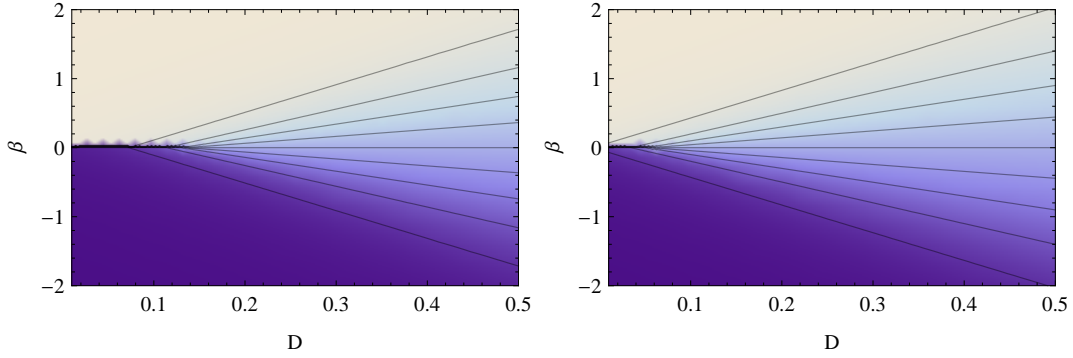


Figure 3: Polarization plots for:
(left) $g_{\uparrow\uparrow} = -6$, $g_{\downarrow\downarrow} = -6$, $g_{\uparrow\downarrow} = 6$, i.e. $g = 6$
(right) $g_{\uparrow\uparrow} = -8$, $g_{\downarrow\downarrow} = -8$, $g_{\uparrow\downarrow} = 0$

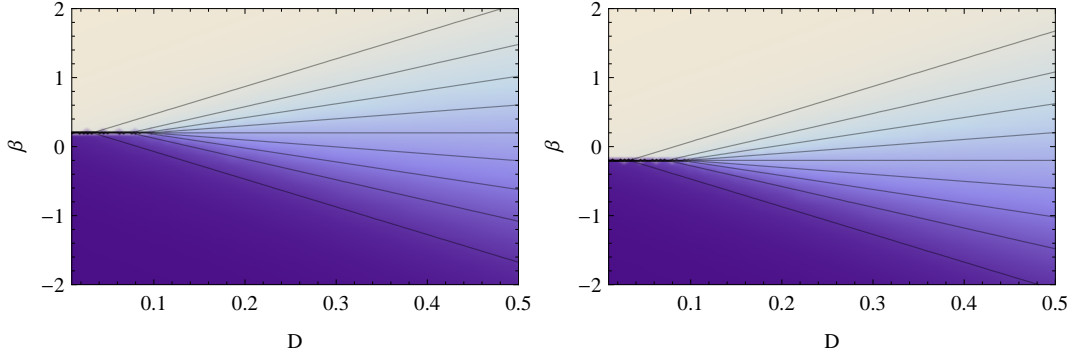


Figure 4: Polarization plots for:
(left) $g_{\uparrow\uparrow} = 0$, $g_{\downarrow\downarrow} = -4$, $g_{\uparrow\downarrow} = 8$
(right) $g_{\uparrow\uparrow} = -4$, $g_{\downarrow\downarrow} = -0$, $g_{\uparrow\downarrow} = 8$

than $g_{\uparrow\uparrow}$ or $g_{\downarrow\downarrow}$. This feature can be produced by sufficiently attractive up-up or down-down contact interactions alone, but this requires a correspondingly larger magnitude of $g_{\uparrow\uparrow}$ or $g_{\downarrow\downarrow}$.

Figure 4 shows what happens when we break the symmetry between $g_{\uparrow\uparrow}$ and $g_{\downarrow\downarrow}$. When we turn on either attractive $g_{\uparrow\uparrow}$ or $g_{\downarrow\downarrow}$ interactions, we can still produce this feature, but the asymmetry causes a vertical shift. The two images are equivalent, so we will discuss the left image for simplicity. This shift occurs because the attractive down-down contact interactions can dominate the electric field when it acts upwards so long as β is small. The phenomenal thing about this is that we have created a system whose polarization is opposite to the sign of the electric field, within a small range of β . This situation appears counterintuitive, but bear in mind that even in this regime increasing β does produce a corresponding change in the polarization. That is, increasing β increases the polarization, even in the regime where the polarization is opposite the direction of β , or indeed anywhere else.

What we have found is that unusual behavior emerges when contact interactions act

oppositely to dipole-dipole interactions. However, these states might not be stable against fluctuations, and this leads us to consider how contact interactions affect the stability of the system.

