Stability of quantum degenerate Fermi gases of tilted polar molecules

Vladimir Veljić[1], Axel Pelster[2], and Antun Balaž[1]

[1]Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Serbia
[2]Research Center OPTIMAS and Department of Physics, Technische Universität Kaiserslautern, Germany

Abstract

A recent experimental realization of an ultracold quantum degenerate gas of ^{40}K^{87}Rb molecules [1] opens up a new chapter in exploring strongly dipolar Fermi gases and many-body phenomena arising in that regime. This includes the deformation of the Fermi surface (FS) for polarized systems, where the electric dipoles have a preferential orientation, which can be achieved using an external field. Compared to atomic magnetic species [2, 3], this effect is significantly increased in ultracold Fermi gases of polar molecules, and the stability of the system is expected to strongly depend on its geometry. Here [4] we generalize a previous Hartree-Fock mean-field theory for the Wigner function, which now takes into account that the cloud shape in the ground state is determined not only by the trap frequencies, but also by the dipoles' orientation. In the special case of a spherically symmetric trap, the cloud is elongated in the direction of the dipoles, similar to the FS. We obtain a universal stability diagram for dipolar fermions and calculate the corresponding FS deformation for an arbitrary orientation of the dipoles, demonstrating the great promise for the exploration of degenerate molecules in electric fields, where the strong dipole-dipole interaction dominates. These results are important for designing future experiments with polar molecules, as well as for the interpretation of measured data, including the dynamics and the time-of-flight expansion.

Motivation

★ Quantum degenerate dipolar Fermi gas of polar molecules was realized for the first time [1]

★ Parameters of the experimental system
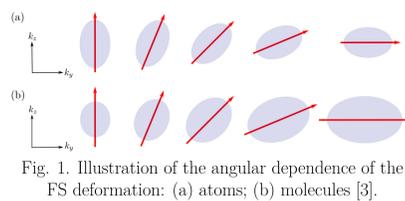
Fig. 1. Illustration of the angular dependence of the FS deformation: (a) atoms; (b) molecules [3].

^{40}K^{87}Rb	$N(\times 10^4)$	ω_x (Hz)	ω_y (Hz)	ω_z (Hz)	T/T_F
	3	$2\pi \times 63$	$2\pi \times 36$	$2\pi \times 200$	0.3

Global equilibrium

★ Our system: quantum degenerate Fermi gas of N polar molecules at $T = 0$ K

★ Molecules: spin-polarized fermions of mass M with tilted electric dipole moments $\mathbf{d} = (d, \theta, \varphi)$

★ Molecules are trapped by a harmonic potential with frequencies $(\omega_x, \omega_y, \omega_z)$

★ Shapes of molecular cloud and FS are assumed to be ellipsoids

★ Ansatz for the Wigner distribution function in global equilibrium is a Heaviside function

$$\nu^0(\mathbf{r}, \mathbf{k}) = \mathrm{H}\left(1 - \sum_{i,j} r_i \mathbb{A}_{ij} r_j - \sum_{i,j} k_i \mathbb{B}_{ij} k_j\right),$$

where matrix elements $\mathbb{A}_{ij}$ ($\mathbb{B}_{ij}$) describe the molecular cloud (Fermi surface) in real (momentum) space
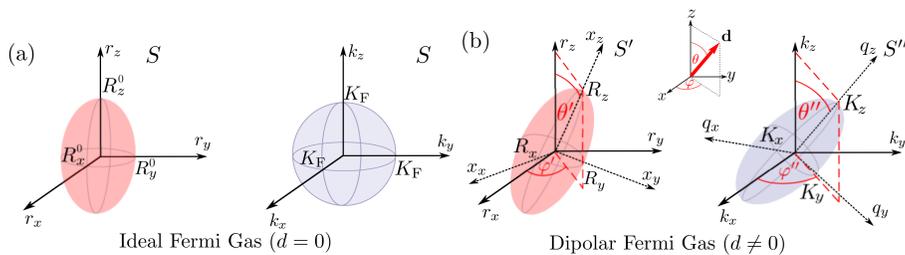

Fig. 2. Schematic illustrations of the most general ansatz for the Fermi surface and molecular cloud.

