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Roton Instability and Phonon Collapse of Two-dimensional Tilted Dipoles

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Abstract. Bose-Einstein condensed gas of two-dimensional tilted dipoles in a thin layer is under consideration. The problem of stability is resolved. Phase diagram for system of two-dimensional dipole atoms in a thin layer is obtained. A formation of density waves and their orientation control possibility via polarizing field are considered. These effects can be experimentally observed for magnetically dipolar atoms at the Feshbach resonance or polar molecules in one-dimensional optical lattices.

1. Introduction

Anisotropy and attraction of dipole-dipole interaction potential are reasons for set of wonderful phenomena. There are density waves (DWs) formation [1], [2], [3], [4], phonon collapse [5], supersolid [7], [8], [9] and anisotropy superfluidity [10] among them. In this regard, great attention is recently paid to the dipole-dipole bosonic systems [11], [12].

In this note we consider two-dimensional (2D) *tilted* dipole atoms in a thin layer at zero temperature. There are two experimental realizations for the model. The first one is atoms with magnetic dipole moment [13], [14] at the Feshbach resonance [15] in a 1D optical lattice [16]. The second one is polar molecules with electrically induced moment [17] in a 1D optical lattice [18]. Also, problem statement (from experimental point of view) is illustrated in the Fig. 1.

Stability criteria defines the phase diagram. The stability criteria is non-negativity of the Bogoliubov spectrum square

$$\varepsilon_{\mathbf{p}}^2 = \frac{p^2}{2m} \left(\frac{p^2}{2m} + 2n_0 U_{2d}(\mathbf{p}) \right) \ge 0, \tag{1}$$

where n_0 is 2D condensate density, m is dipole mass, $U_{2d}(\mathbf{p})$ is Fourier transform of 2D interaction potential of tilted dipoles.

An exposition of a part of results of this note is presented in Ref. [19].

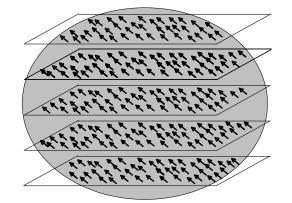


Figure 1. Bose-Einstein condensed gases of 2D tilted dipoles in thin layers, which are formed for a 3D condensate in a 1D optical lattice.

2. Interaction potential

Bogoliubov spectrum calculation is necessary to investigate a stability problem for the system. Therefore, it is necessary to calculate effective part of 2D interaction potential $U_{2d}(\mathbf{r})$ of dipoles in a thin layer. To this aim, let us start from 3D Hamiltonian of the system

$$\hat{H} - \mu_{3d}\hat{N} = \int d\vec{r}\hat{\Psi}(\vec{r})\hat{\Psi}^{+}(\vec{r}) \left(-\frac{\hbar^{2}}{2m}\Delta_{3} + V(\mathbf{r}) + V_{\rm ti}(z) - \mu_{3d}\right) + \frac{1}{2}\int d\vec{r}d\vec{r}'(V_{dd}(\vec{r} - \vec{r}') + g_{3d}\delta(\vec{r} - \vec{r}'))\hat{\Psi}^{+}(\vec{r})\hat{\Psi}^{+}(\vec{r}')\hat{\Psi}(\vec{r}')\hat{\Psi}(\vec{r}'),$$
(2)

where Δ_3 is 3D Laplace operator, $\hat{\Psi}(\vec{\mathbf{r}})$ is 3D field operator, $g_{3d}\delta(\vec{\mathbf{r}})$ is contact van der Waals pseudopotential, μ_{3d} is chemical potential, $V_{\text{ti}}(z)$ is confinement potential in the tight direction, $V(\mathbf{r})$ is confinement potential in thin layer plane,

$$V_{dd}(\vec{\mathbf{r}},\theta) = \frac{d^2}{\vec{\mathbf{r}}^5} (\mathbf{r}^2 - 3(x\sin\theta + z\cos\theta)^2)$$

is dipole-dipole potential, d is dipole moment, and dipoles are tilted at angle θ to z axis. Arrows is used for 3D vectors and bold type is used for 2D vectors

$$\vec{\mathbf{r}} = \{\mathbf{r}, z\}, \quad \mathbf{r} = \{x, y\}, \quad r = |\mathbf{r}|, \quad \mathbf{r} = |\vec{\mathbf{r}}| = \sqrt{r^2 + z^2}.$$