4 Stability

In this section we examine the stability of the system and how it is affected by contact interactions. We will begin by showing the stable regions in $D - \beta$ space with only dipole-dipole interactions, and then we will show the effects of gradually turning on simple contact interactions. For these simple contact interactions, we constrain the three types of contact interactions—governed by $g_{\uparrow\uparrow}$, $g_{\downarrow\downarrow}$, and $g_{\uparrow\downarrow}$ —to oppositely mirror the dipole-dipole interactions. That is, up-up and down-down contact interactions are attractive while up-down contact interactions are repulsive, and all three have equal strength characterized by the parameter g . Explicitly, $g_{\uparrow\downarrow} = -g_{\uparrow\uparrow} = -g_{\downarrow\downarrow} = g$.

We are motivated to explore this constraint because of the unusual behavior this contact interaction paradigm has on the polarization. The feature we found appeared regardless of the combination of contact interactions we chose within this contact interaction paradigm of mirroring the dipole-dipole interactions. Therefore, we find it natural to include all three types of contact interactions and adjust them with the single parameter g . In further work we may relax this constraint to explore more diverse possibilities.

Without contact interactions the stability diagram is just a single curve that separates the stable region from the unstable region. This is represented by the right-most contour in the plots in Figure 5. The region to the left of the curve is stable, and the region to the right is unstable. We know the system is unstable when the dispersion relation is imaginary.

Figure 5 shows how the stable region shrinks as g is turned on and increased. The image on the left is a contour-density plot of the stability thresholds. The rightmost contour shows what values of D and β border instability for $g=0$ (no contact interactions). As g increases, the g -contours move inwards from both sides of the graph, showing reduced regions of stability in D - β space with increasing g . The image on the right has the same contours, but the color gradient shows the polarization of the system at the stability threshold for each point. That is, for each point in D - β space, it shows the polarization of those values of D , β , and the value of g for which that point borders instability. The apparent low-polarization strip along the left side of this image is due to numerical instability.

As we turn g on and gradually increase it, using the dipole-dipole mirroring constraint where $g_{\uparrow\downarrow} = -g_{\uparrow\uparrow} = -g_{\downarrow\downarrow} = g$, the stable region shrinks inwards from both sides, as you can see from Figure 5. On the left side of the diagram where D is small, the dipole-dipole interactions are weak, allowing the electric field to polarize the gas, bringing most dipoles into the up state. Since the gas is polarized and D is small, the up-up contact interactions are prevalent here. With the dipole-dipole interactions dominated by the contact-interactions here, which are attractive in this situation, there is an appreciable attractive force between all of the molecules with little to no repulsive force to keep them from clumping up and maintain their stability, so all of the molecules will be pulled in. This will increase their energies, exciting them out of their bound ground state. This is what happens in the region where D is small with this choice of contact interactions, and so it is unstable until D becomes large enough to provide strong enough repulsive interactions to stabilize the system against the attractive contact interactions.

In the upper-middle part of the stability diagram, where β is large and D is at a maximum

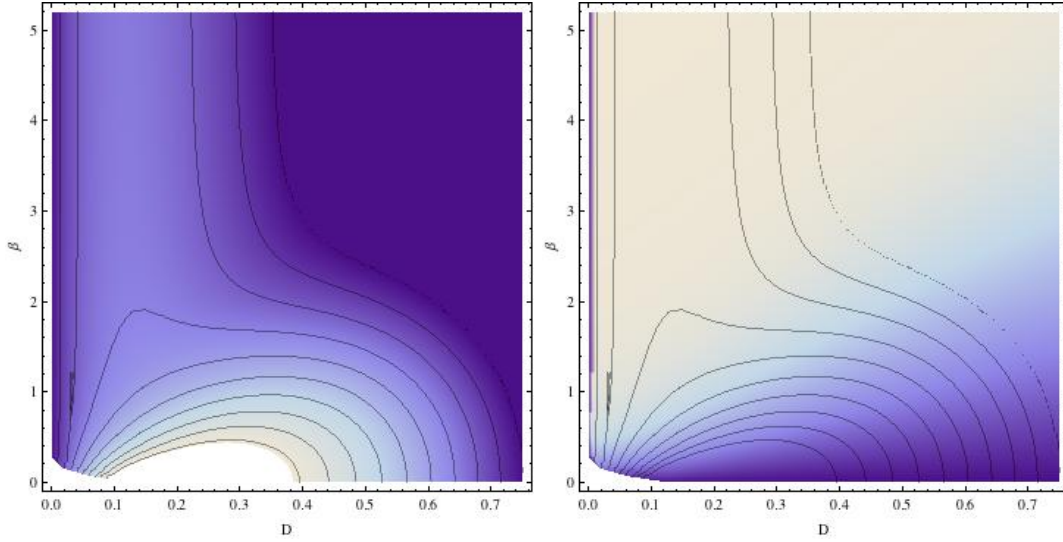


Figure 5: (left) Stability contour-density plot; the region at the bottom is blank and the zero-g contour is jagged due to numerical instabilities in our methods (right) Stability contour plot with a color gradient representing the polarization

