3-body collisions of ultracold atoms: From van der Waals universality to quantum droplets

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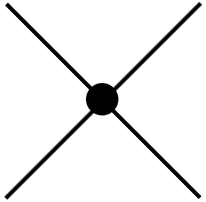
Outline:

- *Background: Few-body collisions at low energies*
- *Three-body collisions at strong and weak interactions*
- *Many-body effects induced by three-body collisions (droplets, etc…)*
    - *Adding to Tobias' discussion of May 13th*
- *Outlook*

- **What is the equivalent of "a" for threshold *elastic* scattering of three particles?**

Collision of two free particles

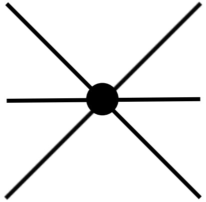


Threshold law

$$\frac{\tan(\delta_l(k))}{k^{2l+1}} \underset{k\to 0}{=} a_l$$

Scattering length $a_0 \equiv a \; [\mathrm{Length}^1]$

Collision of three free particles



(*Expected*) Threshold law

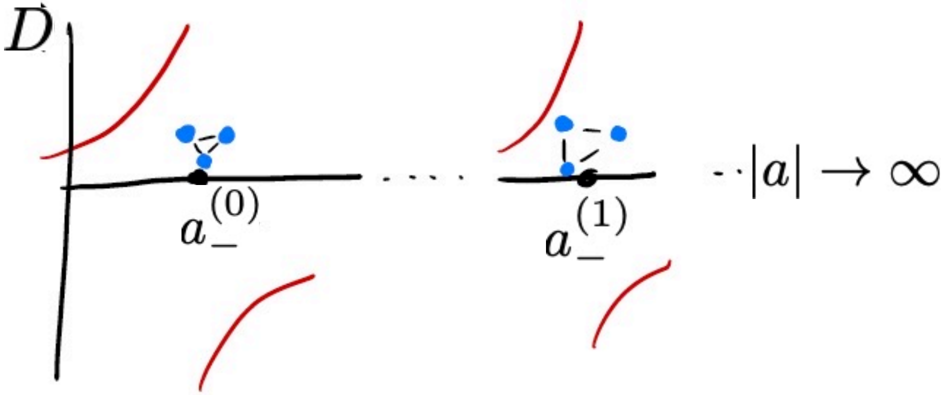
- c.f. D'Incao JPB, 51, 043001 (2018)

$$\frac{\tan(\delta_\lambda(K))}{K^{2\lambda+4}} \underset{K\to 0}{=} D_\lambda \qquad l_{eff} = \lambda + 3/2$$

Scattering hypervolume $D_0 \equiv D \; [\mathrm{Length}^4]$

- Imaginary part: Recombination
- Real part: Elastic scattering

Importance of the hypervolume?



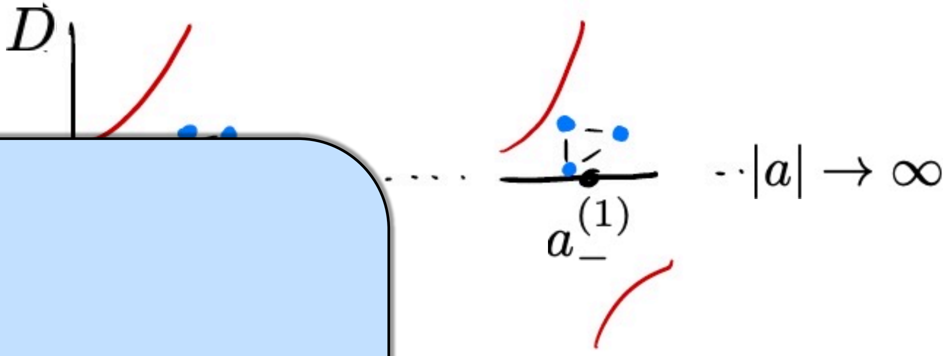
Few-body

- **Three-body bound state at threshold**
  - “Three-body unitarity”

- **Zero scattering length**
  - Finite hypervolume
  - Three-body interaction dominates

$$\Psi^{(3)}(R) \propto \frac{D}{R^4}$$

Importance of the hypervolume?



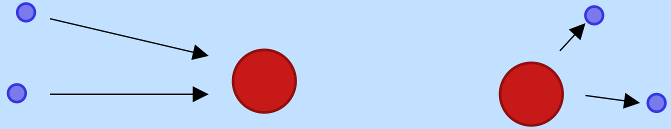
Few-body

- **Three-bo**
  - "Three

- **Zero scatt**
  - Finite
  - Three-

Nuclear physics

- **EFT**
- **Low-energy collisions?**



Importance of the hypervolume?

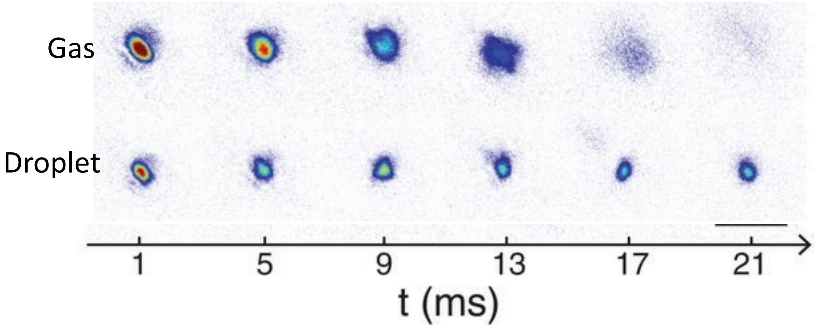
Wu, Phys. Rev., 115, 1390 (1959)

Many-body $$\mathcal{E}(n) = \frac{2\pi\hbar^2 n^2 a}{m}\left\{1 + \frac{128}{15\sqrt{\pi}}\sqrt{na^3} + \left[\frac{8(4\pi - 3\sqrt{3})}{3}\ln(na^3) + \frac{D}{12\pi a^4} + \pi r_s/a + 118.5\right]na^3 + \ldots\right\}$$

Tan, PRA, 78, 013636 (2008)

LHY, Phys. Rev., 106, 1119 (1957)

- **Quantum Droplets (of few-body origin)**
  - Bulgac PRL 89, 050402 (2002)



C. R. Cabrera et al., Science **359**, 301 (2018)

- **Quantum Unbinding (Bose SF Liquid to Gas)**
  - Zwerger JSM 103104 (2019)
  - Kora, Boninsegni, Son, Zhang PNAS 117, 27231 (2020)