★ Matrix $\mathbb{A}$ is determined by a new position of the ellipsoidal molecular cloud, and has a diagonal form in the coordinate system S': $\mathbb{A}' = \mathbb{R}^T(\theta', \varphi')\mathbb{A}\mathbb{R}(\theta', \varphi')$

★ Matrix $\mathbb{B}$ is determined by the orientation of the dipoles, and has a diagonal form in the coordinate system S'': $\mathbb{B}'' = \mathbb{R}^T(\theta'', \varphi'')\mathbb{B}\mathbb{R}(\theta'', \varphi'')$

$$\mathbb{A}' = \begin{pmatrix} R_x'^2 & 0 & 0 \\ 0 & R_y'^2 & 0 \\ 0 & 0 & R_z'^2 \end{pmatrix}, \quad \mathbb{B}'' = \begin{pmatrix} K_x''^2 & 0 & 0 \\ 0 & K_y''^2 & 0 \\ 0 & 0 & K_z''^2 \end{pmatrix}, \quad \mathbb{R}(\theta, \varphi) = \begin{pmatrix} \cos\theta\cos\varphi & -\sin\varphi & \sin\theta\cos\varphi \\ \cos\theta\sin\varphi & \cos\varphi & \sin\theta\sin\varphi \\ -\sin\theta & 0 & \cos\theta \end{pmatrix},$$

where R_i' and K_i'' denote equilibrium radii and momenta of the atomic cloud and FS in direction i

★ The total number of fermions is (we drop prime and double prime symbols from R_i' and K_i'')

$$N = \frac{1}{48} R_x R_y R_z K_x K_y K_z$$

Total energy of the system

★ Total energy of the system in the Hartree-Fock mean-field theory

$$E = \frac{N}{8}\left(\sum_i \frac{\hbar^2 K_i^2}{2M} + \sum_{i,j} \frac{M\omega_i^2 \mathbb{R}_{ij}'^2 R_j^2}{2}\right) - \frac{6N^2 c_0}{\overline{R}^3}\left[F_A\left(\frac{R_x}{R_z}, \frac{R_y}{R_z}, \theta, \varphi, \theta', \varphi'\right) - F_A\left(\frac{K_z}{K_x}, \frac{K_z}{K_y}, \theta, \varphi, \theta'', \varphi''\right)\right]$$

where $\overline{R} = (R_x R_y R_z)^{1/3}$, c_0 is the interaction strength and F_A is a new generalized anisotropy function

$$F_A(x, y, \theta, \varphi, \tilde{\theta}, \tilde{\phi}) = \left(\sum_i \mathbb{R}_{iz}\tilde{\mathbb{R}}_{ix}\right)^2 f\left(\frac{y}{x}, \frac{1}{x}\right) + \left(\sum_i \mathbb{R}_{iz}\tilde{\mathbb{R}}_{iy}\right)^2 f\left(\frac{x}{y}, \frac{1}{y}\right) + \left(\sum_i \mathbb{R}_{iz}\tilde{\mathbb{R}}_{iz}\right)^2 f(x, y)$$

★ FS orientation coincides with the orientation of the dipoles, i.e., $\theta'' = \theta$ and $\varphi'' = \varphi$

★ The variational parameters R_i, K_i, θ', and φ' are determined by minimizing the total energy under the constraint that the particle number N is fixed to a given value

★ Note that the generalized anisotropy function satisfies [3]

$$F_A(x, y, \theta, \varphi, 0, 0) = f_A(x, y, \theta, \varphi) = \sin^2\theta\cos^2\varphi\, f\left(\frac{y}{x}, \frac{1}{x}\right) + \sin^2\theta\sin^2\varphi\, f\left(\frac{x}{y}, \frac{1}{y}\right) + \cos^2\theta\, f(x, y)$$

Stability diagram

★ Relative DDI strength: $\varepsilon_{\mathrm{dd}} = \frac{d^2}{4\pi\varepsilon_0}\sqrt{\frac{M^3}{\hbar^5}}(\omega_x\omega_y\omega_z N)^{1/6}$
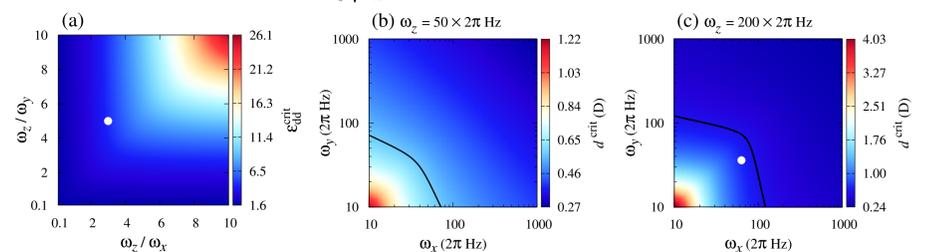

Fig. 3. (a) Universal stability diagram for harmonically trapped ultracold dipolar Fermi gases at quantum degeneracy. (b), (c) Critical value of the electric dipole moment d^{crit}, below which a stable ground state of $N = 3 \times 10^4$ ultracold molecules of ^{40}K^{87}Rb exists. Black lines correspond to $d^{\mathrm{perm}} = 0.567$ D. The dipoles are oriented along z axis.

