8. OCTOBER 2014

TALES OF QUANTUM MECHANICS

A JOURNEY FROM FEW- TO MANY-BODY PHYSICS

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ICTP SAIFR International Centre for Theoretical Physics South American Institute for Fundamental Research

São Paulo International Schools on Theoretical Physics

FAPESP ICTP unesp IFT

Mini-school on Few-body Physics

B

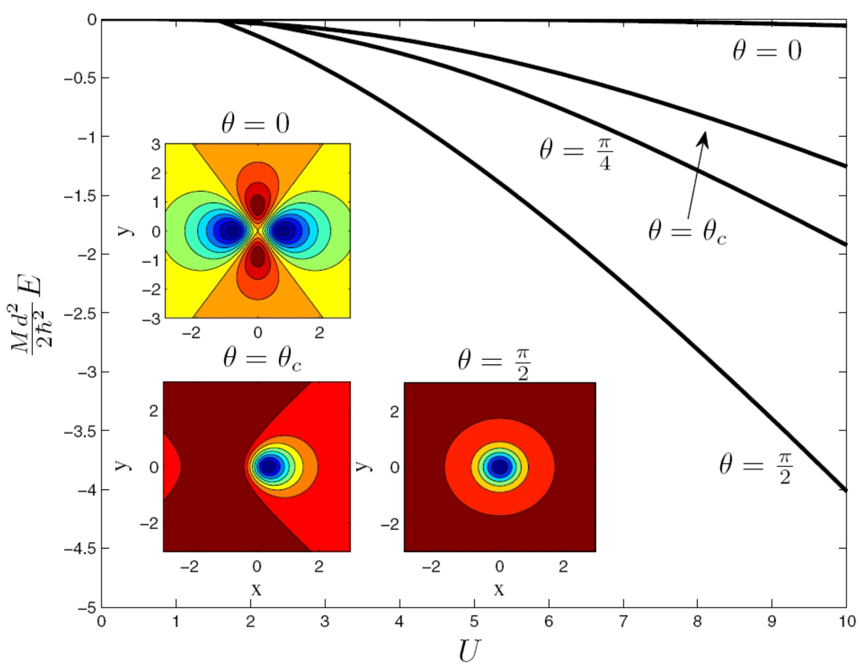
BOUND STATES – GOOGLE STYLE!

Bound dimers in bilayers of cold polar molecules

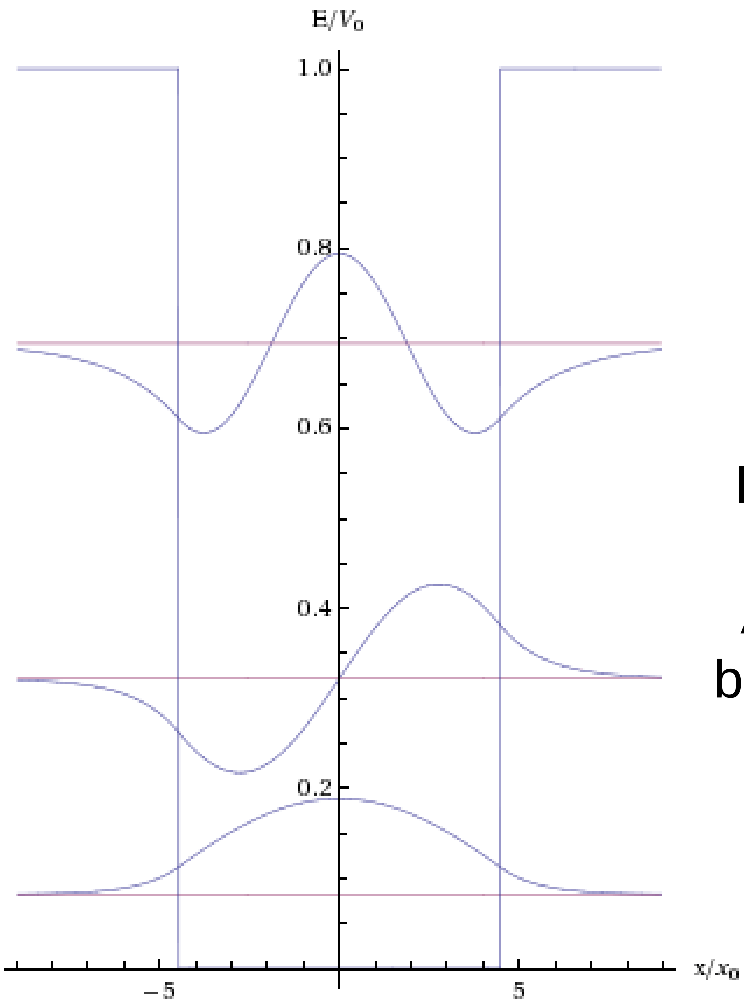
A G Volosniev, N T Zinner, D V Fedorov, A S Jensen and B Wunsch

Google images first page!

J. Phys. B: At. Mol. Opt. Phys. **44** 125301 2011



QUANTUM MECHANICS 101



When do bound states form?

Consider 1D finite square well potential

Ground state solution for **ANY** strength

Excited state solution **REQUIRES** finite strength

Attractive potential of ANY strength produces bound state in 1D. Finite strength required in 3D

1D and 3D are very similar

BOUND STATE CRITERIA

Consider weak potential limit

Landau

$$1\text{D} : E \sim -\frac{m}{\hbar^2}\left[\int_{-\infty}^{\infty} V(x)dx\right]^2 \sim \frac{mU^2l^2}{\hbar^2}$$

Gaussian example

$$V(r) = -Ue^{-r^2/l^2}$$

$$\frac{mUl^2}{\hbar^2} \ll 1$$

Asymptotic wave function $\psi(r) \sim \exp(-\frac{\hbar}{\sqrt{m|E|}}r)\,, \quad r \to \infty$

Tail-dominated for very small energies
Non-classical behavior prevails!

BOUND STATE CRITERIA

Two-dimensional case

Landau

$$2\text{D}: E \sim -\frac{\hbar}{ml^2}\exp\left[-\frac{\hbar^2}{m}\left(\int d^2\boldsymbol{r}V(\boldsymbol{r})\right)^{-1}\right]$$

Gaussian example

$$V(r) = -Ue^{-r^2/l^2}$$

$$\frac{mUl^2}{\hbar^2} \ll 1$$

Huge difference to 1D

Weakly bound states are truly weakly bound!

BOUND STATE CRITERIA

Bound state criterion in 2D $$\int d^2 r V(r) < 0$$

Even if we assume $$\int d^2 \boldsymbol{r} V(\boldsymbol{r}) = 0, \ V(\boldsymbol{r}) \neq 0$$

we find $$E \sim -\exp\left[-\frac{1}{\lambda^2}\right], \quad V(\boldsymbol{r}) = \lambda \tilde{V}(\boldsymbol{r})$$

2D binds but only weakly. Interesting to study dimensional interpolation to 3D via d=2+ε

B. Simon, Ann. Phys. **97,** 279 (1976)

A.G. Volosniev *et al.*, PRL **106**, 250401 (2011)

A.G. Volosniev *et al.*, J. Phys. B **44**, 125301 (2011)

A CAVEAT ABOUT RANGE

So far we considered short-range interactions

$$V(r) = -Ue^{-r^2/l^2}$$

Standard criterion

$$r^2 V(r) \to 0, \quad r \to \infty$$

For low-energy scattering it is more complicated

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LOW-ENERGY SCATTERING (IN 3D)

Scattering wave function	$\psi(\boldsymbol{r}) \sim e^{ik_z z} + f(k_z, \boldsymbol{k})\frac{e^{ikr}}{r}, \quad r \to \infty$
Scattering cross section	$\sigma_{\text{elastic}} \propto \lvert f(k_z, \boldsymbol{k})\rvert^2, \quad \lvert\boldsymbol{k}\rvert = k_z$
Low-energy limit	$\lim_{\boldsymbol{k}\to 0} f(k_z, \boldsymbol{k}) \propto a$
However, only valid when	$V(r) \propto r^{-\nu}, \text{ and } \nu > d$

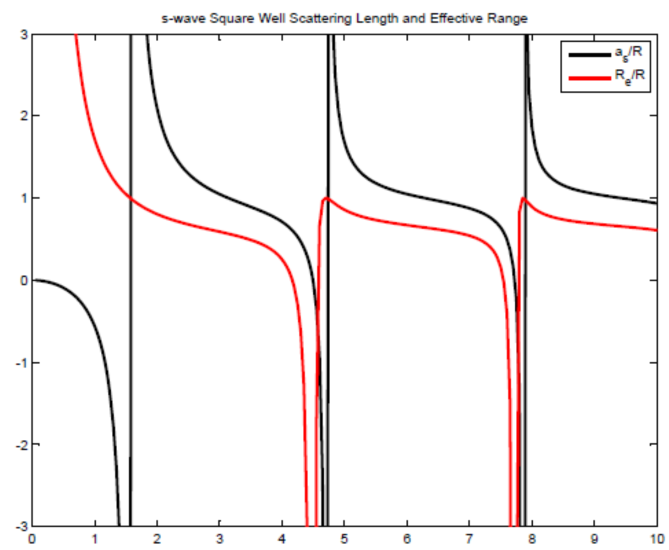
In 3D, the dipolar interaction violates this,
but luckily the van der Waals r^6 does not.

SCATTERING AND BOUND STATES

Consider the finite square well

$$V(r) = \begin{cases} -V_0 & , \; r < R \\ 0 & , \; r > R \end{cases}$$

$$\frac{a}{R} = 1 - \frac{\tan(s)}{s}, \quad s = \left[\frac{2mV_0R^2}{\hbar^2}\right]^{1/2}$$



Resonant when bound state appears!