In the sufficiently thin layer the motion in the tight direction is frozen at the lowest level, the excited levels being practically not populated. Therefore, in the expansion of 3D field operator on basis $\{\varphi_k^{ti}(z)\}$ in the tight direction

$$\hat{\Psi}(\vec{\mathbf{r}}) = \sum_{k=0}^{\infty} \varphi_k^{\text{ti}}(z) \hat{\Psi}_k(\mathbf{r}), \quad \hat{\Psi}_k(\mathbf{r}) = \int dz \varphi_k^{\text{ti*}}(z) \hat{\Psi}(\vec{\mathbf{r}})$$

we can neglect all $\hat{\Psi}_k(\mathbf{r})$ for k > 0. Here the eigenfunctions $\varphi_k^{\text{ti}}(z)$ and eigenenergies E_k^{ti} are determined from the following equation

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dz^2}+V_{\rm ti}(z)\right)\varphi_k^{\rm ti}(z)=E_k^{\rm ti}\varphi_k^{\rm ti}(z).$$

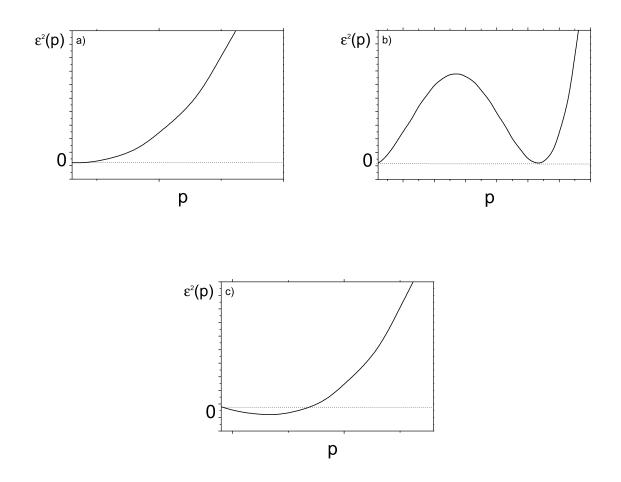


Figure 2. Bogoliubov spectrums for three phases. a) Stable homogeneous gas. b) Phase with roton instability with respect to density wave formation. c) Phase with phonon instability with respect to long-wave-lenght collapse.

Thus, we can consider k = 0 element

$$\hat{\Psi}(\vec{\mathbf{r}}) \approx \varphi_0^{\mathrm{ti}}(z)\hat{\Psi}(\mathbf{r}), \quad \hat{\Psi}(\mathbf{r}) = \int dz \varphi_0^{\mathrm{ti}*}(z)\hat{\Psi}(\vec{\mathbf{r}}), \tag{3}$$

where $\hat{\Psi}(\mathbf{r})$ is effective 2D field operator, which is satisfied to bosonic commutation relations.

After substituting (3) in (2), effective 2D Hamiltonian for thin-layer motion is obtained in the following form

$$\hat{H} - \mu \hat{N} = \int \hat{\Psi}^{+}(\mathbf{r}) \left(-\frac{\hbar^{2}}{2m} \Delta_{2} - \mu + V(\mathbf{r}) \right) \hat{\Psi}(\mathbf{r}) d\mathbf{r} + \int U_{2d}(\mathbf{r} - \mathbf{r}') \hat{\Psi}^{+}(\mathbf{r}) \hat{\Psi}^{+}(\mathbf{r}') \hat{\Psi}(\mathbf{r}') \hat{\Psi}(\mathbf{r}) d\mathbf{r} d\mathbf{r}'$$
(4)

with effective 2D interaction

$$U_{2d}(\mathbf{r} - \mathbf{r}') = \int dz dz' |\varphi_0^{\rm ti}(z)\varphi_0^{\rm ti}(z')|^2 (g_{3d}\delta(\vec{\mathbf{r}} - \vec{\mathbf{r}}) + V_{dd}(\vec{\mathbf{r}} - \vec{\mathbf{r}}))$$
(5)