Fermi Surface Deformation

★ Cylindrical symmetry of the FS remains in a plane perpendicular to the direction of the dipoles $\mathbf{d}$

$$K_x = K_y$$

★ Deformation of the Fermi surface

$$\Delta = K_z / K_x - 1$$

★ FS deformation Δ of polar molecules strongly depends on the trap frequencies and dipoles' orientation

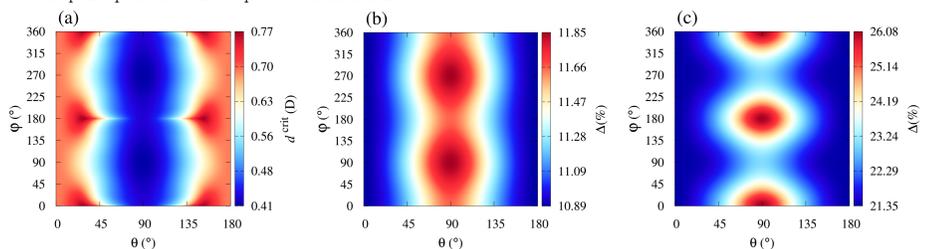Fig. 4. Δ as a function of ω_x and ω_y for $\omega_z = 2\pi \times 200$ Hz.

Fig. 5. (a) Angular stability diagram of trapped ^{40}K^{87}Rb: critical value of the electric dipole moment d^{crit} as a function of dipoles' orientation for the same parameters as in experiments of Ref. [1]. (b), (c) Angular dependence of Δ for a fixed $d = 0.25$ D and trap frequencies: $(\omega_x, \omega_y, \omega_z) = 2\pi \times (63, 36, 200)$ Hz and $(\omega_x, \omega_y, \omega_z) = 2\pi \times (50, 500, 900)$ Hz.

Time-of-flight expansion

★ Dynamics is described by the quantum Boltzmann approach within the relaxation-time approximation

★ System is in the collisional regime at very low temperature → self-consistently determined τ [2]

★ Number of molecules is $N = 3 \times 10^4$ and the dipoles are parallel to z axis

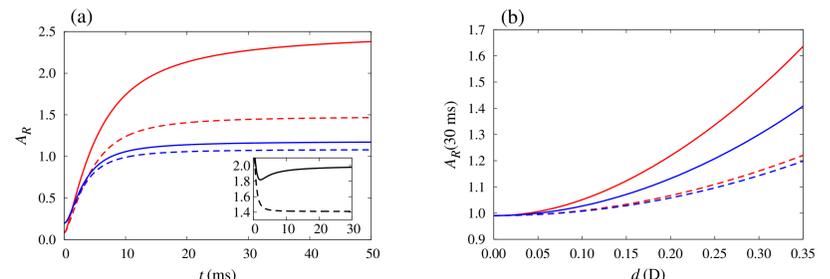★ A_R is calculated using the imaging angle of 68.5° [1], in geometry of Ref. [2]

Fig. 6. (a) Aspect ratio A_R for ^{40}K^{87}Rbs of molecular cloud as a function of time t in TOF expansion. (b) Aspect ratio $A_R(t = 30$ ms) as a function of electric dipole moment d. Top red lines are obtained for $d = 0.5$ D and $(\omega_x, \omega_y, \omega_z) = 2\pi \times (63, 36, 500)$ Hz, while the bottom blue lines correspond to $d = 0.22$ D and $(\omega_x, \omega_y, \omega_z) = 2\pi \times (63, 36, 200)$ Hz. Inset is done for $d = 0.35$ D and $(\omega_x, \omega_y, \omega_z) = 2\pi \times (250, 150, 100)$ Hz.

Conclusions and outlook

★ Fermi surface deformation strongly depends on the orientation of the dipoles of polar molecules

★ Self-consistent τ needed for describing the TOF dynamics of polar molecules

★ Obtained equations of motion for scaling parameters applicable to other non-equilibrium scenarios, e.g., parametric modulation of trap frequencies or strength of the dipolar interaction

References

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