Dipole-induced Fermi-surface anisotropy in strongly dipolar quantum gases

Vladimir Veljić

Thinking of MY mentor

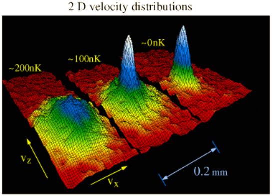
- He didn't just teach me the job - **he set the standard**
- In the hardest moments and the proudest ones, in every challenge and every victory - **I am using the toolkit he gave me**
- My professional DNA is largely shaped by his influence - **the work I do today stands on the foundation he built**

ANTUN'S LEGACY CONTINUES!

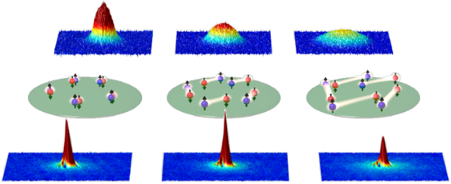
Contents

Ultracold quantum gases

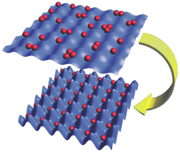
- Bose-Einstein condensation
- Quantum degenerate Fermi gases
- Tunability of interactions and geometry
- BEC-BCS crosssover
- Optical lattices - simulating solid state physics



Science **269**, 198 (1995)



Phys. Rev. Lett. **114**, 230401 (2015)



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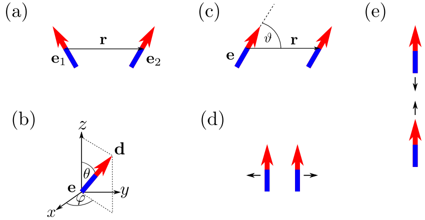
Dipole-dipole interaction (DDI)



- DDI potential: $V_{\mathrm{dd}}(\mathbf{r}) = \frac{C_{\mathrm{dd}}}{4\pi} \frac{\mathbf{r}^2 - 3(\mathbf{e}\cdot\mathbf{r})^{\mathbf{2}}}{|\mathbf{r}|^5}$
- $C_{\mathrm{dd}} = \mu_0 m^2$ for magnetic dipole moment m
  Dipolar atoms: $^{53}\mathrm{Cr}$, $^{164}\mathrm{Dy}$, $^{167}\mathrm{Er}$, ...
- $C_{\mathrm{dd}} = d^2/\varepsilon_0$ for electric dipole moment d
  Dipolar molecules: $^{40}\mathrm{K}^{87}\mathrm{Rb}$, $^{23}\mathrm{Na}^{40}\mathrm{K}$, ...

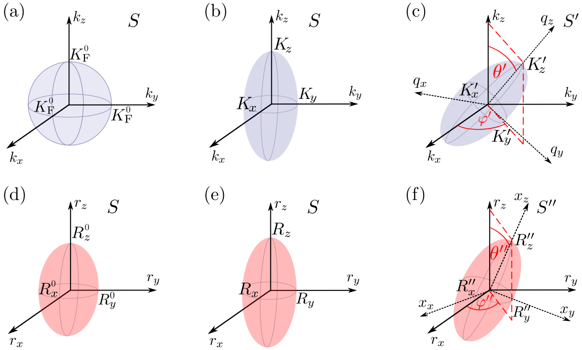
Motivation

- Observation of the Fermi surface (FS) deformation

Science **345**, 1484 (2014)

- Realization of the degenerate Fermi gas of polar molecules

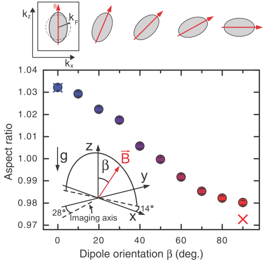
Science **363**, 853 (2019)



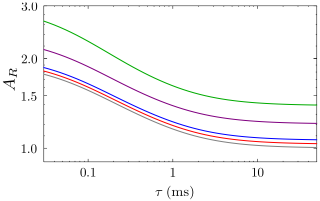
Phys. Rev. A **77**, 061603(R) (2008)

