## eResearch 2016

## Dipolar quantum gases

#### Danny Baillie

Physics, University of Otago

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#### MARSDEN FUND

TE PŪTEA RANGAHAU A MARSDEN





Te Whare Wānanga o Otāgo

NEW ZEALAND

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$$n(E) = e^{-(E-\mu)/k_BT}$$



$$n(E) = \frac{1}{e^{(E-\mu)/k_BT}+1}$$



$$n(E) = \frac{1}{e^{(E-\mu)/k_BT} - 1}$$

# First BEC



$$n(E) = \frac{1}{e^{(E-\mu)/k_BT} - \eta}$$

$$E = \frac{p^2}{2m} + V_{tr}(\mathbf{x}) + 2gn(\mathbf{x})$$

$$V_{tr}(\mathbf{x}) = \frac{1}{2}m\omega_\rho^2(\rho^2 + \lambda^2 z^2)$$

$$N = \left(\frac{k_BT}{\hbar\omega}\right)^3 \zeta_3^\eta \left(e^{\mu/k_BT}\right)$$

$$n(\mathbf{x}) = \left(\frac{2\pi\hbar^2}{mk_BT}\right)^{-3/2} \zeta_3^\eta \left(e^{[\mu-V_{tr}(\mathbf{x})-2gn(\mathbf{x})]/k_BT}\right)$$

$$egin{cases} \eta = 1 & \textit{Boson} \ \eta = -1 & \textit{Fermion} \end{cases}$$

# Dipolar gases

	1																	18
1	1 1.0079 H Hydrogen	2				Perio	dic Tal	ble of t	he Eler	nents			13	14	15	16	17	2 4.0025 He Helium
2	3 6.941 Li Lithium	4 9.0122 Be Beryllum											5 10.811 B Baron	6 12.011 C Carbon	7 14.007 N Nitrogen	8 15.999 O Oxygen	9 18.998 F Flourine	10 20.180 Ne Neon
3	11 22.990 Na Sodium	12 24.305 Mg Magasian	3	4	5	6	7	8	9	10	11	12	13 26.982 Al Alamisiam	s4 20.005 Si Silicon	15 30.974 P Phosphorus	16 32.005 S Sulphur	17 35.453 CI Chlorine	18 39.948 Ar <sub>Argon</sub>
4	19 30.095 K Potassium	20 40.078 Ca Calcium	21 44.955 Sc Scandum	22 47.867 Ti Titanium	23 50.942 V Varadum	24 51.995 Cr Chronium	25 54.933 Mn Manganese	26 55.845 Fe Iron	27 58.933 Co Cobalt	28 58.093 Ni Nickel	29 63.545 Cu Copper	30 es.39 Zn Zinc	31 09.723 Ga Gallum	32 72.64 Ge Germanium	33 74.922 As Aruenic	34 78.95 Se Selesium	35 79.904 Br Bromine	36 83.8 Kr Krypton
5	37 85.468 Rb Rebidien	38 87.62 Sr Strontium	39 88.905 Y Yitrium	40 91.224 Zr Zirconium	41 92.905 Nb Niobium	42 95.94 Mo Molybderum	43 95 Tc Technetium	44 101.07 Ru Rathenium	45 102.91 Rh Rhodium	46 105.42 Pd Palladum	47 107.87 Ag Silver	48 112.41 Cd Cadmium	49 114.82 In Indum	50 118.71 Sn Tin	51 121.76 Sb Antimony	52 127.6 Te Tellurium	53 125.9      odine	54 131.29 Xe Xenon
6	55 132.91 Cs Caesium	56 137-33 Ba Barium	Lanthanide	72 178.49 Hf Halfnium	73 180.95 Ta Tastalum	74 183.84 W Tungsten	75 105.21 Re Rhenium	76 190.23 Os Osmium	77 192.22 Ir Iridum	78 195.08 Pt Platinum	79 196.97 Au Gold	80 200.59 Hg Mercury	81 204.38 TI Thalium	82 207.2 Pb Lead	83 208.95 Bi Biamath	84 209 Po Polonium	85 210 At Astatine	86 222 Rn Radon
7	87 223 Fr Francium	88 225 Ra	Actinide	57 138.91	58 140.12	59 140.91 Pr	60 144.24 Nd	61 145 Pass	62 150.36 Sm	63 151.95 Fu	64 157.25 C d	65 158.93 Th	66 102.50	67 164.93	68 167.25	69 168.93 Tan	70 173.04 Vb	71 174.97
				Lanthanum	Cerium	Praseodymium	Neodymium	Promethium	Samarium	Europium	Gadolinium	Terbium	Dysprosium	Holmium	Erbium	Thulum	Ytterbium	Lutetium
	z mai Symbol Name			89 227 Ac Actinium	90 232.04 Th Tharium	91 233.04 Pa Protectinium	92 238.03 U Uranium											

- BEC Cr 2005, 2008
- Dipolar Fermi KRb 2008
- Dipolar Bose KRb 2010
- BEC Dy 2011
- Fermi Dy 2012
- BEC Er 2012

	$\mu_{m}/\mu_{B}$	$\frac{\text{dipolar}}{\text{contact}} = \frac{g_d}{g}$
<sup>87</sup> Rb	1	0.0064
$^{52}\mathrm{Cr}$	6	0.15
$^{168}\mathrm{Er}$	7	0.38
<sup>164</sup> Dy	10	1.3
KRb		20