Depends on range and strength in a combined fashion

Generically one finds

$$\psi_k(r) \sim \frac{\sin(k(r-a))}{r} \sim 1 - \frac{a}{r}$$

A LIMIT OF GREAT UTILITY

Simplify the potential by making the range small, a zero-range approach

For a>0, we need a bound state with the right limit $$\psi(r) \propto \frac{e^{-r/a}}{r}$$

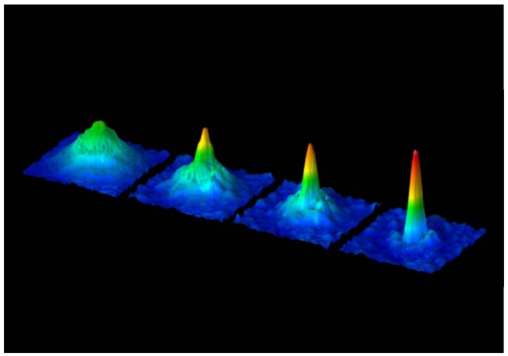
Two-body bound state energy $$E \sim -\frac{\hbar^2}{ma^2}$$

Universal two-body state since it only depends on low-energy scattering properties of the potential

Naturally obtained from limits of other finite-range potentials

One parameter model of interaction between particles

WHY IS THIS RELEVANT?



[87]Rb Rempe group, MPQ

Cold atomic gases!

1) Extremely cold, T~10-100nK
2) Extremely dilute, n~10$^{12-15}$ cm^{-3}

$$l_0 = n^{-1/3} \sim 10^{-4} - 10^{-5}\mathrm{cm} \sim 10^3 - 10^4 a_0 \gg r_{\mathrm{vdW}}$$

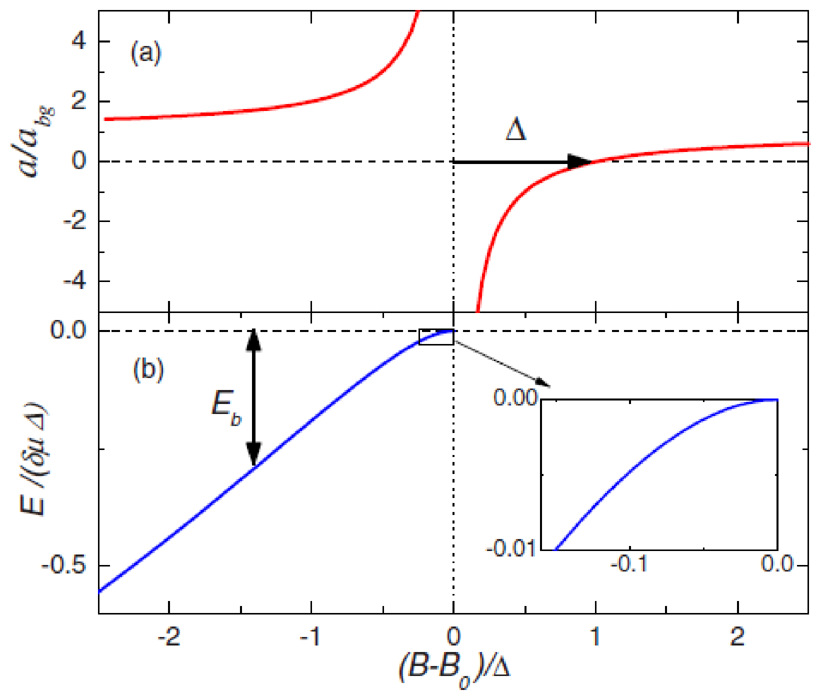
$$\lambda_{\mathrm{dB}} \sim \frac{\hbar}{\sqrt{mk_BT}} \gg l_0, \;\; k \sim \frac{1}{\lambda_{\mathrm{dB}}} \ll \frac{1}{l_0} \ll \frac{1}{r_{\mathrm{vdW}}}$$

Low-energy (elastic) scattering dominates

A NEAT FEATURE

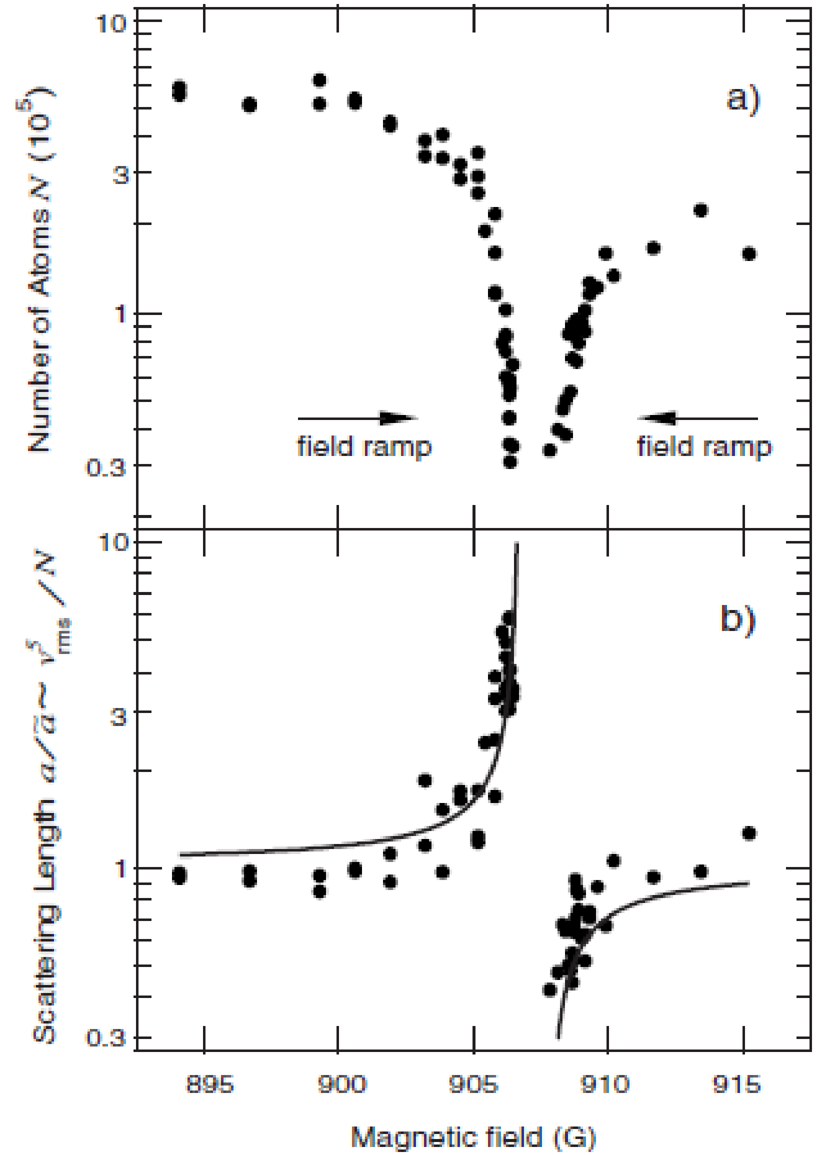
Interactions are tunable!

Feshbach resonance



C. Chin *et al.*, RMP **82**, 1225 (2010)

S. Inouye *et al.*, Nature **392**, 151 (1998)



UNIVERSALITY?

Tune onto the resonance itself where scattering length diverges but collision energy is still low

$$a \to \pm\infty, \ k \ll \frac{1}{r_{\mathrm{vdW}}}$$

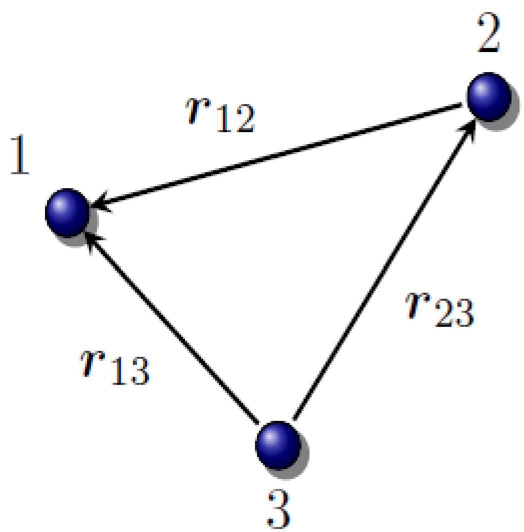
Anything I calculate in this limit *cannot* depend on scattering length!

An example is a Fermi gas

$$E_{\mathrm{tot}} = \xi \frac{\hbar^2 k_F^2}{2m}$$

The regime of diverging a is termed the universal regime

UNIVERSAL THREE-BODY PHYSICS



Zero-range model

$$\left.\frac{\partial \ln(r_{jk}\Phi)}{\partial r_{jk}}\right|_{r_{jk}=0} = -\frac{1}{a}$$

Exact radial solution when a diverges

$$f_0^{(n)}(\rho) = \sqrt{\rho} K_{i\xi}(\kappa^{(n)}\rho) \simeq \sqrt{\rho}|\Gamma(i\xi)| \sin\left(\xi \ln(\kappa^{(n)}\rho) + \theta\right)$$