Thesis goals

- Generalization of the Hartree-Fock mean-field theory to describe trapped Fermi gases with tilted dipoles at $T = 0\,\mathrm{K}$
- Extending of the existing theoretical models for dynamics of dipolar fermions for all experimentally relevant regimes



Science **345**, 1484 (2014)



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Contents

Ground state

- Second–quantized Hamiltonian for dipolar Fermi gases:

$$\hat{H}=\int d\mathbf{r}\hat{\Psi}^\dagger(\mathbf{r})\left[-\frac{\hbar^2}{2M}\Delta+V_{\rm trap}(\mathbf{r})\right]\hat{\Psi}(\mathbf{r})+\frac{1}{2}\iint d\mathbf{r}d\mathbf{r}'\hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}^\dagger(\mathbf{r}')V_{\rm dd}(\mathbf{r}-\mathbf{r}')\hat{\Psi}(\mathbf{r}')\hat{\Psi}(\mathbf{r})$$

- Wigner function:

$$\nu^0(\mathbf{r},\mathbf{k})=\int d\mathbf{s}\, e^{i\mathbf{k}\cdot\mathbf{s}}\left\langle\hat{\Psi}^\dagger\left(\mathbf{r}+\frac{\mathbf{s}}{2}\right)\hat{\Psi}\left(\mathbf{r}-\frac{\mathbf{s}}{2}\right)\right\rangle,\text{ with } n(\mathbf{r})=\int\frac{d\mathbf{k}}{(2\pi)^3}\nu(\mathbf{r},\mathbf{k})$$

- Total energy of the system in Hartree-Fock approximation:

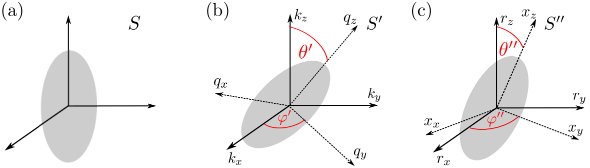
$$E_{\rm kin}=\iint\frac{d\mathbf{r}d\mathbf{k}}{(2\pi)^3}\frac{\hbar^2k^2}{2M}\nu^0(\mathbf{r},\mathbf{k})\,,$$

$$E_{\rm trap}=\iint\frac{d\mathbf{r}d\mathbf{k}}{(2\pi)^3}V_{\rm trap}(\mathbf{r})\nu^0(\mathbf{r},\mathbf{k})\,,$$

$$E_{\rm dd}^{\rm D}=\frac{1}{2}\iiiint\frac{d\mathbf{r}d\mathbf{r}'d\mathbf{k}d\mathbf{k}'}{(2\pi)^6}V_{\rm dd}(\mathbf{r}-\mathbf{r}')\nu^0(\mathbf{r},\mathbf{k})\,\nu^0(\mathbf{r}',\mathbf{k}')\,,$$

$$E_{\rm dd}^{\rm E}=-\frac{1}{2}\iiiint\frac{d\mathbf{r}d\mathbf{r}'d\mathbf{k}d\mathbf{k}'}{(2\pi)^6}V_{\rm dd}(\mathbf{r}')\mathrm{e}^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}'}\nu^0(\mathbf{r},\mathbf{k})\,\nu^0(\mathbf{r},\mathbf{k}')\,.$$

Wigner function ansatz



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- Ansatz for the Wigner function at zero temperature:

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

$$\mathbb{A}''=\begin{pmatrix} 1/R_x''^2 & 0 & 0 \\ 0 & 1/R_y''^2 & 0 \\ 0 & 0 & 1/R_z''^2 \end{pmatrix} \quad \text{and} \quad \mathbb{B}'=\begin{pmatrix} 1/K_x'^2 & 0 & 0 \\ 0 & 1/K_y'^2 & 0 \\ 0 & 0 & 1/K_z'^2 \end{pmatrix},$$

$$\mathbb{R}(\theta,\varphi)=\begin{pmatrix} \cos\theta\cos\varphi & -\sin\varphi & \sin\theta\cos\varphi \\ \cos\theta\sin\varphi & \cos\varphi & \sin\theta\sin\varphi \\ -\sin\theta & 0 & \cos\theta \end{pmatrix}$$

