Theory of dipolar gases (I)

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Contact interaction

In typical experiments up to now the atoms interact via short-range isotropic interactions.

The interaction is given by the s-wave scattering length “a”.

\[ V(\vec{r} - \vec{r}') \approx \frac{4\pi\hbar^2 a}{m} \delta(\vec{r} - \vec{r}') \equiv g\delta(\vec{r} - \vec{r}') \]
Dipole-dipole interaction

\[ U_{dd}(\mathbf{r}) = \frac{C_{dd}}{4\pi} \frac{(e_1 \cdot e_2) r^2 - 3 (e_1 \cdot \mathbf{r}) (e_2 \cdot \mathbf{r})}{r^5} \]

\[ C_{dd} \leftrightarrow \frac{\mu_0 \mu^2}{d^2/\varepsilon_0} \]

(magnetic dipoles)

(13.1)

(13.2)

\[ U_{dd}(\mathbf{r}) = \frac{C_{dd}}{4\pi} \frac{1 - 3 \cos^2 \theta}{r^3} \]

(13.2)

(13.3)
Dipolar gases: all the way from very weak to huge
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\[ \varepsilon_{dd} \equiv \frac{C_{dd}}{3g} \]
Polar molecules

\[ \hat{H} = B \hat{J}^2 \]

\[ |J, M\rangle \Rightarrow BJ(J+1) \]

\[ \langle 0,0 | d | 0,0 \rangle = 0 \quad \langle 1,M | d | 0,0 \rangle \neq 0 \]
Polar molecules

\[ \hat{H} = B\hat{J}^2 - \vec{d} \cdot \vec{E} \]
Polar molecules

\[ \hat{H} = B\hat{J}^2 - \vec{d} \cdot \vec{E} \]

\[ \langle \phi_0 | d | \phi_0 \rangle \neq 0 \]
Pseudopotential

\[ U_{SR}(r) + U_{dd}(\vec{r}) \rightarrow g(d)\delta(r) + U_{dd}(\vec{r}) \]

[From Bortolotti et al., PRL 97, 160402 (2006)]
Dipolar BECs: Nonlocal Gross-Pitaevskii equation

\[ H = \int dr \hat{\psi}^+ (\vec{r}) \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_T (r) - \mu \right] \hat{\psi} (\vec{r}) \]

\[ + \frac{1}{2} \iint d\vec{r} d\vec{r}' \hat{\psi}^+ (\vec{r}) \hat{\psi}^+ (\vec{r}') U (\vec{r} - \vec{r}') \hat{\psi} (\vec{r}') \hat{\psi} (\vec{r}) \]

\[ U (\vec{r}) = g \delta (r) + U_{dd} (\vec{r}) \]
Dipolar BECs: Nonlocal Gross-Pitaevskii equation

\[ \hat{H} = \int d\mathbf{r} \hat{\psi}^\dagger(\mathbf{r}) \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_T(\mathbf{r}) - \mu + \frac{1}{2} g \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}) \right] \hat{\psi}(\mathbf{r}) \]

\[ + \frac{1}{2} \int d^3r d^3r' \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') U_{dd}(\mathbf{r} - \mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}), \]

\[ \hat{\psi}(\mathbf{r}) \equiv \psi(\mathbf{r}) \]
Dipolar BECs: Nonlocal Gross-Pitaevskii equation

\[ i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) - \mu + g|\psi(\mathbf{r}, t)|^2 \right. \]
\[ \left. + \frac{C_{dd}}{4\pi} \int d\mathbf{r}' \frac{1 - 3 \cos^2 \theta}{|\mathbf{r} - \mathbf{r}'|^3} |\psi(\mathbf{r}', t)|^2 \right] \psi(\mathbf{r}, t) \]
Stability: homogeneous space

\[ \hat{\psi}(\mathbf{r}) = \sum_{\mathbf{p}} \hat{a}_{\mathbf{p}} \exp[i\mathbf{p} \cdot \mathbf{r}/\hbar] \sqrt{V}. \]

\[ \hat{H} = \sum_{\mathbf{p}} \frac{p^2}{2m} \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}} + \frac{1}{2V} \sum_{\mathbf{p}_1, \mathbf{p}_2, \mathbf{q}} (g + \tilde{U}_{dd}(\mathbf{q})) \hat{a}_{\mathbf{p}_1}^\dagger \hat{a}_{\mathbf{p}_2}^\dagger \hat{a}_{-\mathbf{q}} \hat{a}_{\mathbf{p}_2} \hat{a}_{\mathbf{p}_1} \]

\[ \tilde{U}_{dd}(\mathbf{q}) = \frac{C_{dd}}{3} (3 \cos^2 \theta_q - 1) \]