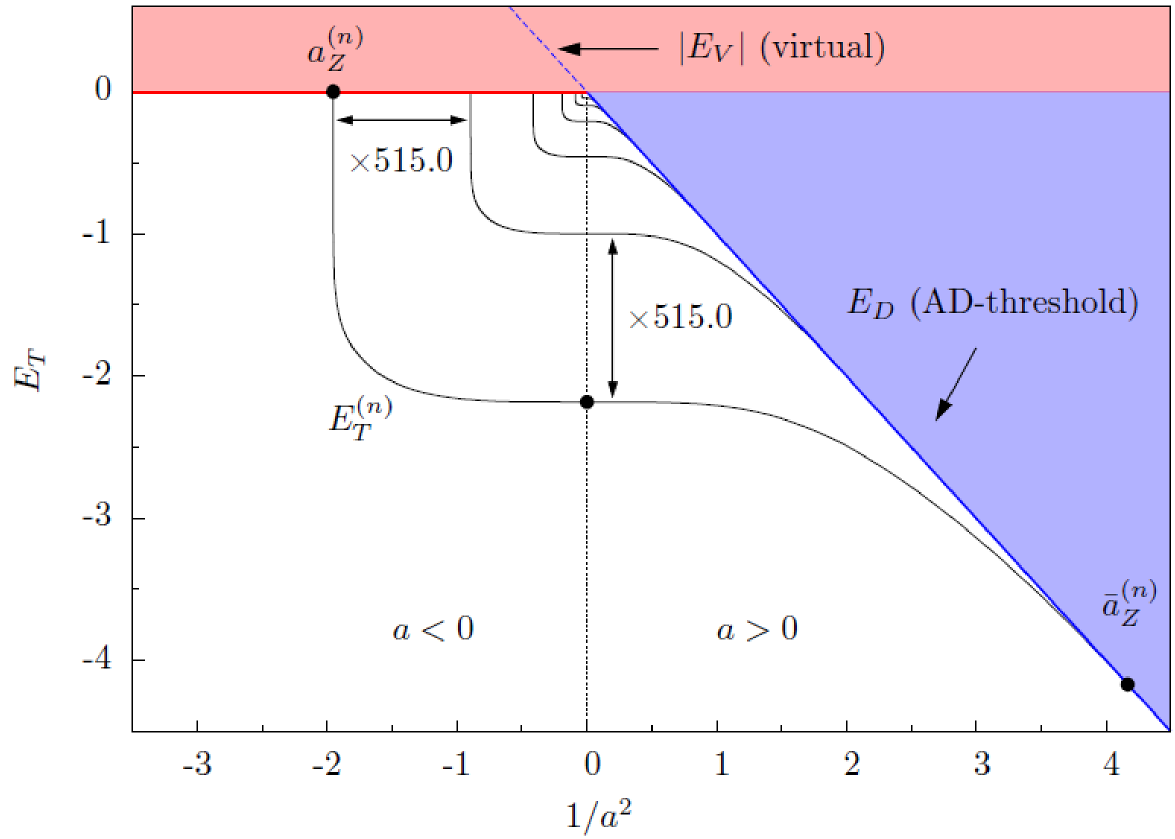
$$\rho^2 = x_i^2 + y_i^2 = \frac{1}{3}(r_{12}^2 + r_{13}^2 + r_{23}^2)$$

Log-periodic behavior! This is the Efimov effect!

$$\frac{\kappa^{(n)}}{\kappa^{(0)}} = e^{-\pi n/\xi} \simeq 22.7^{-n}, \quad \text{or} \quad \frac{E^{(n)}}{E^{(0)}} = e^{-2\pi n/\xi} \simeq 515.0^{-n}$$