Thomas-Fermi radii and momenta

- Total energy of the system:

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

- Generalized anisotropy function:

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

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- Particle number conservation:

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

- The minimization of $E_{\rm tot}$ leads to the set of 10 equations for 10 variational parameters $(R_i'',K_i',\theta',\varphi',\theta'',\varphi'')$

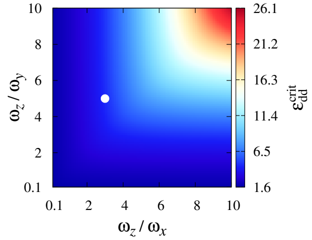
Contents

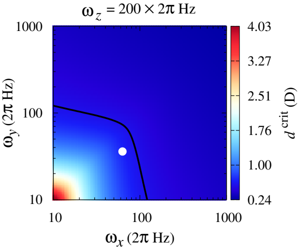
Stability diagrams

- Non-dimensional form of equations: species-independent!
- Relative interaction strength:

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

- Stability only depends on the trap aspect ratios and the dipoles' orientation





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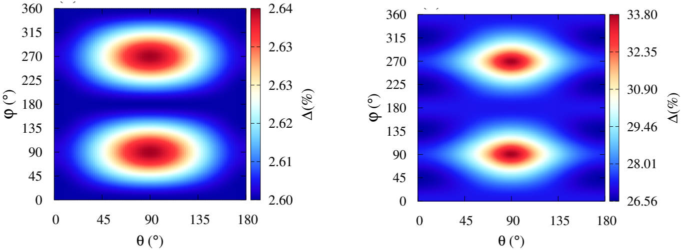
Fermi surface deformation

- Our theory confirms that Fermi surface (FS):
  1. follows the dipoles' orientation $(\theta'=\theta, \varphi'=\varphi)$
  2. remains cylindrically symmetric ellipsoid $(K'_x=K'_y)$
- Fermi surface deformation:

$$\Delta=\frac{K'_z}{K'_x}-1$$

- $N = 6.7 \cdot 10^4$, (579, 91, 611) Hz



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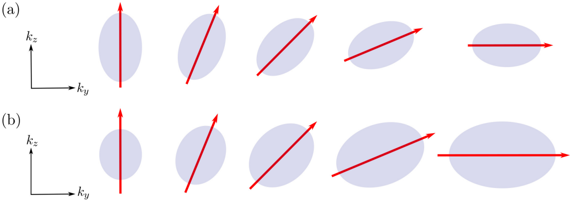
Fermi surface deformation

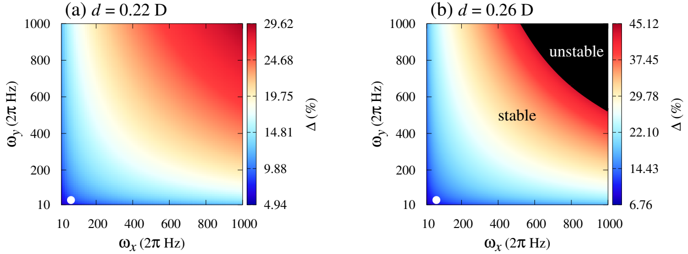
- Dipolar atoms → rigid FS; Polar molecules → soft FS



- FS deformation and its angular distribution can be tuned by changing the trap frequencies and dipoles' orientation
- For stronger DDI we expect increased critical temperature of Cooper pairing, but also a higher degree of tunability

Fermi surface deformation - KRb

- FS deformation is much larger in gases of polar molecules
- $N = 3 \cdot 10^4$, $\omega_z = 2\pi \times 200$ Hz, $\theta = \varphi = 0$
- Even small changes in the dipolar moment strength can significantly affect the systems' stability