- **Collective modes/Excitation shifts**

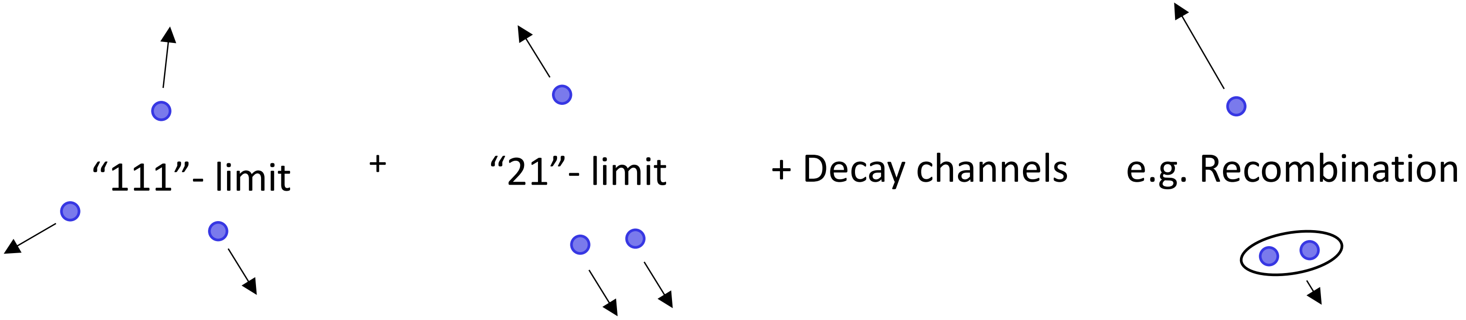
Many-body origin (QM Fluctuations)

1. **Why hasn't the hypervolume been measured *experimentally*?**
    - Diluteness compared to two-body collisions

2. **What complicates our *theoretical* understanding of the hypervolume?**
    - Complexities/singularities in the three-body continuum

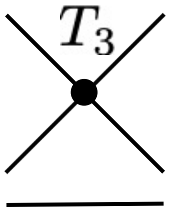
- **<u>Complexities</u> of the three-body continuum**

1. Asymptotic limits:



• Complexities of the three-body continuum

2. Scattering processes: $\hat{U}_{00} =$



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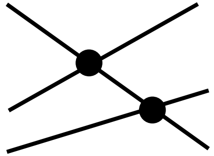


+ …) + “True” three-body

Disconnected process
- “Spectator” scattering

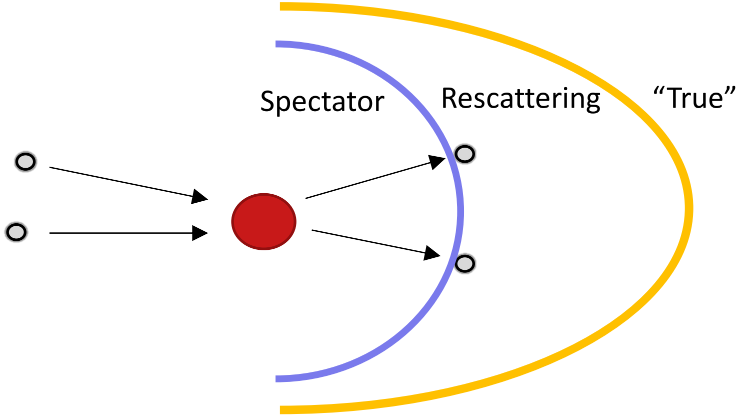
$$\delta^{(3)}(\mathbf{p}_1 + \mathbf{p}_2 - \mathbf{p}_1' - \mathbf{p}_2')T_3$$

Rescattering process
- Double, triplet, quadruple…

$$\frac{T_3 T_1}{E_{\text{inc.}} - E_{\text{int.}} + i0}$$

Usual $|\langle \mathbf{p}|\hat{U}_{00}|\mathbf{p}'\rangle|^2$ gives unphysical results

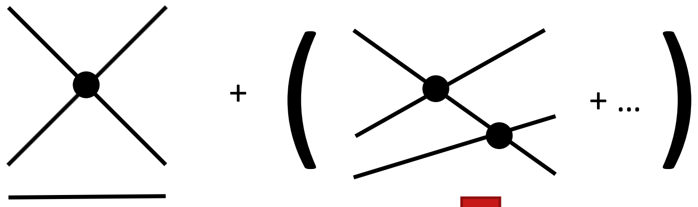
- Finite collisions rates can be constructed
  - Potapov, Taylor PRA 16, 2264 (1977)
  - Potapov, Taylor PRA 16, 2276 (1977)



- **<u>Complexities</u> of the three-body continuum**

3. Singularities at threshold:
   - Amado, Rubin PRL 25, 194 (1970)

$\hat{U}_{00} =$



\+ "True" three-body

Expansion for $L_{3B} = 0$: $$U_{00}(E \to +i0)|_{\text{Connected}} \approx \frac{A}{E} + \frac{B}{\sqrt{E}} + C \ln E + O(1)$$

The *expected* threshold behavior $\dfrac{\tan(\delta_\lambda(K))}{K^{2\lambda+4}} \underset{K\to 0}{=} D_\lambda$ is therefore *hidden* by singular processes.

Progress in threshold elastic three-body scattering calculations

- **Spinless (equal mass) bosons**

Weak interactions	Strong interactions
Wave function expansion: Soft-sphere • Zhu, Tan arXiv:1710.04147	EFT: g_3 effective three-body coupling constant (contact) • c.f. Braaten, Nieto EPJ 11, 143 (1999) Wave function expansion: Hard sphere • Tan PRA 78, 013636 (2008) • Defined hypervolume – connected to EFT $g_3(\|a\|^{-1}) = 6(D + 12\pi^2 a^3 r_s + 977.736695 a^4)$

See: S. Tan KITP FBS 16

Open questions

- General methods (Im(D) $\neq 0$)
- Van der Waals $D(r_{\mathrm{vdW}}, a)$?

This talk

Scattering amplitude expansion

- Mestrom, Colussi, Secker, Kokkelmans PRA 100, 050702(R) (2019)
- Mestrom, Colussi, Secker, Groeneveld, Kokkelmans PRL 124 (14), 143401 (2020)

Alt-Grassberger-Sandhas (AGS) equations

AGS, Nucl. Phys. B **2**, 167 (1967)

$$|\Psi_{3\text{b}}(0+i0)\rangle = |\mathbf{0},\mathbf{0}\rangle + G_0(0+i0)U_{00}(0+i0)|\mathbf{0},\mathbf{0}\rangle$$

$$U_{00}(z) = \sum_{\alpha=1}^{3} T_\alpha(z)G_0(z)U_{\alpha 0}(z)$$

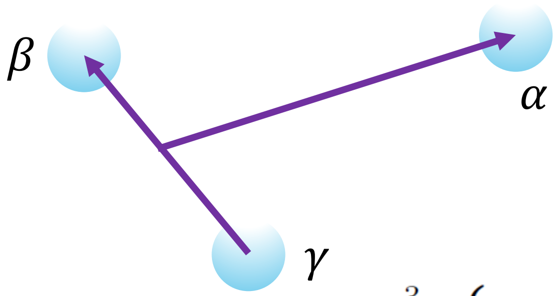
$$U_{\alpha 0}(z) = G_0^{-1}(z) + \sum_{\substack{\beta=1 \\ \beta\neq\alpha}}^{3} T_\beta(z)G_0(z)U_{\beta 0}(z)$$

$$\text{for } \alpha = 1,2,3,$$

α	**configuration**
0	A + B + C
1	A + BC
2	B + CA
3	C + AB

- $G_0(E) = (E - H_0)^{-1}$ three-body free Green's function
- T_α transition operator of two-body subsystem
  - Partial-wave + Weinberg expansion
    - Weinber, Phys. Rev. 131, 440 (1963), Mestrom, Secker, Kroeze, Kokkelmans PRA 99, 012702 (2019)