## Dipolar energy



$$E = \frac{p^2}{2m} + V_{tr}(\mathbf{x}) + 2gn(\mathbf{x}) + \Phi_D(\mathbf{x})$$
$$\Phi_D(\mathbf{x}) = \int d\mathbf{x}' U_{dd}(\mathbf{x} - \mathbf{x}')n(\mathbf{x}')$$
$$U_{dd}(\mathbf{r}) = \frac{C_{dd}}{4\pi r^3} (1 - 3\cos^2 \theta)$$
$$\tilde{U}_{dd}(\mathbf{k}) = C_{dd} (\cos^2 \theta_{\mathbf{k}} - 1/3)$$

## Exchange interaction

#### Hartree-Fock approximation

$$\langle \hat{\psi}^{\dagger}(\mathbf{x}) \hat{\psi}^{\dagger}(\mathbf{x}') \hat{\psi}(\mathbf{x}') \hat{\psi}(\mathbf{x}) \rangle \approx \underbrace{\widetilde{n(\mathbf{x})n(\mathbf{x}')}}_{n(\mathbf{x})n(\mathbf{x}')} + \underbrace{\widetilde{\eta}|\langle \hat{\psi}^{\dagger}(\mathbf{x}) \hat{\psi}(\mathbf{x}') \rangle|^{2}}_{\text{Exchange/Fock}}, \ \eta = \pm 1$$

Including exchange interaction

$$E = \frac{p^2}{2m} + V_{tr}(\mathbf{x}) + 2gn(\mathbf{x}) + \Phi_D(\mathbf{x}) + \eta \Phi_E(\mathbf{x}, \mathbf{p})$$

$$W(\mathbf{x}, \mathbf{p}) = \frac{1}{e^{(E-\mu)/k_BT} - \eta}$$

$$\Phi_D(\mathbf{x}) = \int d\mathbf{x}' U_{dd}(\mathbf{x} - \mathbf{x}')n(\mathbf{x}')$$
harder
$$\Phi_E(\mathbf{x}, \mathbf{p}) = \int d\mathbf{p}' \tilde{U}_{dd}(\mathbf{p} - \mathbf{p}')W(\mathbf{x}, \mathbf{p}')$$
very hard

## Magnetostriction

## What is magnetostriction?



## Magnetostriction



Aikawa, Baier, Frisch, Mark, Ravensbergen, and Ferlaino, "Observation of Fermi surface deformation in a dipolar gas", Science **345**, 1484 (2014) Baillie and Blakie, "Magnetostriction and exchange effects in trapped dipolar Bose and Fermi gases", Phys. Rev. A **86**, 023605 (2012)

$$AR = \sqrt{\frac{\langle k_z^2 \rangle}{\langle k_\gamma^2 \rangle}} = 1 + \left\{ 1 - \sin^2 \beta [1 + \cos^2(\gamma - \varphi)] \right\} \frac{3c_\alpha g_d N^{1/6}}{4\pi \hbar \omega a_{h\alpha}^3},$$
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### What about bosons?





## Dipolar instability



Lahaye, Metz, Fröhlich, Koch, Meister, Griesmaier, Pfau, Saito, Kawaguchi, and Ueda, "*d*-wave collapse and explosion of a dipolar Bose-Einstein condensate", Phys. Rev. Lett. **101**, 080401 (2008)

## Dipolar quantum gases



## Effect of exchange interaction on stability

$$rac{\partial n(\mathbf{x})}{\partial \mu} = rac{n_\mu(\mathbf{x})}{1 + [2g - C_{
m dd}/3 - C_{
m dd}\xi_\eta(\mathbf{x})]n_\mu(\mathbf{x})},$$

where we have defined

$$\begin{split} n_{\mu}(\mathbf{x}) &\equiv \int \frac{d\mathbf{k}}{(2\pi)^3} W_{\mu}(\mathbf{x}, \mathbf{k}), \\ \xi_{\eta}(\mathbf{x}) &\equiv -\eta \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{W_{\mu}(\mathbf{x}, \mathbf{k})}{n_{\mu}(\mathbf{x})} \frac{\partial \Phi_{E}(\mathbf{x}, \mathbf{k})}{C_{\mathrm{dd}} \partial n(\mathbf{x})}, \end{split}$$

$$\begin{split} \frac{\partial \Phi_E(\mathbf{x}, \mathbf{k})}{\partial n(\mathbf{x})} &= \left[1 - C_{\mathrm{dd}} \xi_\eta(\mathbf{x}) n_\mu(\mathbf{x})\right] \int \frac{d\mathbf{k}'}{(2\pi)^3} \tilde{U}_{\mathrm{dd}}(\mathbf{k} - \mathbf{k}') \frac{W_\mu(\mathbf{x}, \mathbf{k}')}{n_\mu(\mathbf{x})} \\ &- \eta \int \frac{d\mathbf{k}'}{(2\pi)^3} \tilde{U}_{\mathrm{dd}}(\mathbf{k} - \mathbf{k}') W_\mu(\mathbf{x}, \mathbf{k}') \frac{\partial \Phi_E(\mathbf{x}, \mathbf{k}')}{\partial n(\mathbf{x})}. \end{split}$$



Baillie, Bisset, and Blakie, "Stability of a trapped dipolar quantum gas", Phys. Rev. A **91**, 013613 (2015)

- Position grids Cosine-Hankel ( $\rho$ , z): 200 × 200
- Momentum grids Spherical  $(p_r, p_{\theta})$ : 300 × 30
- Almost 2.9GB to store 4D grid

- Licence
- Parallel options:
  - Built-in for FFT, eigenvalues, matrix multiply, sort
  - Different assumptions as different tasks
  - parfor
  - Distributed Computing Server
  - openMP in mex