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Contents

Boltzmann - quantum kinetic equation

- Second–quantized Hamiltonian for dipolar Fermi gases:

$$\hat{H}=\int d\mathbf{r}\hat{\Psi}^\dagger(\mathbf{r},t)\left[-\frac{\hbar^2}{2M}\Delta+V_{\text{trap}}(\mathbf{r})\right]\hat{\Psi}(\mathbf{r},t)+\frac{1}{2}\int d\mathbf{r}d\mathbf{r}'\hat{\Psi}^\dagger(\mathbf{r},t)\hat{\Psi}^\dagger(\mathbf{r}',t)V_{\text{dd}}(\mathbf{r}-\mathbf{r}')\hat{\Psi}(\mathbf{r}',t)\hat{\Psi}(\mathbf{r},t)$$

- Wigner function:

$$\nu(\mathbf{r},\mathbf{k},t)=\int d\mathbf{s}\, e^{i\mathbf{k}\cdot\mathbf{s}}\left\langle\hat{\Psi}^\dagger\left(\mathbf{r}+\frac{\mathbf{s}}{2},t\right)\hat{\Psi}\left(\mathbf{r}-\frac{\mathbf{s}}{2},t\right)\right\rangle, \text{ with } n(\mathbf{r},t)=\int\frac{d\mathbf{k}}{(2\pi)^3}\nu(\mathbf{r},\mathbf{k},t)$$

- Dynamics of the system:

$$\frac{\partial\nu(\mathbf{r},\mathbf{k},t)}{\partial t}+\frac{\hbar\mathbf{k}}{M}\nabla_{\mathbf{r}}\nu(\mathbf{r},\mathbf{k},t)+\nabla_{\mathbf{k}}V(\mathbf{r},\mathbf{k},t)\nabla_{\mathbf{r}}\nu(\mathbf{r},\mathbf{k},t)-\nabla_{\mathbf{r}}V(\mathbf{r},\mathbf{k},t)\nabla_{\mathbf{k}}\nu(\mathbf{r},\mathbf{k},t)=I_{\text{coll}}[\nu](\mathbf{r},\mathbf{k},t)$$

- Hartree-Fock mean-field potential:

$$V(\mathbf{r},\mathbf{k},t)=V_{\text{trap}}(\mathbf{r})+\int d\mathbf{r}'V_{\text{dd}}(\mathbf{r}-\mathbf{r}')n(\mathbf{r}',t)-\int\frac{d\mathbf{k}'}{(2\pi\hbar)^3}\tilde{V}_{\text{dd}}(\mathbf{k}-\mathbf{k}')\nu(\mathbf{r},\mathbf{k}',t)$$

- Relaxation-time approximation: $I_{\text{coll}}[f]=-\frac{\nu-\nu^{\text{hy}}}{\tau}$

Ansatz for Wigner function

- Ansatz for global equilibrium distribution function at zero temperature:

$$\nu^0(\mathbf{r},\mathbf{k})=\Theta\left(1-\sum_i \frac{r_i^2}{R_i^2}-\sum_i \frac{k_i^2}{K_i^2}\right)$$

R_i and K_i are Thomas-Fermi radii and momenta

- Scaling ansatz:

$$\nu(\mathbf{r},\mathbf{k},t)\rightarrow\Gamma(t)\nu^0(\boldsymbol{\mathcal{R}}(\mathbf{r},t),\boldsymbol{\mathcal{K}}(\mathbf{r},\mathbf{k},t))$$

Rescaled variables: $\mathcal{R}_i(\mathbf{r},t)=\frac{r_i}{b_i(t)}$ and $\mathcal{K}_i(\mathbf{r},\mathbf{k},t)=\frac{1}{\sqrt{\theta_i(t)}}\left[k_i-\frac{M\dot{b}_i(t)r_i}{\hbar b_i(t)}\right]$

- Normalization factor:

$$\Gamma(t)^{-1}=\prod_i b_i(t)\sqrt{\theta_i(t)}$$

Phys. Rev. A **68**, 043608 (2003)