M. Thøgersen, arXiv:0908.0852v1

THE UNIVERSAL SPECTRUM



M. Thøgersen, arXiv:0908.0852v1

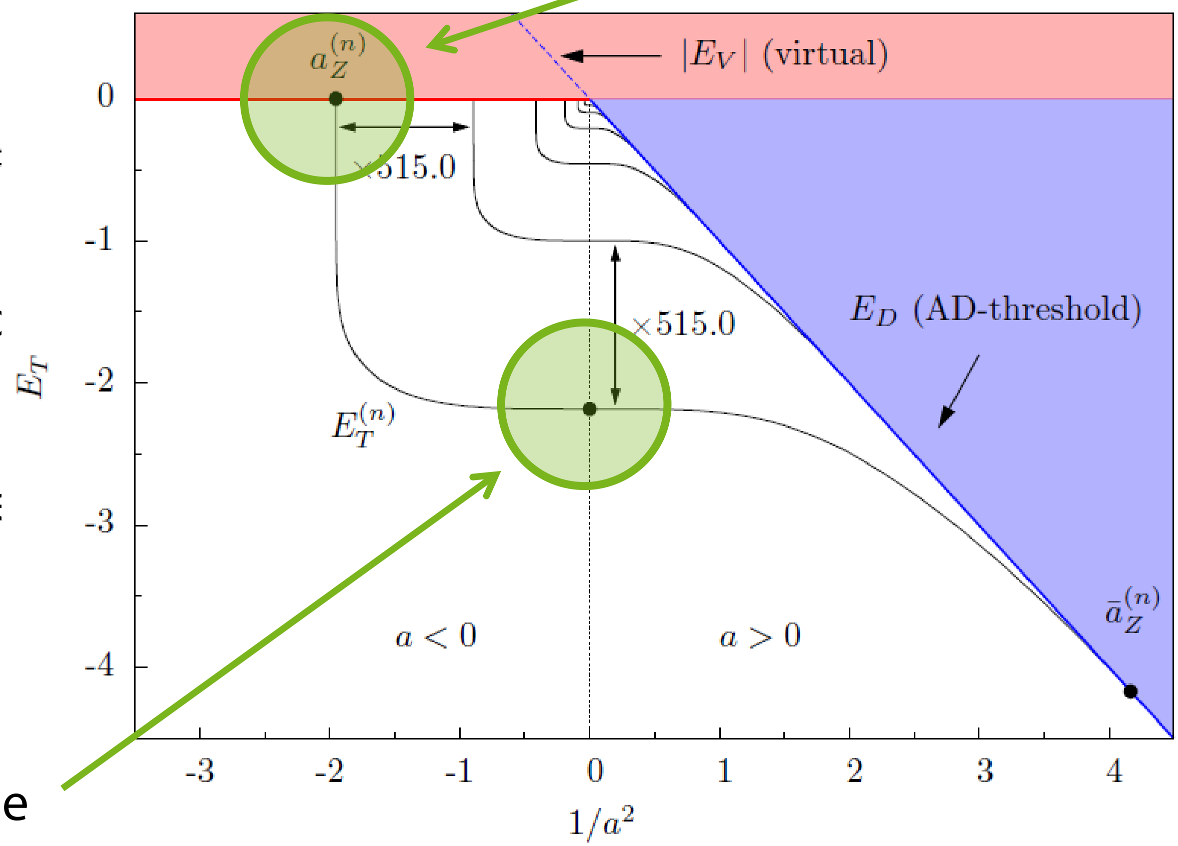
A HUGE PROBLEM

Importantly, it also fixes this scale, called a_

$f_0^{(n)}(\rho) =$ ... $\rho) + \theta\Big)$

Must introc ... -body

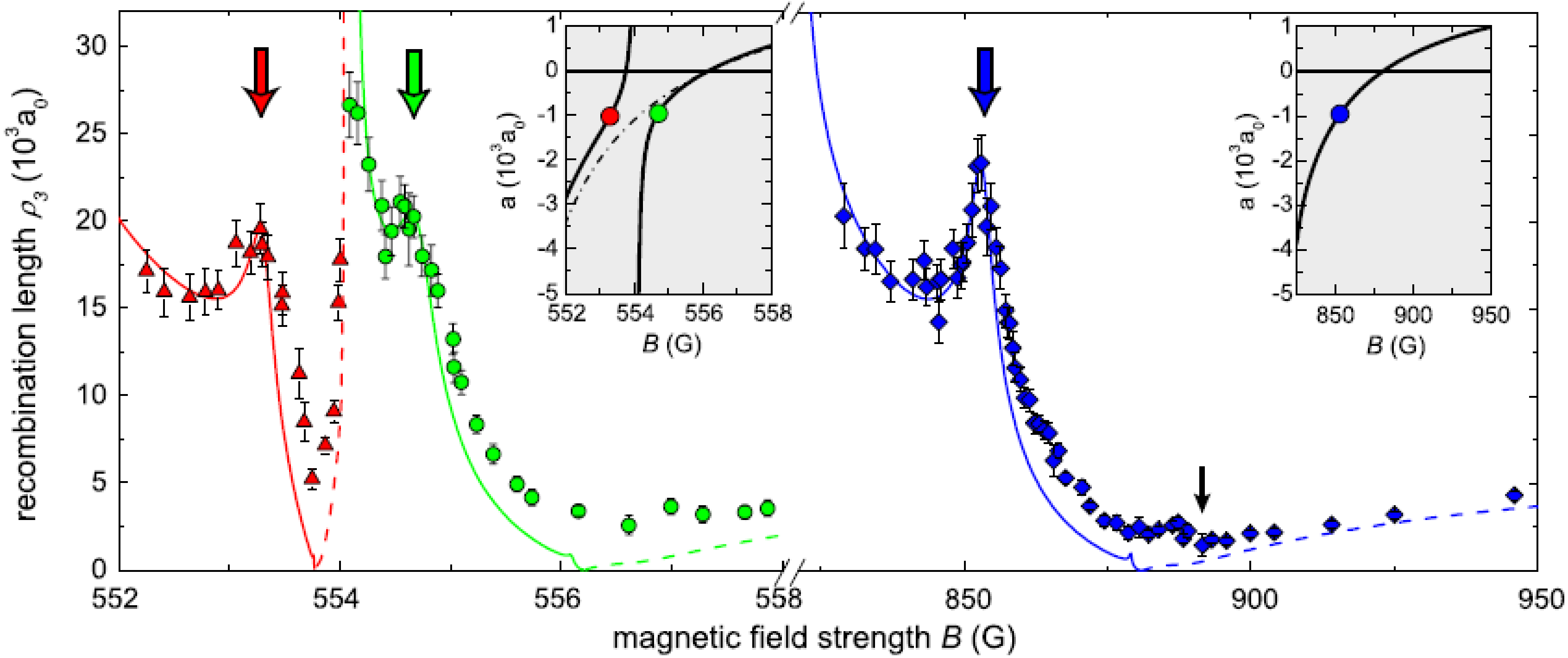
This effe ... s the



Fixes this scale

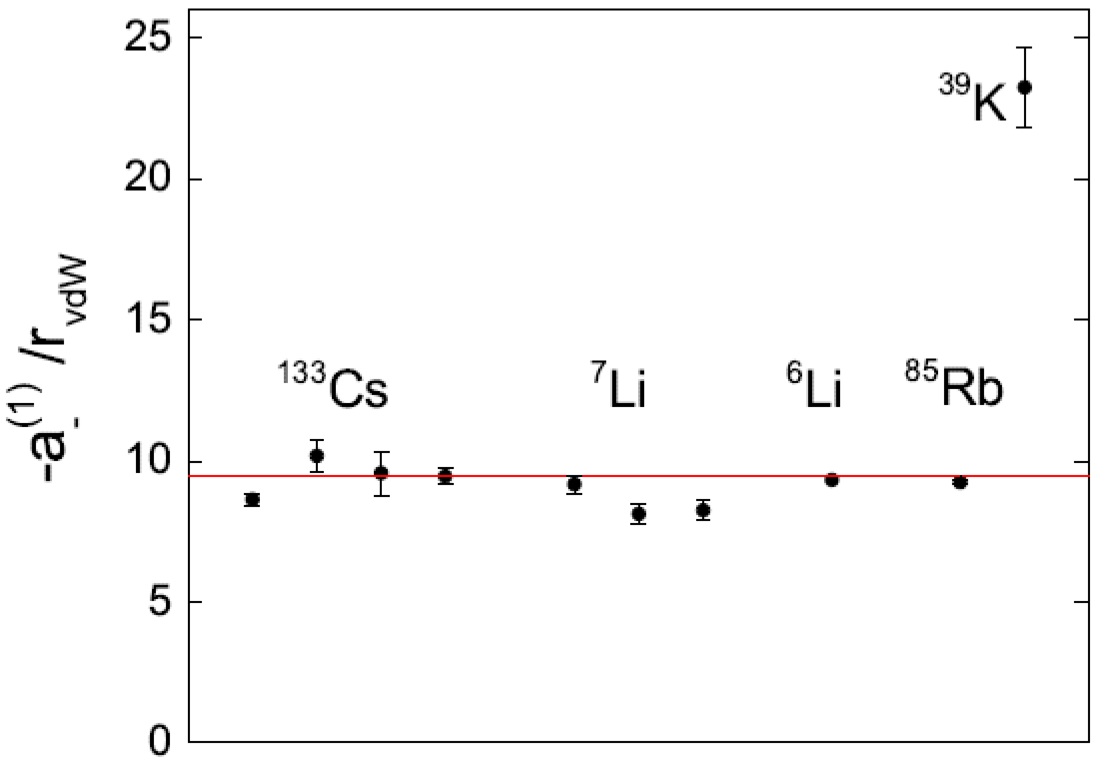
OBSERVATIONS

Observations of a_- in ^{133}Cs at different resonances



M. Berninger *et al.*, PRL **107**, 120401 (2011)

AN INTERESTING FINDING



A conspiracy of numbers?

M. Berninger *et al.*, PRL **107**, 120401 (2011)
C. Chin, arXiv:1111.1484v1

IMPLICATIONS

Could imply no three-body parameter at all

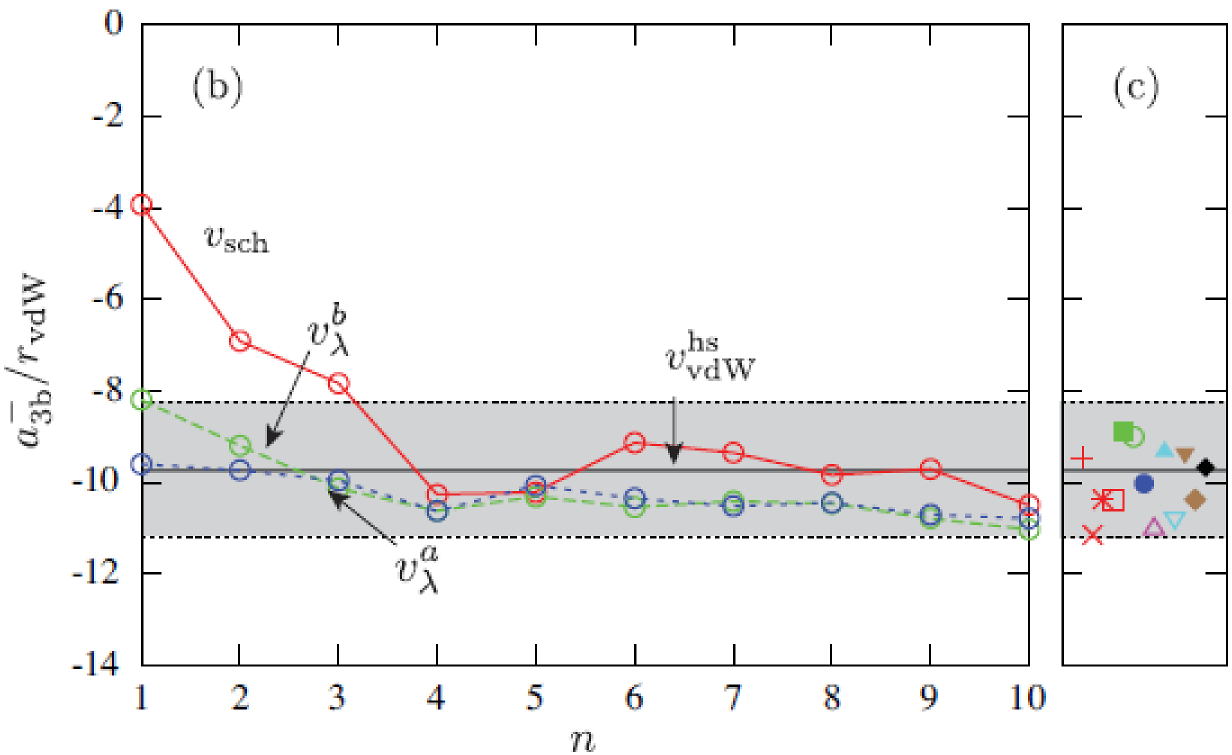
All physics given by the two-body van der Waals length

This implies increased universality of the three-body problem!

Perhaps not really surprising since zero-range models are intrinsically incomplete. Calibration to *ab initio* is extremely difficult

How does the van der Waals length enter more specifically?

THEORETICAL IDEAS



J. Wang et al., arXiv:1201.1176v1
C. Chin, arXiv:1111.1484v1

ABANDON ZERO-RANGE?

Zero-range potentials are extremely convenient so good motivation for keeping them around

Consider the cut-off in the zero-range model as a physical two-body length similar to Cheng Chin's ideas.

Could also consider a zero-range model with extra parameters,

$$f(k)^{-1} = -\frac{1}{a} + \frac{1}{2} r_{\mathrm{eff}} k^2 + \dots$$

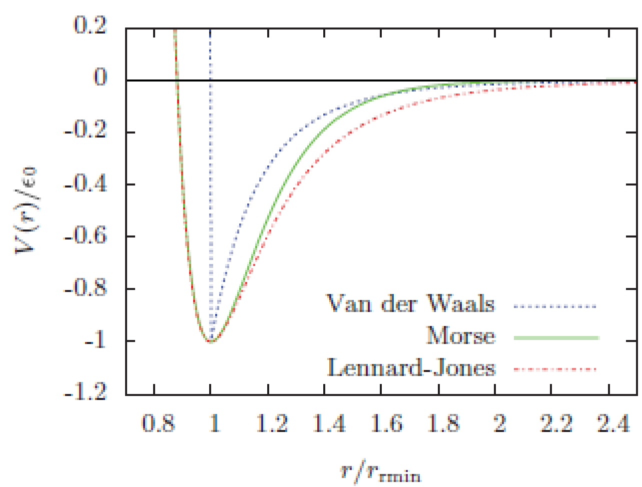
Effective range is typically related to width of the Feshbach resonance

$$r_{\mathrm{eff}} \propto \frac{1}{\Delta}$$

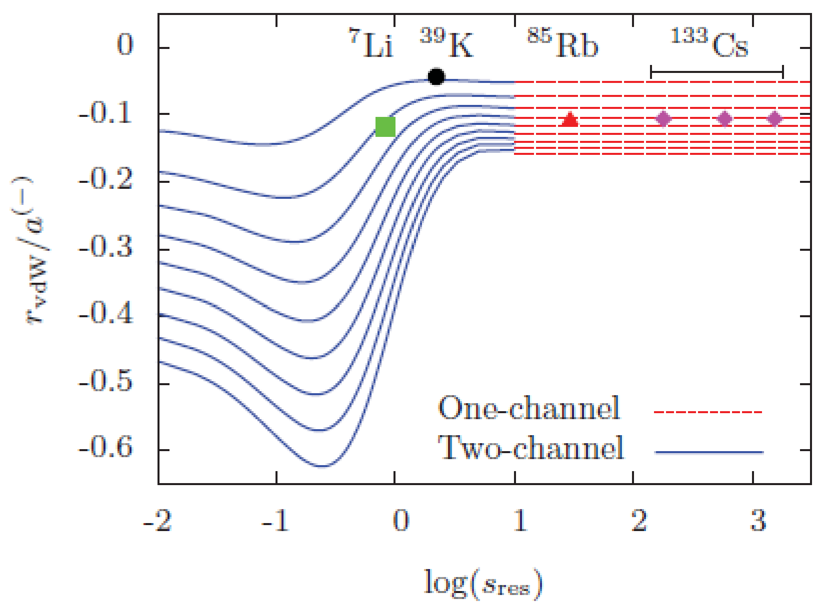
A good test of the theory is to look at different widths!

IDEA: Two-body hard-core becomes a three-body hard-core!

Atomic two-body potential has a strong hard-core part!