Elastic scattering amplitude



$$\boldsymbol{p}_\alpha = \frac{1}{2}(\boldsymbol{P}_\beta - \boldsymbol{P}_\gamma) \qquad (\alpha\beta\gamma = 123, 231, 312)$$

$$\boldsymbol{q}_\alpha = \frac{2}{3}\left(\boldsymbol{P}_\alpha - \frac{1}{2}(\boldsymbol{P}_\beta + \boldsymbol{P}_\gamma)\right)$$

$$\langle \mathbf{p}, \mathbf{q} | U_{00}(0) | \mathbf{0}, \mathbf{0} \rangle = \sum_{\alpha=1}^{3} \left\{ \delta(\mathbf{q}_\alpha) \langle \mathbf{p}_\alpha | T(0) | \mathbf{0} \rangle + A_1 \frac{a^2}{q_\alpha^2} + A_2 \frac{a^3}{q_\alpha} + A_3\, a^4 \ln\left(\frac{q_\alpha |a|}{\hbar}\right) \right.$$
$$\left. + A_4 \frac{p_\alpha^2 + \frac{3}{4} q_\alpha^2}{q_\alpha^2} a + \frac{1}{3} \frac{1}{(2\pi)^6} \frac{D}{m\hbar^4} + O\left(q_\alpha \ln\left(\frac{q_\alpha |a|}{\hbar}\right), \frac{p_\alpha^2}{q_\alpha} \right) \right\}$$

where $\boldsymbol{p} \equiv \boldsymbol{p}_1$

$\boldsymbol{q} \equiv \boldsymbol{q}_1$

Elastic scattering amplitude

$$
\begin{aligned}
\langle \mathbf{p}, \mathbf{q} | U_{00}(0) | \mathbf{0}, \mathbf{0} \rangle = \sum_{\alpha=1}^{3} \Bigg\{ & \delta(\mathbf{q}_\alpha) \langle \mathbf{p}_\alpha | T(0) | \mathbf{0} \rangle + A_1 \frac{a^2}{q_\alpha^2} + A_2 \frac{a^3}{q_\alpha} + A_3 \, a^4 \ln\left(\frac{q_\alpha |a|}{\hbar} \right) \\
& + A_4 \frac{p_\alpha^2 + \frac{3}{4} q_\alpha^2}{q_\alpha^2} a + \frac{1}{3} \frac{1}{(2\pi)^6} \frac{D}{m \hbar^4} + O\left(q_\alpha \ln\left(\frac{q_\alpha |a|}{\hbar} \right), \frac{p_\alpha^2}{q_\alpha} \right) \Bigg\}
\end{aligned}
$$

Elastic scattering amplitude

Spectator scattering

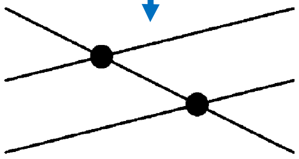
$$\langle \mathbf{p}, \mathbf{q} | U_{00}(0) | \mathbf{0}, \mathbf{0} \rangle = \sum_{\alpha=1}^{3} \left\{ \boxed{\delta(\mathbf{q}_\alpha) \langle \mathbf{p}_\alpha | T(0) | \mathbf{0} \rangle} + A_1 \frac{a^2}{q_\alpha^2} + A_2 \frac{a^3}{q_\alpha} + A_3\, a^4 \ln\left(\frac{q_\alpha |a|}{\hbar} \right) \right.$$
$$\left. + A_4 \frac{p_\alpha^2 + \frac{3}{4} q_\alpha^2}{q_\alpha^2} a + \frac{1}{3} \frac{1}{(2\pi)^6} \frac{D}{m\hbar^4} + O\left(q_\alpha \ln\left(\frac{q_\alpha |a|}{\hbar} \right), \frac{p_\alpha^2}{q_\alpha} \right) \right\}$$

Elastic scattering amplitude

Spectator scattering

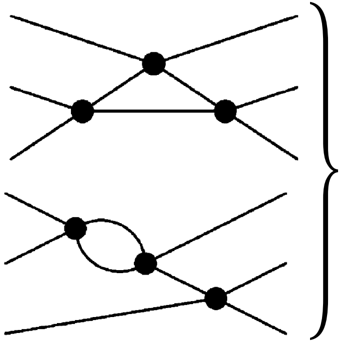
$$\langle \mathbf{p}, \mathbf{q} | U_{00}(0) | \mathbf{0}, \mathbf{0} \rangle = \sum_{\alpha=1}^{3} \Bigg\{ \delta(\mathbf{q}_\alpha) \langle \mathbf{p}_\alpha | T(0) | \mathbf{0} \rangle + A_1 \frac{a^2}{q_\alpha^2} + A_2 \frac{a^3}{q_\alpha} + A_3\, a^4 \ln\left(\frac{q_\alpha |a|}{\hbar}\right)$$

$$+ A_4 \frac{p_\alpha^2 + \frac{3}{4} q_\alpha^2}{q_\alpha^2} a + \frac{1}{3} \frac{1}{(2\pi)^6} \frac{D}{m\hbar^4} + O\left(q_\alpha \ln\left(\frac{q_\alpha |a|}{\hbar}\right), \frac{p_\alpha^2}{q_\alpha} \right) \Bigg\}$$



A_1, A_2, A_3 – Universal constants.

Elastic scattering amplitude



Spectator scattering

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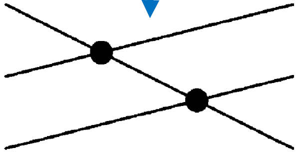

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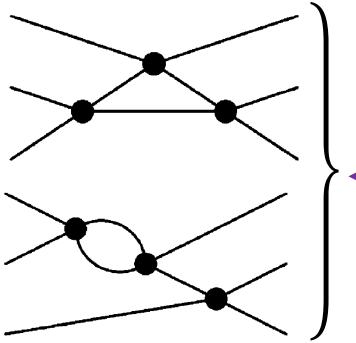
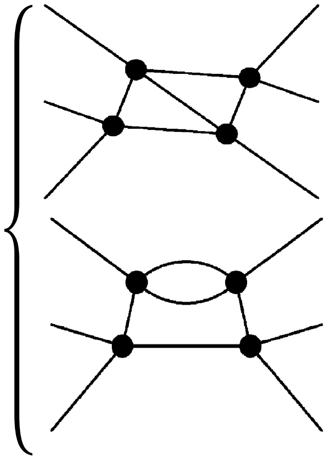
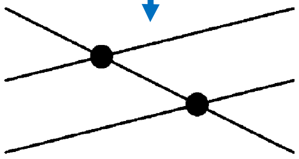
Elastic scattering amplitude