\[ \hat{a}_0, \hat{a}_0^\dagger \simeq \sqrt{N} \]

\[ \hat{H} = \sum_{\mathbf{p} \neq 0} \frac{p^2}{2m} \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}} + \frac{n_0}{2} \sum_{\mathbf{p}} (g + \tilde{U}_{dd}(\mathbf{q}))(2 \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}} + \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{-\mathbf{p}}^\dagger + \hat{a}_{\mathbf{p}} \hat{a}_{-\mathbf{p}}) \]

\[ \epsilon(\mathbf{p}) = \sqrt{\frac{p^2}{2m} \left[ \frac{p^2}{2m} + 2n_0 (g + \tilde{U}_{dd}(\mathbf{p})) \right]} \]
Stability: homogeneous space

\[ \varepsilon(\vec{p}) = \sqrt{\frac{p^2}{2m} \left[ \frac{p^2}{2m} + 2gn_0 \left( 1 + \frac{C_{dd}}{3g} \left( 3\cos^2 \theta_p - 1 \right) \right) \right]} \]

For a short-range interacting gas with \( a < 0 \)

\[ \varepsilon(\vec{p}) = \sqrt{\frac{p^2}{2m} \left[ \frac{p^2}{2m} - 2|g|n_0 \right]} \approx p\sqrt{\frac{-|g|n_0}{m}} = ip|c_s| \]
Stability: homogeneous space

\[ \varepsilon(\vec{p}) = \sqrt{\frac{p^2}{2m} \left[ \frac{p^2}{2m} + 2gn_0 \left( 1 + \frac{C_{dd}}{3g} (3\cos^2 \theta_p - 1) \right) \right]} \]

\[ \varepsilon(\vec{p}) \equiv p \sqrt{\frac{gn_0}{m}} \sqrt{1 + \frac{C_{dd}}{3g} (3\cos^2 \theta_p - 1)} \]

If \( \varepsilon_{dd} > 1 \) one has dynamical instability (phonon instability) but only in some directions
Stability: trapped case

\[ \psi(\rho, z) = \frac{\sqrt{N}}{\pi^{3/4} l_\rho l_z^{1/2}} e^{-z^2/2l_z^2} e^{-\rho^2/2l_\rho^2} \]

\[ E = \frac{N \hbar^2}{2m} \left\{ \frac{1}{l_z^2} + \frac{2}{l_\rho^2} \right\} + \frac{Nm}{4} \left\{ 2\omega_\rho^2 l_\rho^2 + \omega_z^2 l_z^2 \right\} \]

\[ + \frac{gN^2}{2(2\pi)^{3/2} l_z l_\rho^2} + \frac{C_{dd} N^2}{3(2\pi)^{3/2} l_\rho^2 l_z} f(\kappa), \quad \kappa = l_\rho/l_z \]

\[ f(\kappa) \equiv \left\{ \frac{2\kappa^2 + 1}{\kappa^2 - 1} - \frac{3\kappa^2}{(\kappa^2 - 1)^{3/2}} \arctan[\sqrt{\kappa^2 - 1}] \right\} \]
Stability: trapped case

\[ \langle U_{dd} \rangle < 0 \]

\[ \langle U_{dd} \rangle > 0 \]
Geometry-Dependent Stability of Trapped Condensates

Phonon instability also occurs in homogeneous non-dipolar BECs with the density of the DDI, the dispersion has an anomalous momentum dependence. Along the trap geometry crucially determines the stability properties. This is the case for the homogeneous 3D dipolar BEC is dynamically unstable. This is the so-called phonon instability. The axial and radial trap frequencies and the trap aspect ratio are different than the condensates in pancake BECs. As a result, the curve minimum of the energy of the system:

\[ E = \frac{N\hbar^2}{2m} \left\{ \frac{1}{l_z^2} + \frac{2}{l_\rho^2} \right\} + \frac{Nm}{4} \left\{ 2\omega_\rho^2 l_\rho^2 + \omega_z^2 l_z^2 \right\} + \frac{gN^2}{2(2\pi)^{3/2}l_z l_\rho^2} + \frac{C_{dd}N^2}{3(2\pi)^{3/2}l_\rho^2 l_z^2} f(\kappa), \quad \kappa = l_\rho/l_z \]

\[ f(\kappa) \equiv \left\{ \frac{2\kappa^2 + 1}{\kappa^2 - 1} - \frac{3\kappa^2}{(\kappa^2 - 1)^{3/2}} \text{arctan}[\sqrt{\kappa^2 - 1}] \right\} \]
Geometry-dependent stability

[T. Koch et al., Nat. Phys. 4, 218 (2008);
Trap-dependent stability and d-wave collapse