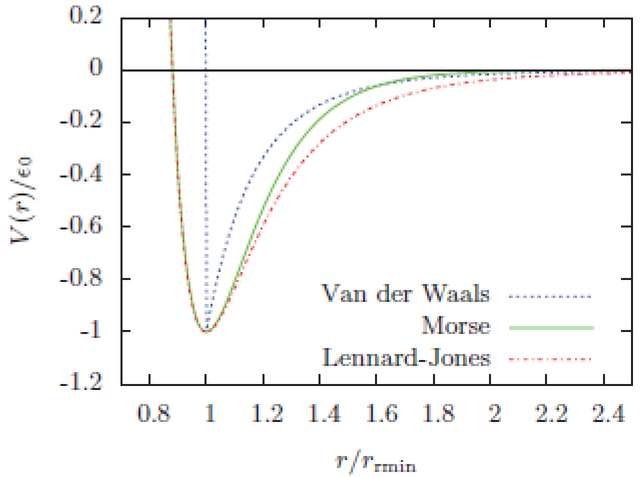


Test different values of three-body cut-off



P.K. Sørensen *et al.*, PRA **86**, 052516 (2012)

A SIMPLE ZERO-RANGE MODEL



van der Waals plus hard-core model

$$V(r) = -\frac{C_6}{r^6}, \quad r > r_c$$

Bound states number is analytical

$$n = \frac{2}{\pi}\left(\frac{r_{\text{vdW}}}{r_c}\right)^2 - \frac{7}{8}$$

Zero-range model relates three-body parameter linearly to a_-

$$a_- = -\delta\,\rho_c = -31.756\,\rho_c$$

Two-body cut-off r_c can be related to three-body cut-off to avoid hard-core

$$\rho_c \geq \sqrt{2} r_c$$

P.K. Sørensen *et al.*, PRA **86**, 052516 (2012)

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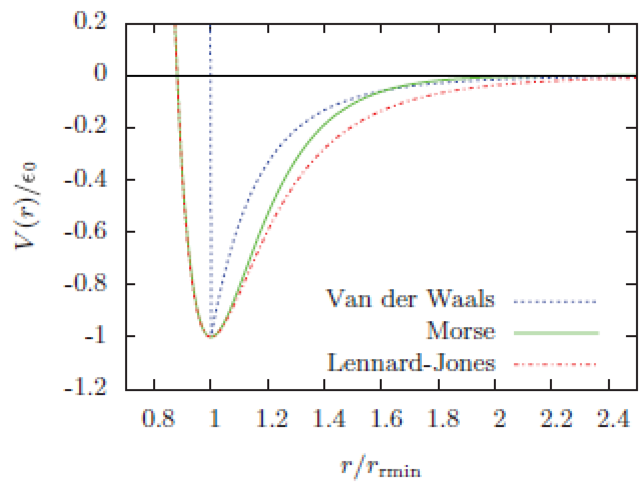
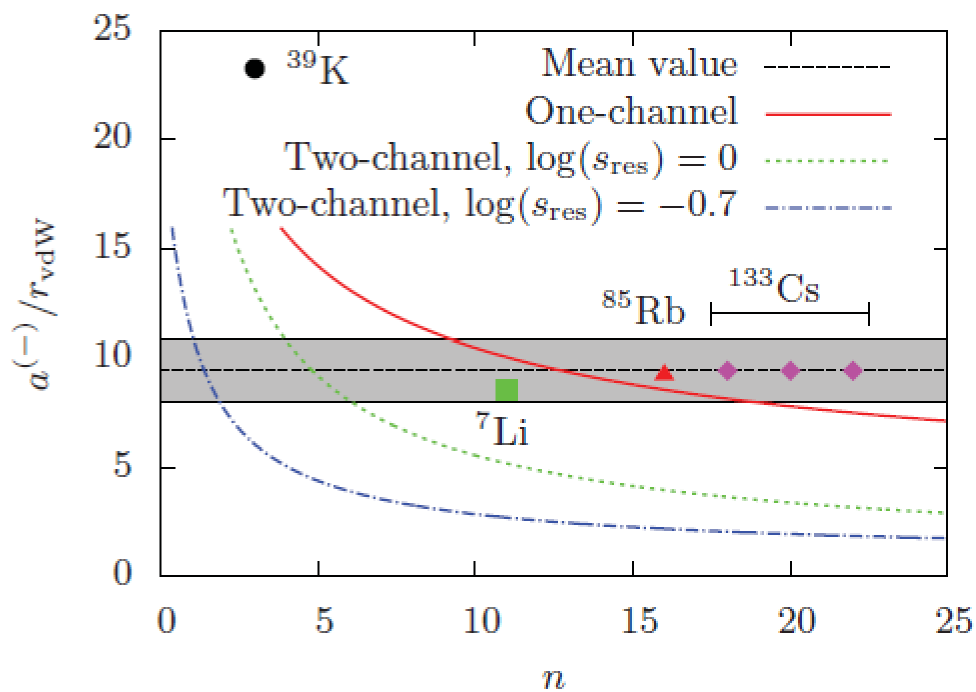
Simple idea: Connect #bound states for Van der Waals plus hard-core to three-body cut-off!

$$\frac{a_-}{r_{\mathrm{vdW}}} = -\frac{2\delta}{\sqrt{(n+\frac{7}{8})\pi}}$$

Atomic two-body potential has a strong hard-core part!





More involved calculations suggest fast convergence to constant value (Naidon *et al.* PRL **112**, 105301 (2014)).

P.K. Sørensen *et al.*, PRA **86**, 052516 (2012)

FURTHER STUDIES

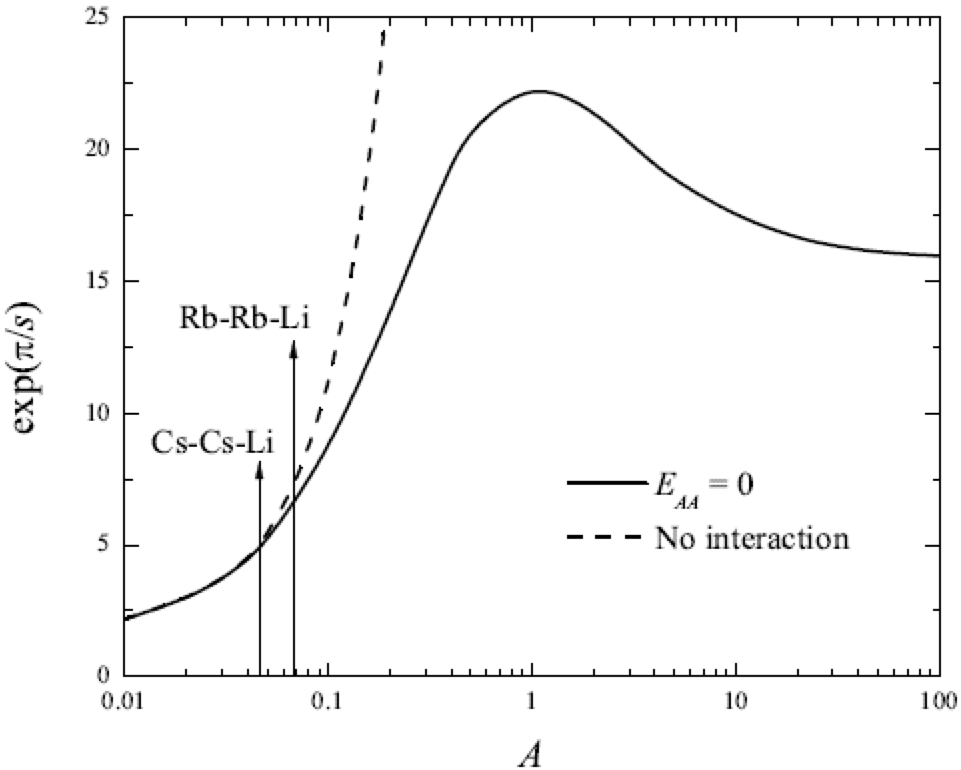
More data needed in the narrow resonance region. Mixtures of different atoms will be very useful in settling these issues!

Momentum-space implementation of multi-parameter zero-range models

Coordinate-space calculations using very accurate molecular potentials from quantum chemistry calculation

MASS IMBALANCED EFIMOV STATES

$$E_n = E_0 \exp\left(-2\pi/s\right)$$



EFIMOV IN TWO DIMENSIONS?

NO Efimov effect in 2D

Mathematical condition for Efimov effect is 2.3<d<3.8

In 2D attractive potential always has bound state $E_2<0$!

For equal mass bosons, two universal states appear: $16.52E_2$ and $1.21E_2$

However, for mass imbalanced systems there can be more than two three-body bound states!

For Cs-Cs-Li in strict 2D geometry, we expect about 4 three-body bound states

F.F. Bellotti *et al.*, JPB **44**, 205302 (2011),
PRA **85**, 025601 (2012), JPB **46**, 055301 (2013)

MOMENTUM SIGNATURES

Equal mass bosons:

$$n(\mathbf{k}) \underset{k\to\infty}{=} \frac{C}{k^4} + \frac{D}{k^5}\cos[2|s_0|\ln(\sqrt{3}k/\kappa_0)+\varphi] + \cdots$$

Castin and Werner, PRA **83**, 063614 (2011)

Braaten, Kang, and Plater, PRL **106**, 153005 (2011)

Mass imbalanced systems:

$$n(\boldsymbol{k}) \to \frac{C(\mathcal{A}))}{k^4} + \frac{D(\mathcal{A})}{k^5} + \frac{E(\mathcal{A})\cos(s\log(k/k^*))}{k^5}$$

If sub-leading momentum tail can be measured, then mass imbalanced three-body signatures are distinct from equal mass case!

M.T. Yamashita *et al.*, PRA **87**, 062702 (2013).