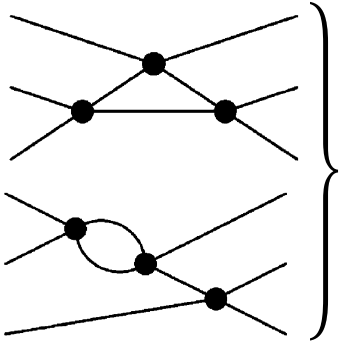
Spectator scattering

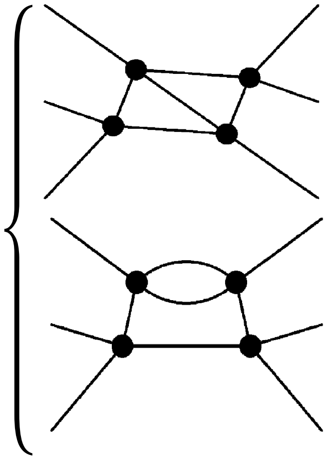
$$\langle \mathbf{p},\mathbf{q}|U_{00}(0)|\mathbf{0},\mathbf{0}\rangle = \sum_{\alpha=1}^{3}\Big\{\delta(\mathbf{q}_\alpha)\langle\mathbf{p}_\alpha|T(0)|\mathbf{0}\rangle + A_1\,\frac{a^2}{q_\alpha^2}+A_2\,\frac{a^3}{q_\alpha}+A_3\,a^4\ln\left(\frac{q_\alpha|a|}{\hbar}\right) + A_4\,\frac{p_\alpha^2+\frac{3}{4}q_\alpha^2}{q_\alpha^2}a + \frac{1}{3}\,\frac{1}{(2\pi)^6}\,\frac{D}{m\hbar^4}+O\left(q_\alpha\ln\left(\frac{q_\alpha|a|}{\hbar}\right),\frac{p_\alpha^2}{q_\alpha}\right)\Big\}$$



A_1, A_2, A_3 – Universal constants.

Elastic scattering amplitude





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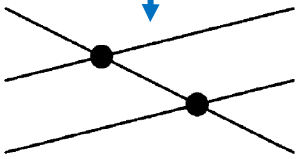
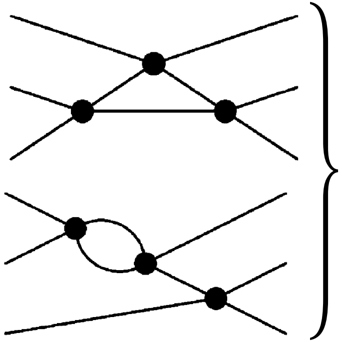
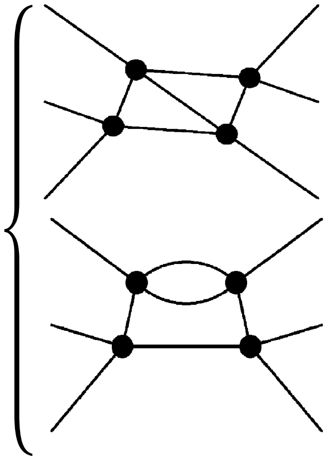


A_4 – Range correction

Elastic scattering amplitude





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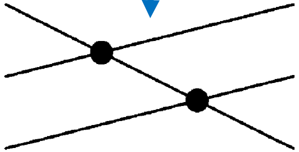


Three-body scattering hypervolume

- Non-perturbative

Outline:

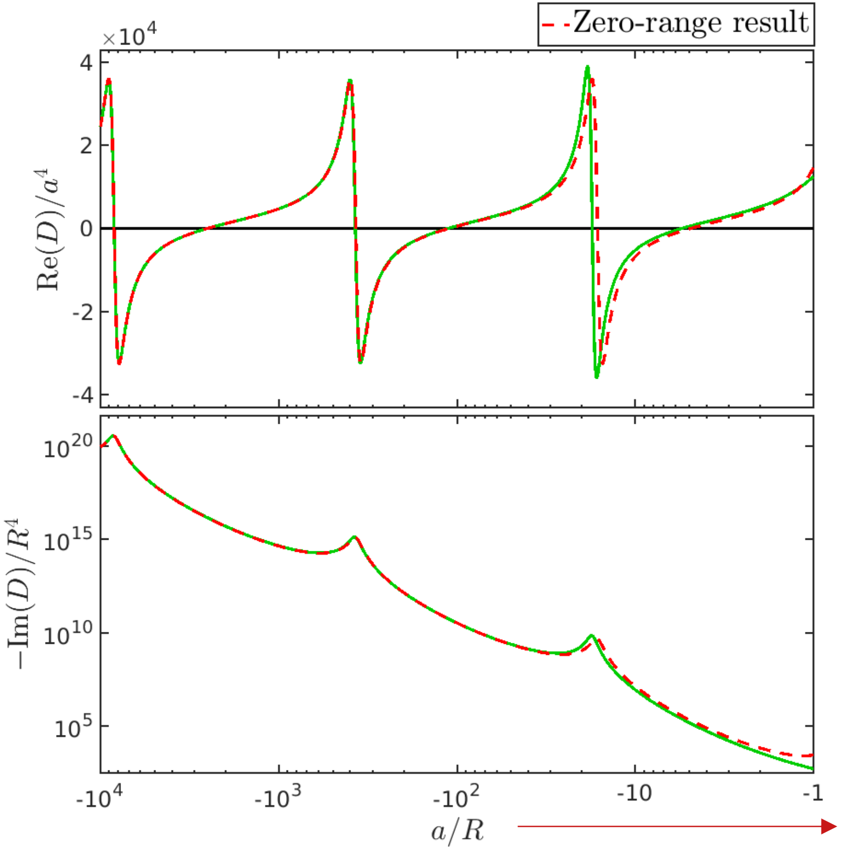
- *Background: Few-body collisions at low energies*

- ***Three-body collisions at strong and weak interactions***
  - Mestrom, Colussi, Secker, Kokkelmans PRA 100, 050702(R) (2019)
  - Mestrom, Colussi, Secker, Groeneveld, Kokkelmans PRL 124 (14), 143401 (2020)

- *Many-body effects induced by three-body collisions (droplets, etc…)*

- *Outlook*

• Results: Near Unitarity (a<0)



Square well radius

Efimov physics

$$\mathrm{Re}(D/a^4) \approx C\left(c_- + \frac{1}{2}b_- \frac{\sin\left(2s_0\ln(a/a_-)\right)}{\sin^2\left(s_0\ln(a/a_-)\right) + \sinh^2(\eta)}\right)$$