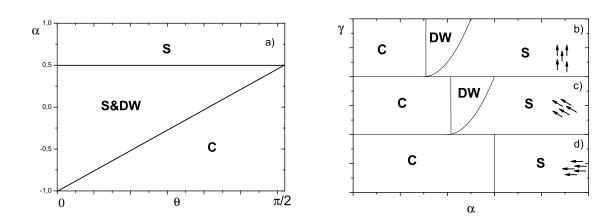


Figure 3. Phase diagrams. a) A phase diagram for two-dimension homogeneous layer is shown; b) homogeneous superfluid phase (S on the figure); c) phonon instability phase with long-wave collapse (C on the figure); and d) roton instability phase with DWs generation (DW on the figure).

and chemical potential $\mu = \mu_{3d} - E_0^{\text{ti}}$ (where Δ_2 is 2D Laplace operator).

Note, that one of the instability possible reasons is negativity of effective 2D potential Fourier transform. Let us calculate the potential $U_{2d}(\mathbf{r})$ and define a condition of it's negativity. We suppose the presence of harmonic trap along tight direction, i.e., $V_{\text{ti}}(z) = (m/2)\omega^2 z^2$, therefore

$$\varphi_{\rm ti}(z) = \exp(-z^2/2z_0^2)/\sqrt{\sqrt{\pi}z_0}$$
 (6)

and $E_0^{\text{ti}} = \hbar \omega/2$. Here $z_0 = \sqrt{\hbar/m\omega}$ is tight-confinement oscillator length and ω is the oscillator frequency.

After substituting (6) in (5), the Fourier transform of the effective 2D potential in first Born approximation is obtained in the following form

$$U_{2d}(\mathbf{p}) = g_s - \frac{g_d}{2} + U_h(\mathbf{p})\sin^2\theta + U_v(\mathbf{p})\cos^2\theta,$$
(7)

where

$$U_{h}(\mathbf{p}) = \frac{2d^{2}}{\hbar} \int_{-\infty}^{+\infty} \exp\left(-\frac{p_{z}^{2}z_{0}^{2}}{2\hbar^{2}}\right) \frac{p_{x}^{2}dp_{z}}{p_{x}^{2} + p_{y}^{2} + p_{z}^{2}},$$
$$U_{v}(\mathbf{p}) = \frac{2d^{2}}{\hbar} \int_{-\infty}^{+\infty} \exp\left(-\frac{p_{z}^{2}z_{0}^{2}}{2\hbar^{2}}\right) \frac{p_{z}^{2}dp_{z}}{p_{x}^{2} + p_{y}^{2} + p_{z}^{2}},$$
$$g_{s} = \frac{2\sqrt{2\pi}\hbar^{2}a_{s}}{mz_{0}} = \frac{g_{3d}}{\sqrt{2\pi}z_{0}}, \ g_{d} = \frac{2\sqrt{2\pi}\hbar^{2}a_{d}}{mz_{0}} = \frac{2\sqrt{2\pi}d^{2}}{3z_{0}}.$$

 a_s is 3D s-wave scattering length and a_d is the length scale characterizing the dipole-dipole interaction.

After substituting (7) in (1), Bogoliubov spectrums for the systems are obtained. There are Bogoliubov spectrums in the Fig. 2.

Some assumptions was used for obtaining relation (7). First, it is the condition of weak interaction $a_s, a_d \ll z_0$ [20]. Second, the condition of the tight-confinement quantization, i.e.,

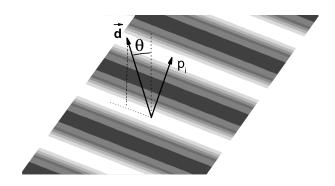


Figure 4. Bose-condensed gas of 2D dipole atoms in a thin layer.

 z_0 to be small. And third, the condition of independence of layers formed by the optical lattice, i.e., small interlayer tunneling and screening interlayer interaction of dipoles. A more precise calculation for independent 2D layers must consider the summation of the ladder diagrams [21], [22] and dipole-dipole scattering problem [23].