Equations

- Equations of motion for scaling parameters:

$$\ddot{b}_i+\omega_i^2 b_i-\frac{\hbar^2 K_i^2\theta_i}{M^2 b_i R_i^2}+\frac{48Nc_0}{Mb_i R_i^2\prod_j b_j R_j}\left[f\left(\frac{b_x R_x}{b_z R_z},\frac{b_y R_y}{b_z R_z}\right)-b_i R_i\frac{\partial}{\partial b_i R_i}f\left(\frac{b_x R_x}{b_z R_z},\frac{b_y R_y}{b_z R_z}\right)\right]$$

$$-\frac{48Nc_0}{Mb_i R_i^2\prod_j b_j R_j}\left[f\left(\frac{\sqrt{\theta_z}K_z}{\sqrt{\theta_x}K_x},\frac{\sqrt{\theta_z}K_z}{\sqrt{\theta_y}K_y}\right)+\sqrt{\theta_i}K_i\frac{\partial}{\partial\sqrt{\theta_i}K_i}f\left(\frac{\sqrt{\theta_z}K_z}{\sqrt{\theta_x}K_x},\frac{\sqrt{\theta_z}K_z}{\sqrt{\theta_y}K_y}\right)\right]=0,$$

$$\dot{\theta}_i+2\frac{\dot{b}_i}{b_i}\theta_i=-\frac{1}{\tau}(\theta_i-\theta_i^{\mathrm{hy}})$$

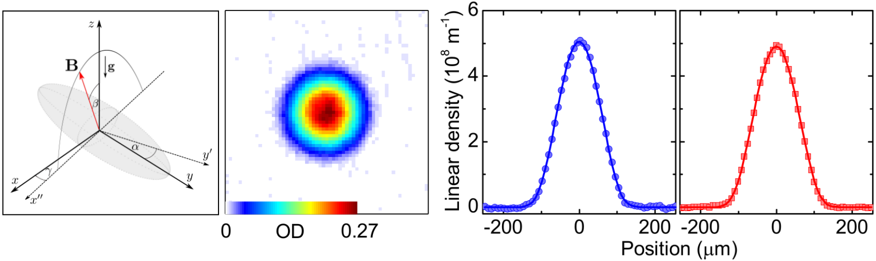
- Strength of dipolar interaction:

$$c_0=\frac{2^{10}C_{\mathrm{dd}}}{3^4\cdot 5\cdot 7\cdot\pi^3}$$

- Collisionless regime: $\tau\to\infty$
- Hydrodynamic regime: $\tau\to 0$, definition: $\prod_i b_i^{\mathrm{hy}}(t)\sqrt{\theta_i^{\mathrm{hy}}(t)}=1$

  Phys. Rev. A **96**, 043608 (2017)

Innsbruck experiment



Science **345**, 1484 (2014)

- Aspect ratios of the atomic cloud and FS in imaging plane:

$$A_R(t)=\sqrt{\frac{\langle r_{\rm v}^2(t)\rangle}{\langle r_{\rm h}^2(t)\rangle}}=\sqrt{\frac{\langle r_z^2(t)\rangle}{\langle r_x^2(t)\rangle\cos^2\alpha+\langle r_y^2(t)\rangle\sin^2\alpha}},\qquad \langle r_i^2(t)\rangle=\frac{1}{8}R_i^2b_i^2(t)$$

$$A_K(t)=\sqrt{\frac{\langle k_{\rm v}^2(t)\rangle}{\langle k_{\rm h}^2(t)\rangle}}=\sqrt{\frac{\langle k_z^2(t)\rangle}{\langle k_x^2(t)\rangle\cos^2\alpha+\langle k_y^2(t)\rangle\sin^2\alpha}},\qquad \langle k_i^2(t)\rangle=\frac{1}{8}K_i^2\theta_i(t)+\frac{1}{\hbar^2}M^2R_i^2\dot{b}_i^2(t)$$