LONG-RANGE INTERACTIONS

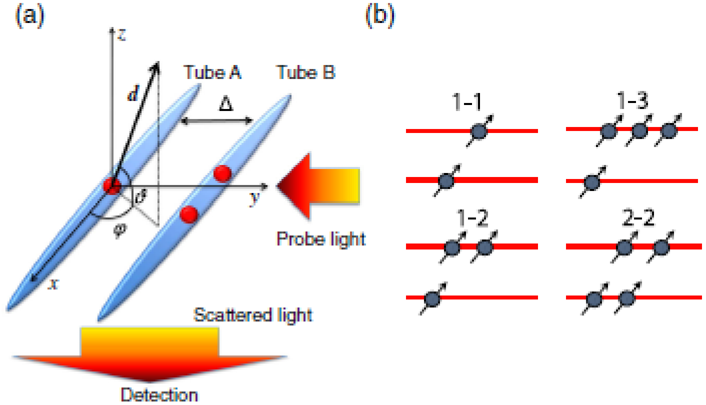
Few-body physics in systems with long-range interactions

DIPOLAR PHYSICS

Few-body physics in 1D tubes

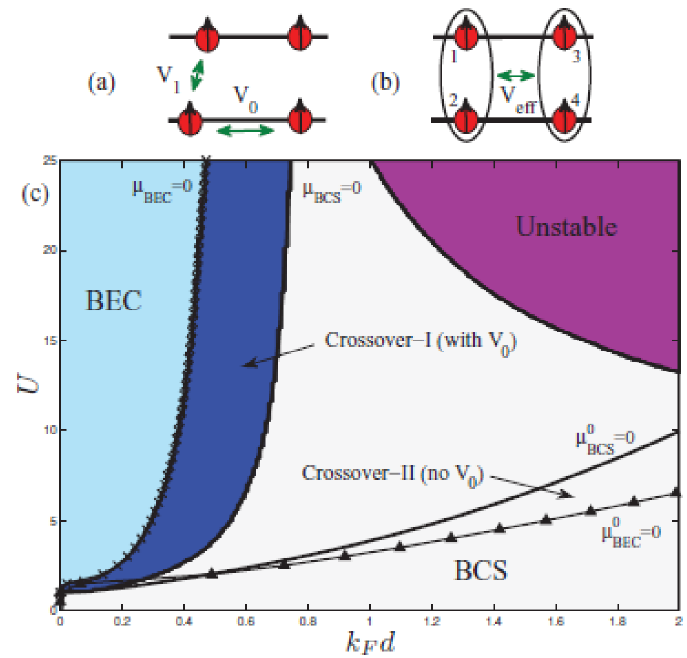
B. Wunsch *et al.*, PRL **107**, 073201 (2011)

N.T. Zinner *et al.*, PRA **84**, 063606 (2011)

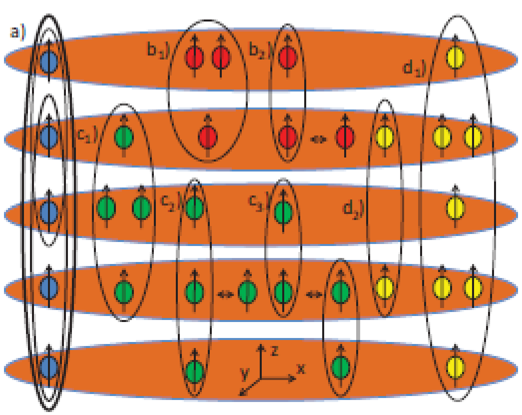


Many-body physics in bilayers

NTZ *et al.*, PRA **85**, 013603 (2012)



Few-body physics in 2D layers



A. G. Volosniev *et al.*, PRL **106**, 250401 (2011)

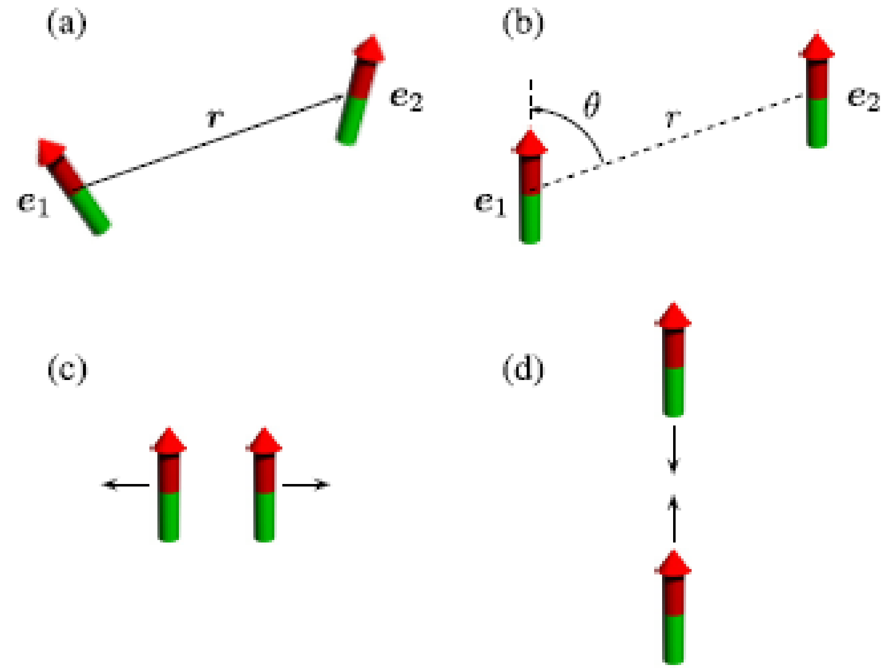
A. G. Volosniev *et al.*, PRA **85**, 023609 (2012)

J. R.. Armstrong *et al.*, EPJD **66**, 85 (2012)

(ULTRA)COLD POLAR MOLECULES

Polar Molecules are interesting due to anisotropic long-range potentials. Novel degenerate quantum states are expected already for weak coupling strength. Even more so for strong interactions.

Controllability is expected to be as good as for non-polar atoms and molecules that are the workhorses of ultracold atomic gas physics.



Drawback is the instability in the head-to-tail configuration that leads to very short lifetimes of the samples.

Solutions proposed are to use fermions and low-dimensionality to minimize overlap and maximize lifetime.

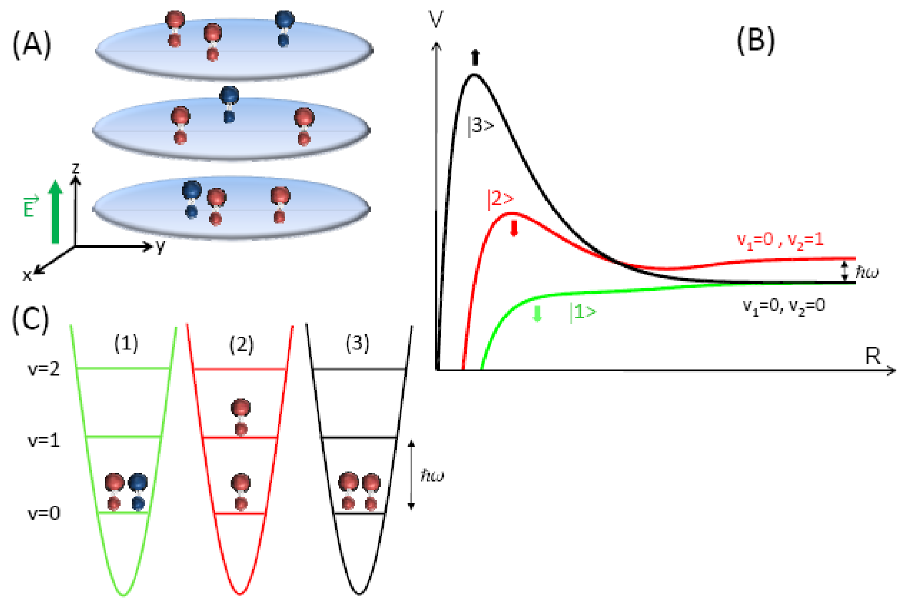
LAYERS WITH DIPOLAR FERMIONS

Jin and Ye groups at JILA

Science 327, 853 (2010)

Nature 464, 1324 (2010)

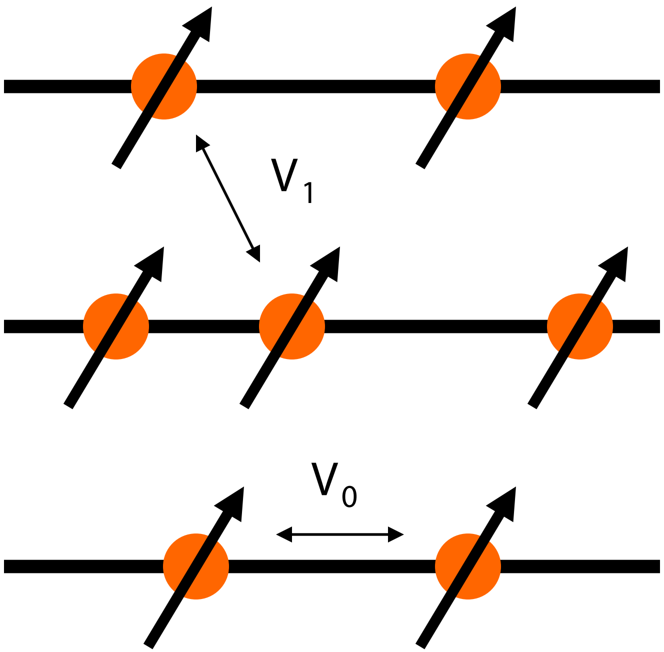
Potassium-Rubidium molecules



Miranda *et al.*, Nature Phys. **7**, 502 (2011)

New results on controlled chemistry through measurements of the sample lifetimes. Single-species fermions in layers have lifetimes of seconds.

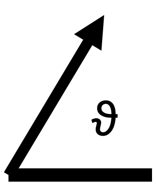
LAYERED SYSTEMS



Single-species fermions confined to (quasi)-2D layers with long-range interactions.