3. Phase diagram

In accordance with (1) there are following phase for system:

- 1. Homogeneous superfluid phase (Fig. 2a), where $\varepsilon_{\mathbf{p}}^2 > 0$ is positive for all momentums \mathbf{p} .
- 2. Phase with phonon instability and long-wave-length collapse (Fig. 2b), where $U_{2d}(0) < 0$ and $\varepsilon_{\mathbf{p}}^2 < 0$ is negative for momentums $p < p_{\text{ph}}$.
- 3. Phase with roton instability and density wave (DW) formation (Fig. 2c), where $U_{2d}(0) > 0$, but there is a certain momentum range $p_1 in which <math>U_{2d}(\mathbf{p}) < 0$, so $\varepsilon_{\mathbf{p}}^2$ touch to zero with roton momentum $\mathbf{p} = \mathbf{p}_r$.

A phase diagram with variables $\theta - \alpha - \gamma$ (where $\gamma = 2\sqrt{2\pi}z_0a_dn_0$ is density parameter and $\alpha = a_s/a_d$) for 2D layer is shown on Fig. 3a. There are a) homogeneous superfluid phase, b) phase with phonon instability and long-wave-length collapse, and c) phase with roton instability and DWs formation. This phases with parameters $\gamma - \alpha$ is shown on fig. 3b-3d for fixed angle θ . There are no DWs if dipoles are parallel to layer plane ($\theta = \pi/2$).

DWs orientation control possibility via (magnetic or electric) field is considered in Fig. 4. Lines of equal phase DWs directed along the projection of the dipole moment on the plane layer. Therefore, it's principally possible to control the orientation of the wave.

4. Experiment

Experimental threshold roton instability in our assessment in implementing following dipole systems:

1) Dysprosium atoms ¹⁶⁴Dy [14]: m = 164 u, $z_0 = 150$ nm, $\hbar\omega = 130$ nK, $\omega/2\pi = 2.7$ kHz, $\theta = 72^{\circ}$, $a_d = 14$ nm, $a_s = 5.5$ nm, a = 0.5 nm, $n_0 = 2.8 \times 10^9$ sm⁻², $\alpha = 0.393$, $\gamma = 0.292$, $\mu = 1.4$ nK, $T_0/4 = 130$ nK.

2) Polar molecules ⁴¹K⁸⁷Rb [28]: m = 128 u, $z_0 = 150$ nm, $\hbar\omega = 168$ nK $\omega/2\pi = 3.5$ kHz, $\theta = 56.8^{\circ}$, $a_d = 30$ nm, $a_s = 5.5$ nm, a = 3 nm, $n_0 = 4.65 \times 10^9$ sm⁻², $\alpha = 0.183$, $\gamma = 0.262$, $\mu = 4.4$ nK, $T_0/4 = 69$ nK.

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Here $T_0 = 2\pi\hbar^2/m$ is degeneracy temperature. The quantity $T_0/4$ is of order of Berezinskii-Kosterlitz-Thouless superfluid transition temperature [24], [25], [26] $T_{BKT} = \xi_s^c T_0/4$ [27] (where $\xi_s^c \equiv n_s(T_{BKT})/n \sim 1$ is superfluid fraction at the transition).

5. Conclusion

We have considered the stability problem for Bose-Einsten condensed gases of 2D tilted dipolar atoms or polar molecules in a thin layers formed for a 3D condensate in a 1D optical lattice. Based on our stability criteria we have obtained the phase diagram in which a stable homogeneous superfluid as well as phonon-collapsed and density-wave phases take place. Rotation of polarizing (magnetic or electric) field around the axis of the optical lattice yields controlling orientation of formed density wave. The effects can be observed for Dy atoms or polar molecules at nK temperatures.

Acknowledgments

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