[Lahaye et al., PRL 101, 080401 (2008)]
2D solitons

**Gross-Pitaevskii equation**

\[
i\hbar \frac{\partial}{\partial t} \psi(\vec{r}, t) = \left\{ \frac{-\hbar^2}{2m} \nabla^2 + V(\vec{r}, t) + \frac{4\pi \hbar^2}{m} N|\psi(\vec{r}, t)|^2 \right\} \psi(\vec{r}, t)
\]

**Dark Solitons (a>0)**

[Burger et al, PRL 83, 5198 (1999)]
[Denschlag et al., Science 287, 97 (2000)]

**Bright solitons (a<0)**

[Strecker et al., Nature 417, 150 (2002)]
[Khaykovich et al., Science 296, 1290 (2002)]

Continuous solitons become unstable in 2D and 3D
2D solitons

\[ \psi(r) = \frac{1}{l_y^{3/2} \pi^{3/4} \Lambda_x \Lambda_z} e^{\frac{1}{2l_y^2} \left( \frac{x^2}{\Lambda_x^2} + \frac{z^2}{\Lambda_z^2} + y^2 \right)} \]

\[ \epsilon \equiv \frac{E}{N \hbar \omega_y} = \frac{1}{4(\Lambda_x^2 + \Lambda_z^2)} + \frac{\tilde{g}}{4\pi \Lambda_x \Lambda_z} \left[ 1 + \epsilon_{dd} \hbar \left( \frac{\Lambda_x}{\Lambda_z}, \frac{1}{\Lambda_z} \right) \right] \]

\[ \tilde{g} = \frac{m}{\hbar^2} \frac{Ng}{\sqrt{2\pi} l_y} \]

\[ h(\alpha, \beta) = -1 + 3 \int_0^1 ds \frac{3\alpha \beta s^2}{[1 + \alpha^2 - 1) s^2]^{1/2} [1 + \beta^2 - 1) s^2]^{1/2}} \]

Without dipole

\[ \epsilon(\Lambda = \Lambda_x = \Lambda_z) = \frac{(1 + \tilde{g}/2\pi)}{2\Lambda^2} \]
2D solitons

Let us consider first what happens for non-dipolar gases. In that case $\epsilon_{dd} = 0$ and $\epsilon(\Lambda_\text{x} = \Lambda_\text{z}) = (1 + \tilde{g}/(2\pi))^{2}\Lambda^2$, hence depending on the sign of $1 + \tilde{g}/(2\pi)$ the system minimises the energy either by expanding without limits, or by contracting without limits. The localised solution is hence unstable. This is once more the well-known instability of solitons in 2D.

The extra term provided by the DDI is quite interesting, since it introduces an additional dependence on $\Lambda_x, \Lambda_z$. This allows (under appropriate conditions) for a minimum in the energy, and hence for a stable self-localised solution! This minimum is characterised by its equilibrium widths $\Lambda_{x,0}$ and $\Lambda_{z,0}$. Note that they are in general not equal. This asymmetry comes of course from the fact that the dipole is along the $z$ direction. In Fig. 1.7 (Nath et al., 2009) we show the stability diagram as a function of $\tilde{g}$ and $\epsilon_{dd}$. There we observe two instability regions for 2D solitons (against collapse and against unlimited expansion). For $\epsilon_{dd} > 1$, there is a critical universal value $\tilde{g}_{\text{cr}}(\beta) \equiv g_{\text{cr}}N/\sqrt{2\pi l_z}$ such that for $N > N_{\text{cr}}$ the minimum of $E(\Lambda_x, \Lambda_z)$ disappears. As a consequence, stable 2D anisotropic self-localised solutions are stable only for a number of particles per soliton below a critical number $N_{\text{cr}}$, which decreases for larger $\epsilon_{dd}$. Beyond this number the 2D soliton collapses. This result is also verified by a direct simulation of the 3D nonlocal Gross-Pitaevskii equation.

In this simplified discussion we have assumed that the problem remains 2D. If the interactions increase the problem becomes 3D, and one may show that the condensate becomes eventually unstable (Pedri and Santos, 2005; Tikhonenkov et al., 2008).

A major difference between bright solitons in non-dipolar and dipolar BECs concerns the soliton-soliton scattering properties. Whereas 1D solitons in non-dipolar...
2D solitons

BECs scatter elastically, the scattering of dipolar solitons is inelastic due to the lack of integrability (Krolikowski et al., 2001). The solitons may transfer centre-of-mass energy into internal vibrational modes, resulting in intriguing scattering properties, including soliton fusion (Pedri and Santos, 2005) (see Fig. 1.8), the appearance of strong inelastic resonances (Nath et al., 2007), and the possibility of observing 2D-soliton spiraling as that already observed in photo-refractive materials (Shih et al., 1997).