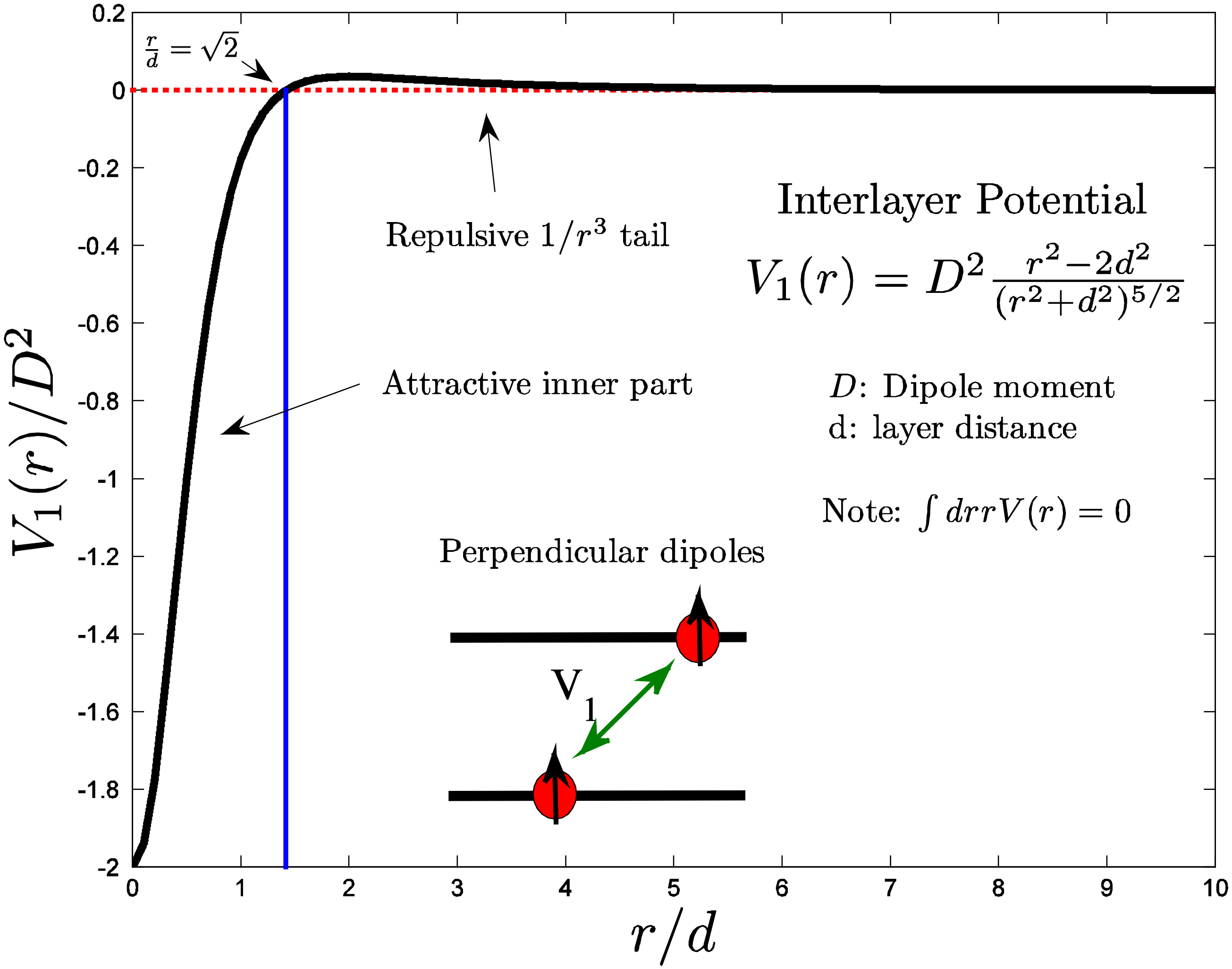
Intralayer interaction within the same layer is repulsive at long distance above ϑ=35°

Interlayer interaction between layers has both attractive and repulsive parts.

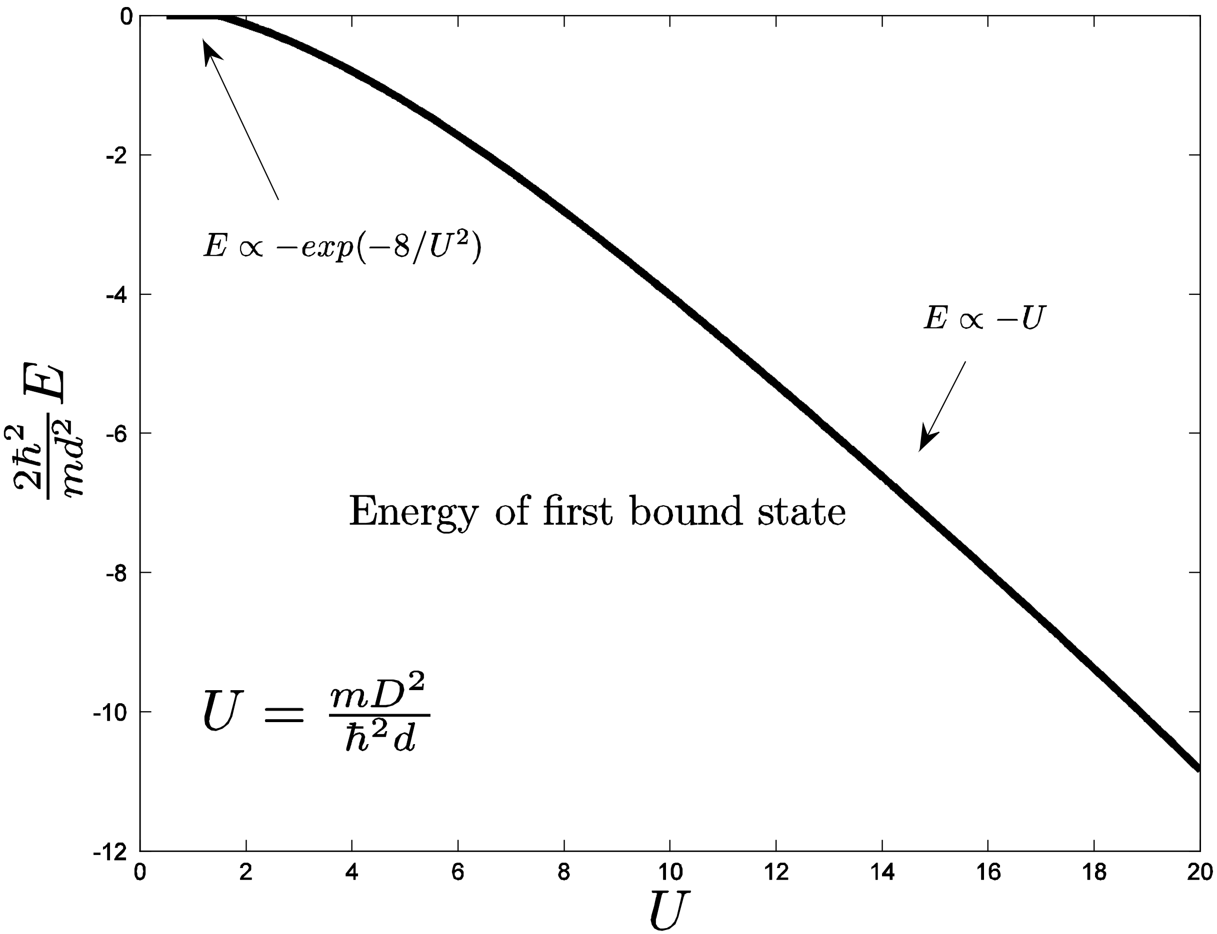


Interesting competition as function of dipole strength and density.

BILAYER WITH PERPENDICULAR DIPOLES



BILAYER WITH PERPENDICULAR DIPOLES

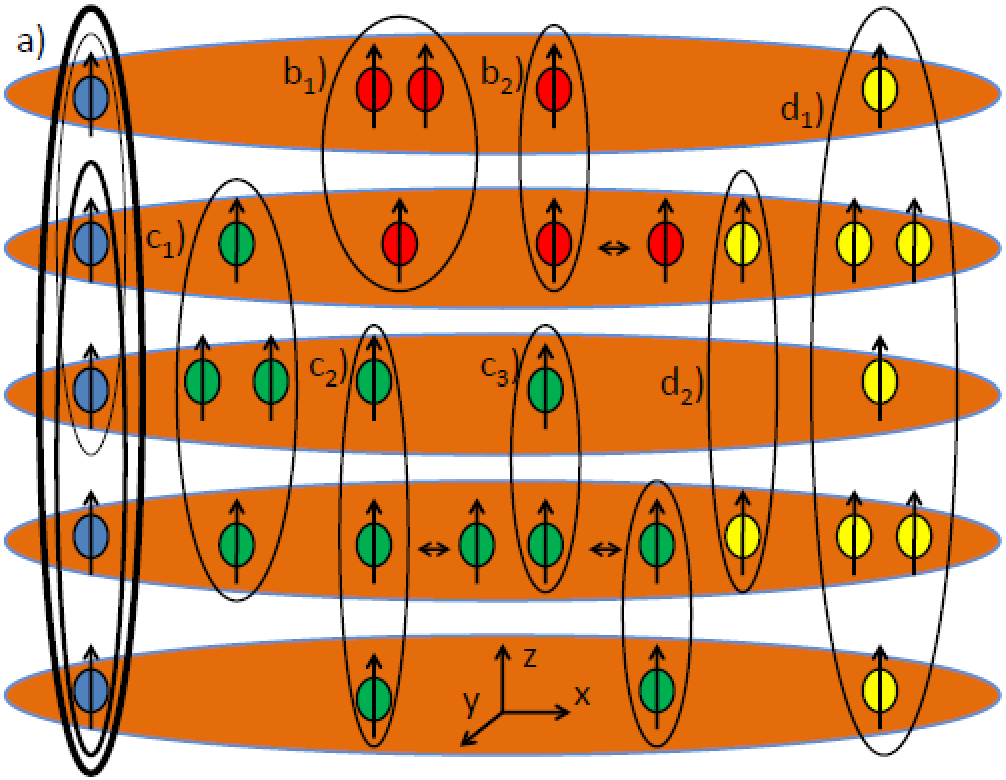


Shih and Wang, PRA **79**, 065603 (2009).

Armstrong *et al.*, EPL **91**, 16001 (2010).

Klawunn et al., PRA **82**, 044701 (2010).