V. Veljić *et al.*, New J. Phys. **20**, 093016 (2018)

Time-of-flight expansion

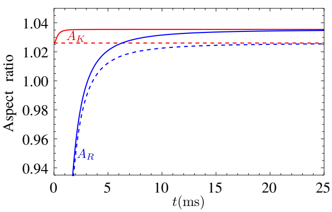
- Ballistic expansion:

$$A_K(0) = \lim_{t\to\infty} A_R(t)$$

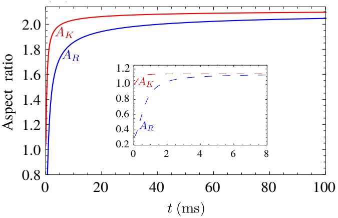
- Non-ballistic expansion:

$$\lim_{t\to\infty} A_K(t) = \lim_{t\to\infty} A_R(t)$$

Collisionless regime



Hydrodynamic regime



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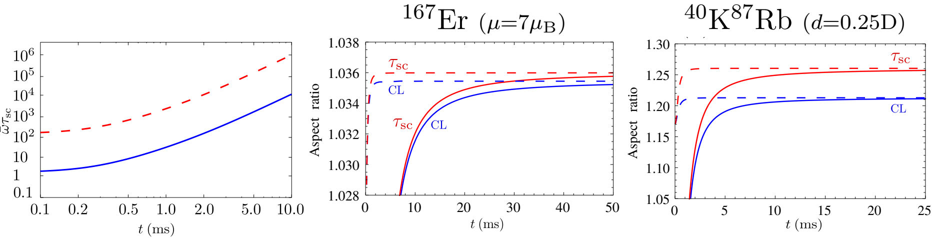
Self-consistent τ

- Self-consistent relaxation time: $\tau_{\mathrm{sc}}(t) \sim \frac{1}{\overline{n}(t)}$
- Mean number density: $\overline{n}(t) = \frac{N}{V(t)}$
- Volume of the gas during the TOF: $V(t) = \frac{4\pi}{3} \prod_i R_i b_i(t)$

Phys. Rev. Lett. **113**, 263201 (2014); Phys. Rev. A **89**, 022702 (2014)



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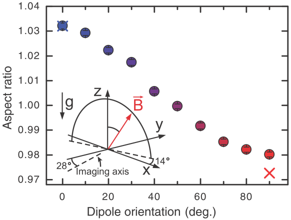
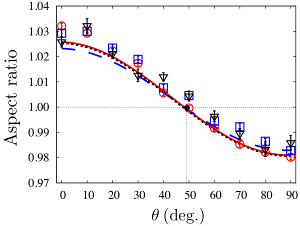
Theory vs Experiment

- Comparison of theoretical results for A_{K} with the experimental results for $A_{\mathrm{R}}(t = 12\,\mathrm{ms})$ for $^{167}\mathrm{Er}$





- $\varphi = 14^\circ$, $\alpha = 28^\circ$
- $N = 6.6 \cdot 10^4$, $(579,\ 91,\ 611)$ Hz
- $N = 6.3 \cdot 10^4$, $(428,\ 91,\ 459)$ Hz
- $N = 6.1 \cdot 10^4$, $(408,\ 212,\ 349)$ Hz

V. Veljić *et al.*, New J. Phys. **20**, 093016 (2018)

Contents

Conclusions

- Generalization of the Hartree-Fock mean-field theory to describe trapped Fermi gases with tilted dipoles at $T = 0\,\mathrm{K}$
  - Stability
  - FS deformation
  - Shape of the gas cloud
- Extending of the existing theoretical models for dynamics of dipolar fermions for all experimentally relevant regimes
  - collisionless, collisional, and hydrodynamic (by self-consistently determined relaxation time)
- Comparison with experimental data and modeling of the dynamics
- These results are published in:
  1. V. Veljić *et al.*, Phys. Rev. A **95**, 053635 (2017)
  2. V. Veljić *et al.*, New J. Phys. **20**, 093016 (2018)
  3. V. Veljić *et al.*, Phys. Rev. Research **1**, 012009 (2019)