before causing instability, the strong electric field overcomes the repulsive dipole-dipole interactions and polarizes the system to a state where most dipoles are in the up state. Since the dipole-dipole interaction between up-up dipoles is repulsive, it creates high-density clumps of up dipoles between rarefied regions. This is a density wave. Within the high-density clumps, because the system is only quasi two-dimensional, there is some “wobble room” in the z -direction, perpendicular to the plane of the trap. Since the dipoles are pressed so close together in these localized regions and are able to slide up and down slightly, they can begin to feel the attractive effects of the dipole-dipole interaction, which acts to pull them on top of each other. That is, when these dipoles are bunched up like this, they start to pile up. If D is made sufficiently strong, the dipoles in the high-density regions will pile up end-to-end, and then be so strongly attracted that they implode. Including the contact interactions in this parameter regime introduces a source of attraction between all the dipoles in the up state, which is most of them since the system is highly polarized in the high field limit. This pulls the localized clumps of up-dipoles closer together, and therefore has the effect of strengthening the dipole-dipole interactions, leading to the same type of instability, but at smaller values of D which were stable without the contact interactions.

In the lower-right portion of the stability diagram, β is small but D is large, and the system is pushed towards a low-polarization state where there are few more up-dipoles than down-dipoles. In the low field limit where β goes to zero, there is the same number of up-dipoles as down-dipoles. Rather than a density wave as in the high field limit just described, a spin wave is set up in this region. That is, there are localized regions of primarily up-dipoles alternating with regions of primarily down-dipoles. Once in this state, things act much as in the high field case, wherein locally polarized regions of dipoles get pushed together and begin to pile up end-to-end due to the dipole-dipole interactions. As before, if D becomes sufficiently large then they will fully pile up end-to-end, collapse, and explode, falling out of

the trap. Adding contact interactions introduces repulsion between up and down dipoles, and acts to quicken the separation of locally polarized regions. Once that spin wave has been set up, the contact interactions serve to further attract the polarized dipoles in each region to their neighbors within those regions, effectively strengthening the dipole-dipole interactions, which cause them to pile up and collapse. The overall effect is that instability occurs at lower D values.

At the bottom of the diagram the g -contours eventually converge to a point. At this g -value, the stable region has contracted until the system is stable for only one value of D and β . The physical nature of the instabilities introduced by deviating from this point along D or β have not yet been explored. Presumably they are of the same types as the instabilities on the fringes of the stable region to the left and right at smaller values of g .

5 Conclusion

Our model of the system assumes that all bosons have the same single-body wavefunction: the product of their center-of-mass movement with their internal state. We extend this to a many-body wavefunction and use the variational principle with the proportion of dipoles in the $|\uparrow\rangle$ state, ν , as our variational parameter to approximate the ground state energy and find the polarization of the system. We extend this model by adding small excitation plane waves to the center-of-mass factor of the wavefunction to allow slight perturbations above the ground state. We solve the Schrodinger equation with this extended wavefunction for the amplitudes of the excitations and the dispersion relations, with which we can determine the stability or instability of the system for a given set of parameter values (D and β).

We have explored the polarization of the system with a variety of contact interactions and found that a feature appears in certain contact interaction regimes. The feature that we've found is a convergence of polarization contours for small D values, i.e. when the dipole-dipole interactions are weak, and it occurs when we include very strong contact interactions that make a highly polarized state more favorable than a low polarization state. We see this in Figures 2-4. However, in Figure 4 the contact interactions are asymmetric; they are only attractive between either two up-dipoles or two down-dipoles. This corresponds to a shift in the feature along the vertical β -axis.

This feature may indicate a first order phase transition in the polarization. That is, a minute change in β across this feature corresponds to a discontinuous change in the polarization from one extremely polarized state to the other. When there is a vertical shift in this polarization feature, we see an anomalous region between the $\beta = 0$ line and the feature in which the polarization of the system is opposite the direction of the external electric field (β). This would indicate that in these parameter regimes, turning on an electric field may induce a polarization opposite to that field. However, the contact interaction strengths necessary to create this polarization feature are extreme, so it is natural to explore the stability of the system around these features and determine if they might actually be realized in a physical system.

To this end, it is useful to consider the polarization plot on the left in Figure 3 in concert with the stability diagrams in Figure 5. Note that the largest g -contour shown on the stability diagrams corresponds to $g = 2.25$. The stable region in $D - \beta$ space when $g = 6$ has not disappeared entirely, but is confined to a small area around $D = 0.2$ where β is small. Referring back to the polarization plot, we see that this stable region does not include any part of the feature created when $g = 6$. Therefore, we conclude that these

features are highly unstable, and will be difficult or impossible to find experimentally.