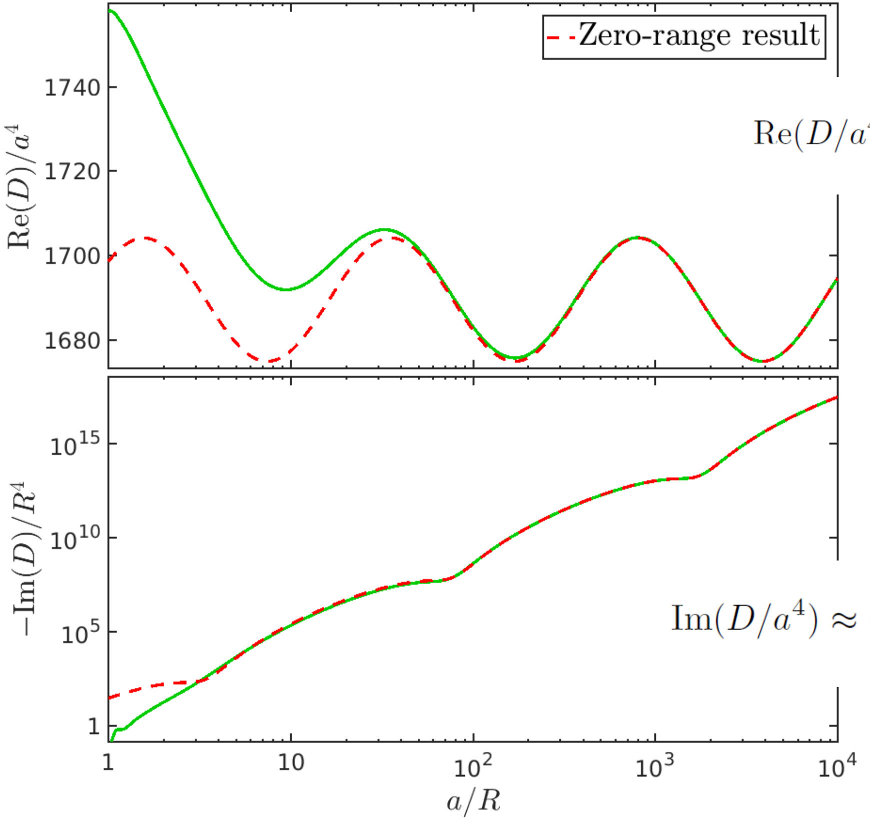
	Our result	Result of Ref. [1]
b_-	3.153(5)	3.16
c_-	1.140(2)	1.14
η	0.068(1)	-

$$\mathrm{Im}(D/a^4) \approx -\frac{1}{2}C_- \frac{\sinh(2\eta)}{\sin^2\left(s_0\ln(a/a_-)\right) + \sinh^2(\eta)}$$

[1] E. Braaten, H.-W. Hammer, T. Mehen, Phys. Rev. Lett., 88, 040401 (2002)

- **Results: Near Unitarity (a>0)**

Efimov physics



$$\mathrm{Re}(D/a^4) \approx C\left(c_+ + \frac{1}{2}b_+(1-e^{-2\eta}) + b_+ e^{-2\eta}\sin^2\left(s_0\,\ln(a/a_+) - \pi/4\right)\right)$$

	Our result	Result of Ref. [1]
b_+	0.0226(5)	0.021
c_+	1.1288(5)	1.13
η	0.068(1)	-

$$\mathrm{Im}(D/a^4) \approx -\frac{1}{2}C_+\left(\frac{1}{4}\left(1-e^{-4\eta}\right) + e^{-2\eta}\left(\sin^2\left(s_0\ln(a/a_+)\right) + \sinh^2(\eta)\right)\right)$$

[1] E. Braaten, H.-W. Hammer, T. Mehen, Phys. Rev. Lett., 88, 040401 (2002)

Re(D) satisfies (Efimov) van der Waals universality near unitarity ✓

What about at zero scattering length…?

- Re(D) $\neq 0$?
- Van der Waals universality
  - Im(D)(a,r_{vdW}) ?
  - Re(D)(a,r_{vdW}) ?

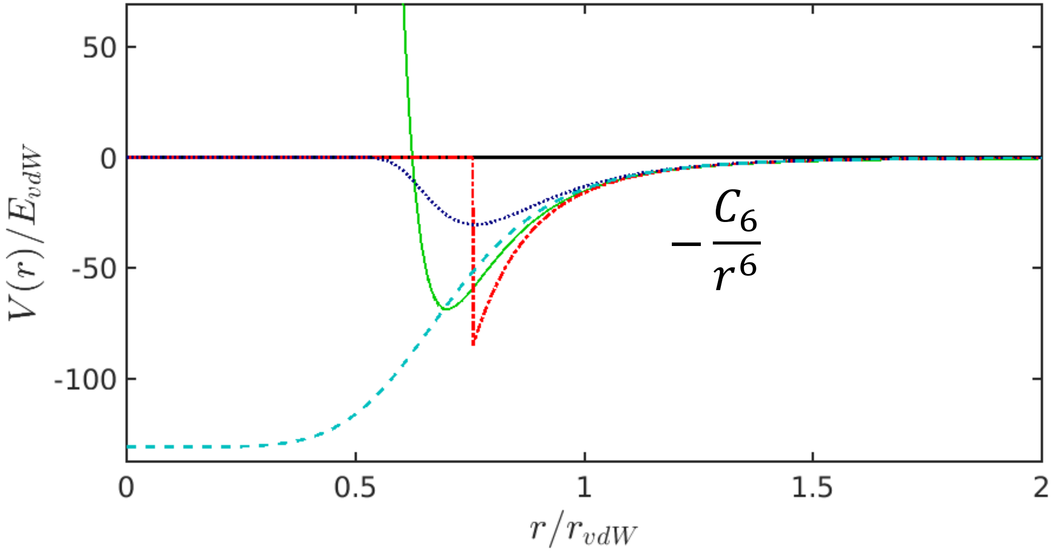
$$\Psi^{(3)}(R) \propto \frac{D}{R^4}$$

Results: van der Waals potentials

Idea: Vary short-range physics & fix long range

Search for universality, i.e. $D(r_{rvdW}, a)$

$$r_{vdW} = \frac{1}{2}\left(\frac{mC_6}{\hbar^2}\right)^{\frac{1}{4}} \quad E_{vdW} = \frac{\hbar^2}{m\, r_{vdW}^2}$$

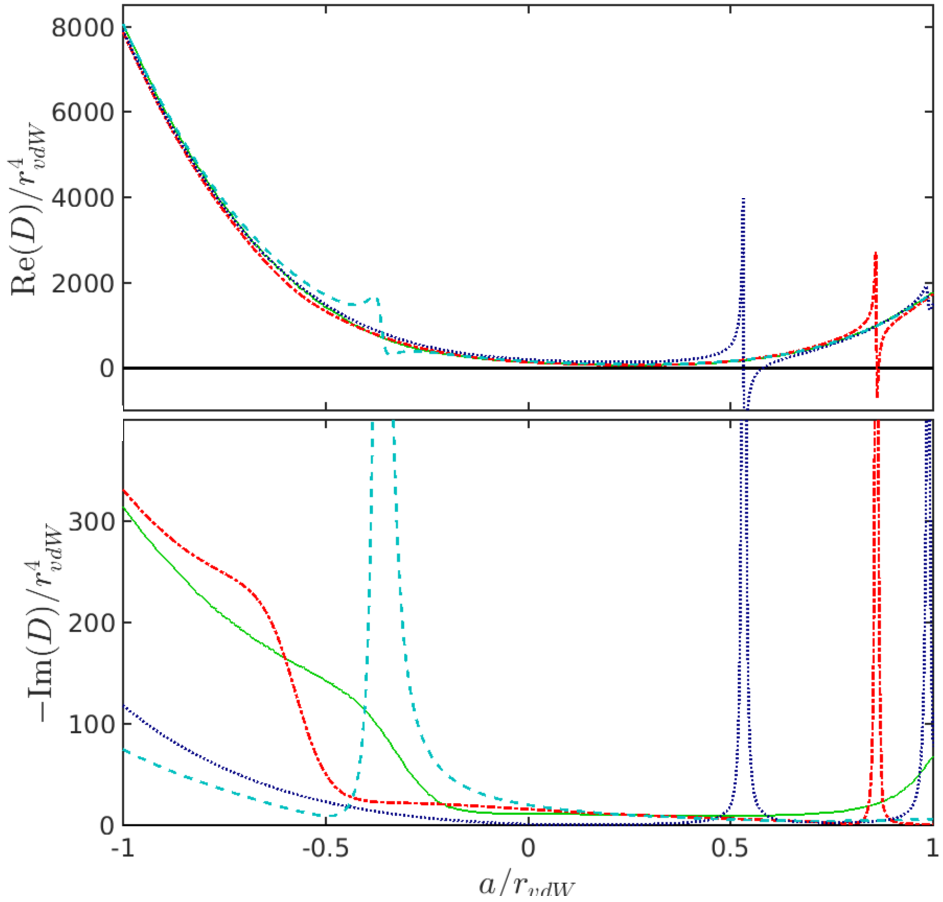


Same idea as Efimov van der Waals universality search

- Wang, D'Incao, Esry, Greene PRL 108, 263001 (2012)
- Naidon, Endo, Ueda PRL 112, 105301 (2014)

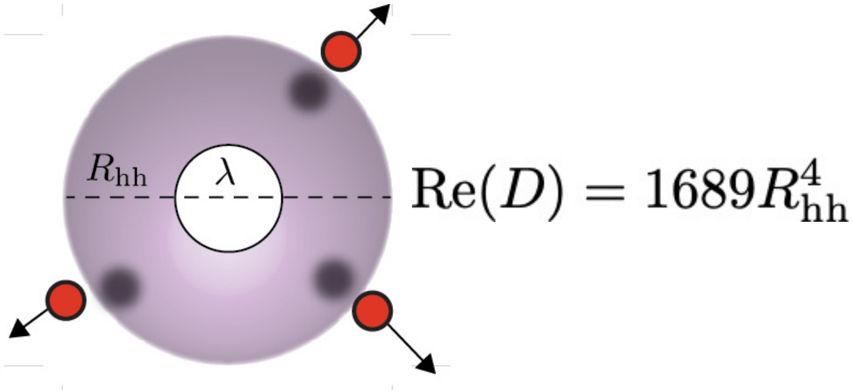
But now near $|a|/r_{vdW} = 0$

- No Efimov states!



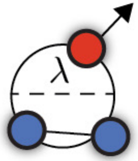
Re(D)

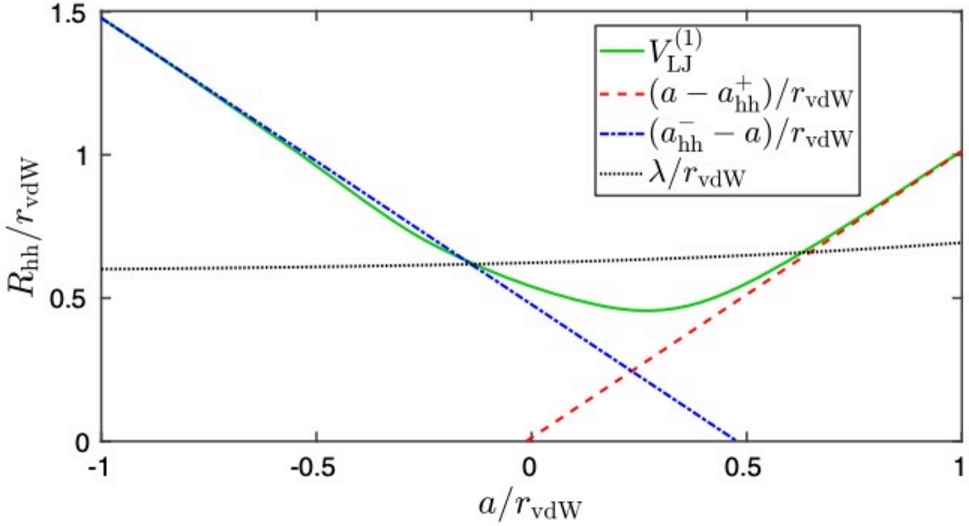
- Hard-hypersphere scattering
- "Single reflection"
  - D'Incao JPB 51, 043001 (2018)



Im(D)

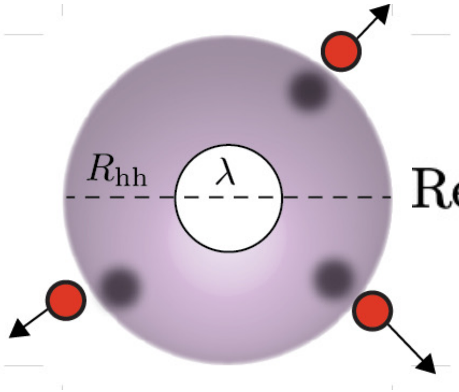
- Non-universal chemistry





Re(D)

- Hard-hypersphere scattering
- "Single reflection"
  - D'Incao JPB 51, 043001 (2018)



$$\mathrm{Re}(D) = 1689 R_{\rm hh}^4$$

Even when a=0, Re(D) remains!

$$\mathrm{Re}(D)(a=0) \approx 200 r_{\rm vdW}^4$$

Stable ground state

$$-\left.\frac{\mathrm{Re}(D)}{\mathrm{Im}(D)}\right|_{a=0} \approx 10$$

$$\mathrm{Re}(D) = 1689(a - R_{\rm hh}^{\pm})^4$$

$$R_{\rm hh}^{+} = -0.01 r_{\rm vdW}$$

$$R_{\rm hh}^{-} = 0.5 r_{\rm vdW}$$

van der Waals universality!

Outline:

- *Background: Few-body collisions at low energies*

- *Three-body collisions at strong and weak interactions*

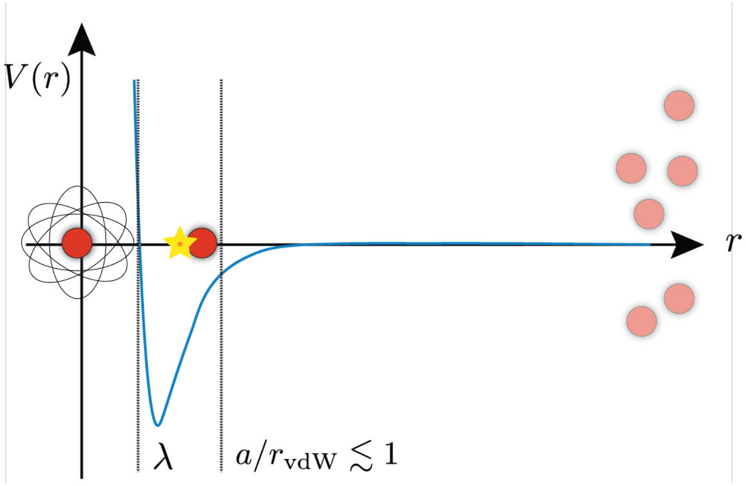
- ***Many-body effects induced by three-body collisions (droplets, etc…)***
    - Mestrom, Colussi, Secker, Groeneveld, Kokkelmans PRL 124 (14), 143401 (2020)
    - Mestrom, Li, Colussi, Secker, Kokkelmans PRA 104, 023321 (2021)

$$\mathcal{E} \approx \frac{\hbar^2 n^2 D}{6m} \qquad D(a, r_{\mathrm{vdW}}) \implies \mathcal{E}(a, r_{\mathrm{vdW}})$$

- *Outlook*

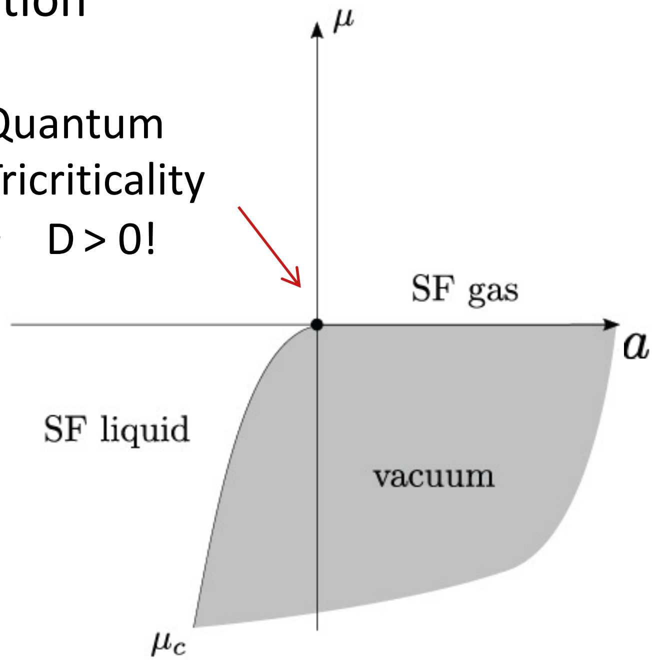
Phase Diagram: Bose particles w/Lennard Jones interaction

- Kora, Boninsegni, Son, Zhang PNAS 117, 27231 (2020)
- W. Zwerger, J. Stat. Mech. (2019)
- M. D. Miller et al., PRB (1977)



Quantum Tricriticality

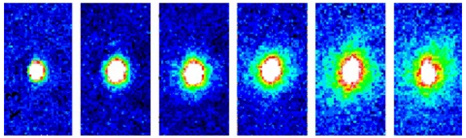
- D > 0!



$$V_{\rm eff}[\psi] = -\mu|\psi|^2 + \frac{4\pi\hbar^2 a}{m}|\psi|^2\psi + \frac{\hbar^2 D}{2m}|\psi|^4\psi$$

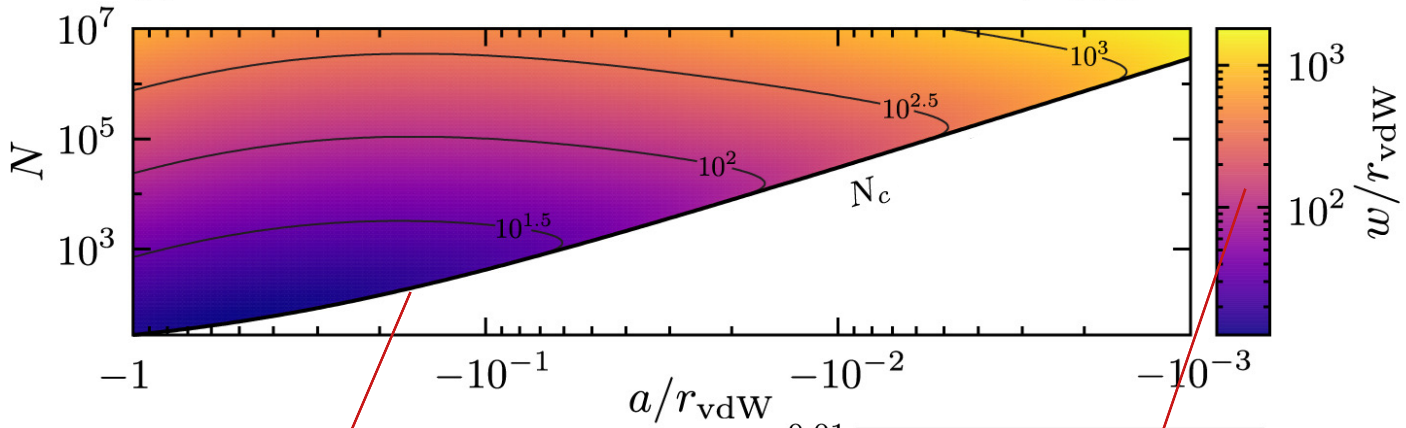
Bosenova

- Cornell/Wiemann, Nat. 412, 295 (2001)

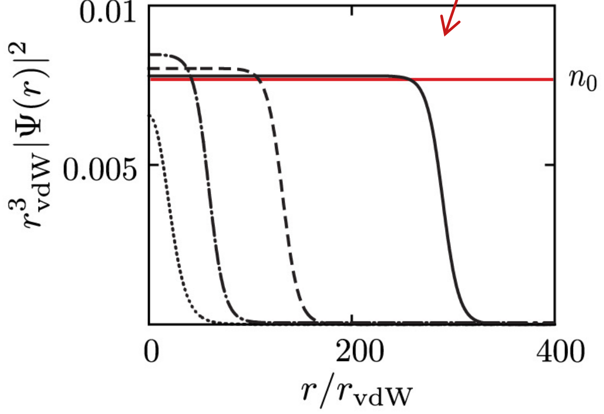


Universal droplet phase diagram

- Mestrom, Colussi, Secker, Groeneveld, Kokkelmans PRL 124 (14), 143401 (2020)



Liquid to gas $N_c \propto \frac{\sqrt{D}}{a^2}$



Droplet profile

Historical Note: This is the *opposite* regime from Bulgac's original proposal for dilute quantum droplets

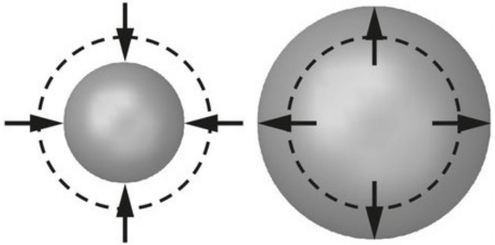
- PRL **89**, 050401 (2002)

Could D also be inferred from collective mode shifts?

- Mestrom, Colussi, Secker, Groeneveld, Kokkelmans PRL 124 (14), 143401 (2020)

Monopole mode

- Compression -> Interaction effects



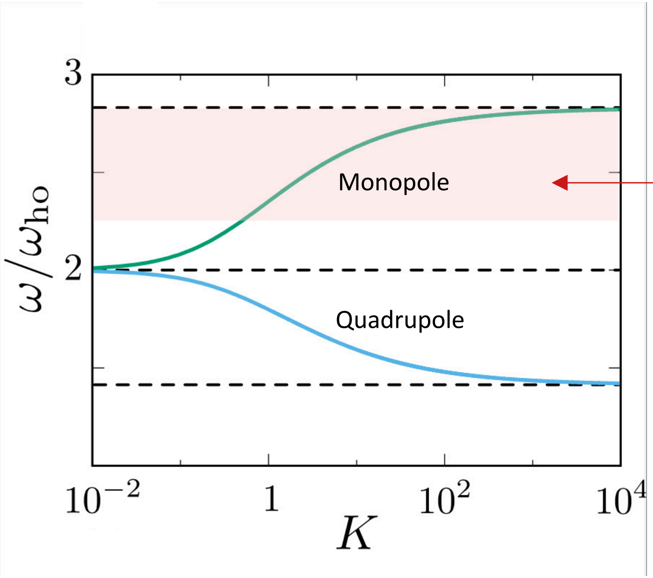
Thomas-Fermi limits

- Two-body $Na/a_{\mathrm{ho}} \gg 1$

$$\omega/\omega_{\mathrm{ho}} \approx 2.23$$

- Three-body $DN^2/a_{\mathrm{ho}}^4 \gg 1$

$$\omega/\omega_{\mathrm{ho}} \approx 2.82$$



$$K = \frac{2DN^2}{9\sqrt{3}\pi^3 a_{\mathrm{ho}}^4} \propto r_{\mathrm{vdW}}^4 m^2$$

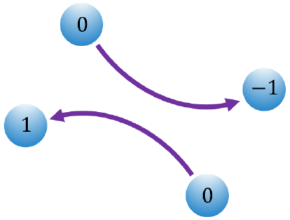
Challenge: How to increase K to see regime of clear three-body shifts?

- Choose species with larger D
  - i.e. K, **Rb**, **Cs**,…
- Choose spherical mode
  - No magnetic dipole-dipole shift

Could D be inferred from the spin phase of the spin – 1 BEC?

- Colussi, Greene, D'Incao PRL 113, 045302 (2014)
- Mestrom, Li, Colussi, Secker, Kokkelmans PRA 104, 023321 (2021)

Spin-exchange pathways



$F_{2b} = 0, 2$

$$c_{2b}^{di} = \frac{1}{3}(a_0 + 2a_2)$$

$$c_{2b}^{ex} = \frac{1}{3}(a_2 - a_0)$$

$F_{3b} = 1, 3$

$$c_{3b}^{di} = \frac{1}{5}(3D_1 + 2D_3)$$

$$c_{3b}^{ex} = \frac{1}{5}(D_3 - D_1)$$

Three-body spin-exchange

- Also vdW universality

For $4\pi c_{2b}^{ex} + c_{3b}^{ex} n < 0$: $F = N$ (Ferromagnetic)

For $4\pi c_{2b}^{ex} + c_{3b}^{ex} n > 0$: $F = 0$ (Antiferromagnetic)

At what density would the spin phase change?

For ^{23}Na and ^{41}K: $n_c \approx 10^{17} \mathrm{cm}^{-3}$

- Spin ground state not changed by three-body collisions

^{87}Rb ($a_0 \approx a_2$) is sensitive to finite-range effects

- Open question…

Could D be inferred from spin-mixing dynamics?

- Mestrom, Li, Colussi, Secker, Kokkelmans PRA 104, 023321 (2021)

Consider a spin-1 BEC with $N_0 = N$ and $N_1 = N_{-1} = 0$ at $t = 0$

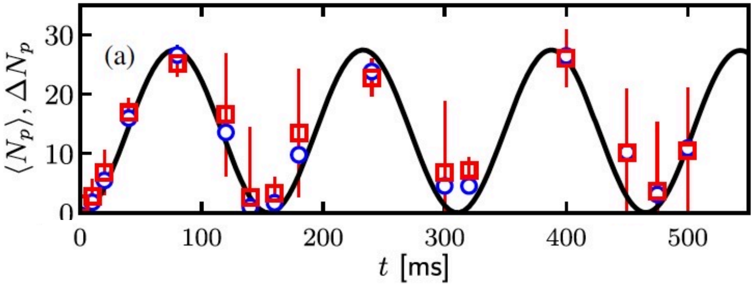
Spin-mixing: $$N_{\pm 1}(t) = \left(\frac{U_s}{\varepsilon_{\mathrm{B}}}\right)^2 \sin^2(\varepsilon_{\mathrm{B}} t/\hbar)$$

$$\varepsilon_{\mathrm{B}} = \sqrt{q_{\mathrm{Z}}(q_{\mathrm{Z}} + 2U_s)}$$

Measurable

Quadratic Zeeman $$U_s = (4\pi n_0 c_{2\mathrm{b}}^{\mathrm{ex}} + n_0^2 c_{3\mathrm{b}}^{\mathrm{ex}})\hbar^2/m$$

Evrard et al., Phys. Rev. Lett. **126**, 063401 (2021)



Idea: Apply a weak magnetic field *B* to cancel out effective two-body interactions.

$$q_{\mathrm{Z}} = -\frac{8\pi\hbar^2 n_0 c_{2\mathrm{b}}^{\mathrm{ex}}}{m}$$

^{41}K: $B = 0.17$ G
^{87}Rb: $B = 0.29$ G
^{23}Na: Scheme fails ($c_{2\mathrm{b}}^{\mathrm{ex}} > 0$)

$$\varepsilon_{\mathrm{B}} = \hbar n_0 \sqrt{2 q_{\mathrm{Z}} c_{3\mathrm{b}}^{\mathrm{ex}}/m}$$
$$= \frac{4\hbar^2 n_0^{3/2}\sqrt{-\pi c_{2\mathrm{b}}^{\mathrm{ex}} c_{3\mathrm{b}}^{\mathrm{ex}}}}{m}$$

Signature of three-body spin mixing:

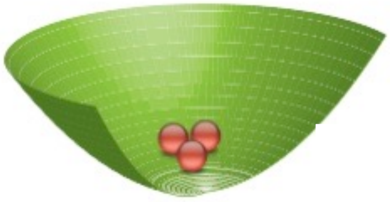
$$\varepsilon_{\mathrm{B}} \propto n_0^{3/2}\sqrt{c_{3\mathrm{b}}^{\mathrm{ex}}}$$

Extensions

- Heteronuclear systems
  - Mestrom, Colussi, Secker, Li, and Kokkelmans, PRA 103, L051303 (2021).
    - Regime of strong three-body interactions/weak losses found near p-wave resonance
  - Wang and Tan, PRA 103, 063315 (2021).
- Spin-polarized fermions
  - 3D: Wang & Tan, Phys. Rev. A **104**, 043319 (2021)
  - 2D: Wang & Tan, arXiv:2205.02658

Open Questions

- 1st Experimental measurement – *seemingly there for the taking!*
- Origin of a=0 vdW universality
- Lower dimensions
  - Confinement induced resonances (c.f. Petrov, Olshanii, others…)
- Long(er) range interactions (i.e. dipolar)



Thanks for your attention!

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