BILAYER WITH PERPENDICULAR DIPOLES



A. G. Volosniev *et al.*, PRL **106**, 250401 (2011)

A. G. Volosniev *et al.*, PRA **85**, 023609 (2012)

J. R.. Armstrong *et al.*, EPJD **66**, 85 (2012)

See also D.S. Petrov PRL **112**, 103201 (2014)

Complexes with three or four particles in a bilayered are unlikely to be bound. Larger chains can be formed and stabilize more complicated complexes.

BILAYER AND MANY-BODY PHYSICS

Solve many-body problem for the bilayer with perpendicular polarization using BCS theory for s-wave part of interlayer interaction.

$$\Delta_k = -\frac{1}{V}\sum_q V_1(k-q)\frac{\Delta_q}{2E_q}\tanh\left(\frac{E_q}{2k_BT}\right)$$

Interested in stronger coupling and crossover so solve the self-consistent equations including the chemical potential.

$$n = \frac{1}{2V}\sum_k\left[1-\frac{\xi_k}{E_k}\tanh\left(\frac{E_k}{2k_BT}\right)\right]$$

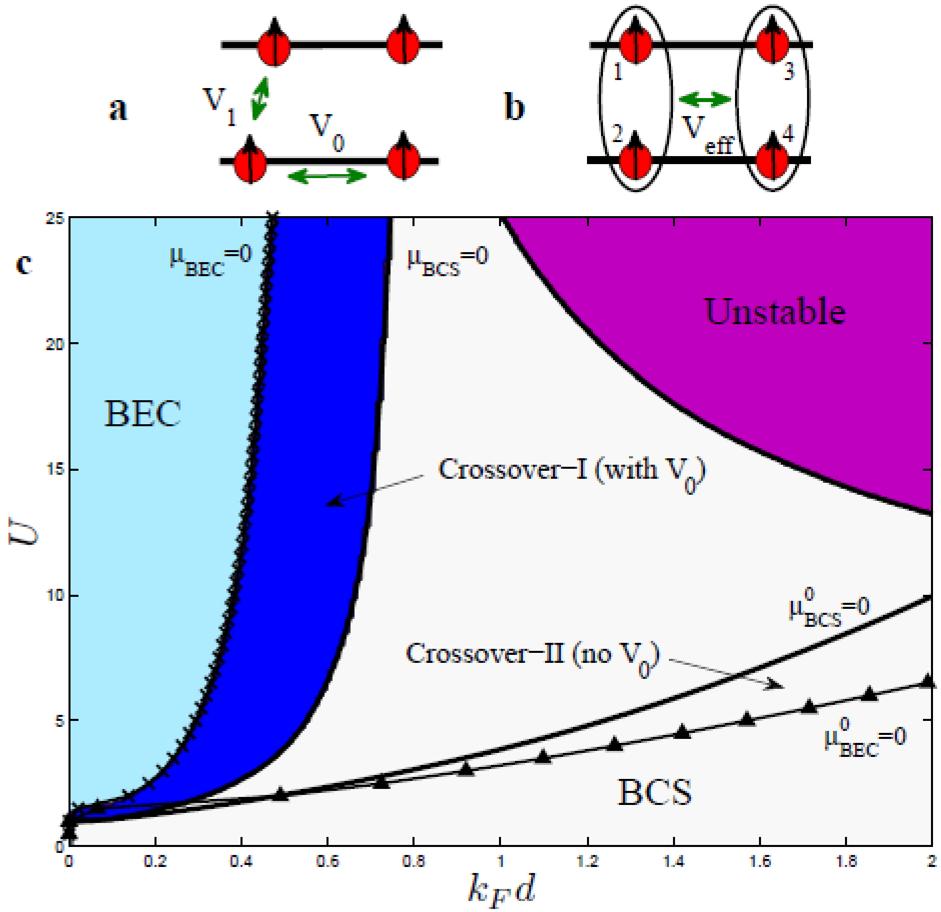
$$\xi_k = \varepsilon_k - \Sigma_k - \mu$$

Include the INTRA-layer term in the self-energy in a self-consistent Hartree-Fock manner.

$$\Sigma_k = \frac{1}{2V}\sum_q\left(V_0(0)-V_0(k-q)\right)\left[1-\frac{\xi_q}{E_q}\tanh\left(\frac{E_q}{2k_BT}\right)\right]$$

In weak-coupling limit it makes little difference, at stronger coupling it changes the position of the crossover from BCS to BEC behavior significantly.

BILAYER AND MANY-BODY PHYSICS



Crossover from BCS to BEC behavior including both attractive and repulsive interactions.

Presence of bilayer dimer bound states defines three lines in the phase diagram:

1) Binding energy equal to Fermi energy

$$\mu^0_{BEC} = E_F - \frac{E_B}{2} = 0$$

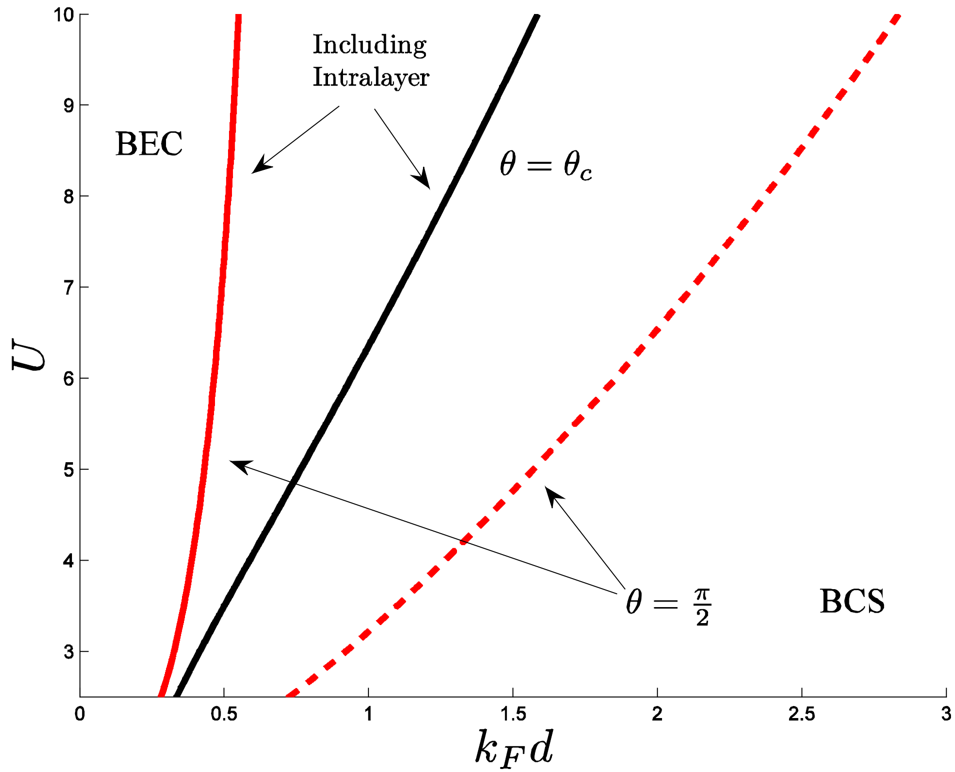
2) Chemical potential of dimer gas vanishes

$$\mu_{BEC} = \frac{1}{2} n V_{eff}(0) + E_F - \frac{E_B}{2} = 0$$

3) Onset of roton instablity

NTZ *et al.*, PRA **85**, 013603 (2012)

NON-PERPENDICULAR DIPOLES



Lines of vanishing chemical potential in the strong-coupling limit.

At ϑ_c the intralayer term is zero in the long-wavelength limit. Thus, there is only one line!

The region of (quasi)-BEC is enlarged compared to $\vartheta=\pi/2$.

Below ϑ_c there is collapse in a single layer already.

Many-body problem: Symmetry of the pairing order parameter should be connected to the structure of the potential and the bound states it allows.

A.G. Volosniev *et al.*, JPB **44**, 125301 (2011)

MESSING WITH 2D QUANTUM GASES

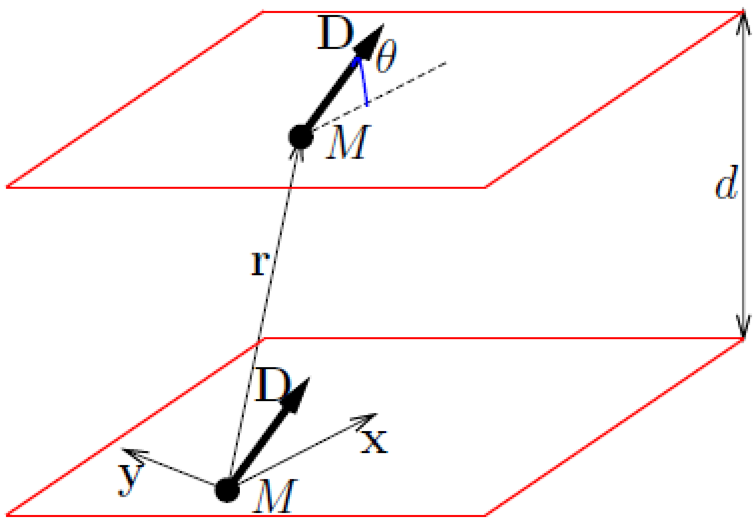
2D quantum gases typically always hold a two-body bound state which is important for many-body physics

Study the system by a maximal disturbance

Get rid of the two-body bound state!

Hard to achieve with normal non-polar atoms but possible with polar molecules!

POLAR MOLECULES IN 2D LAYERS



Interaction is long-range and anisotropic for general ϑ

External electric field aligns the molecules

Peculiar property of the potential:

$$\int d^2 r V(r) = 0$$

Two-body bound state exists for any dipole moment!

J.R. Armstrong *et al.*, EPL **91**, 16001 (2010)
A.G. Volosniev *et al.*, PRL **106**, 250401 (2011)
A.G. Volosniev *et al.*, J. Phys. B **44**, 125301 (2011)

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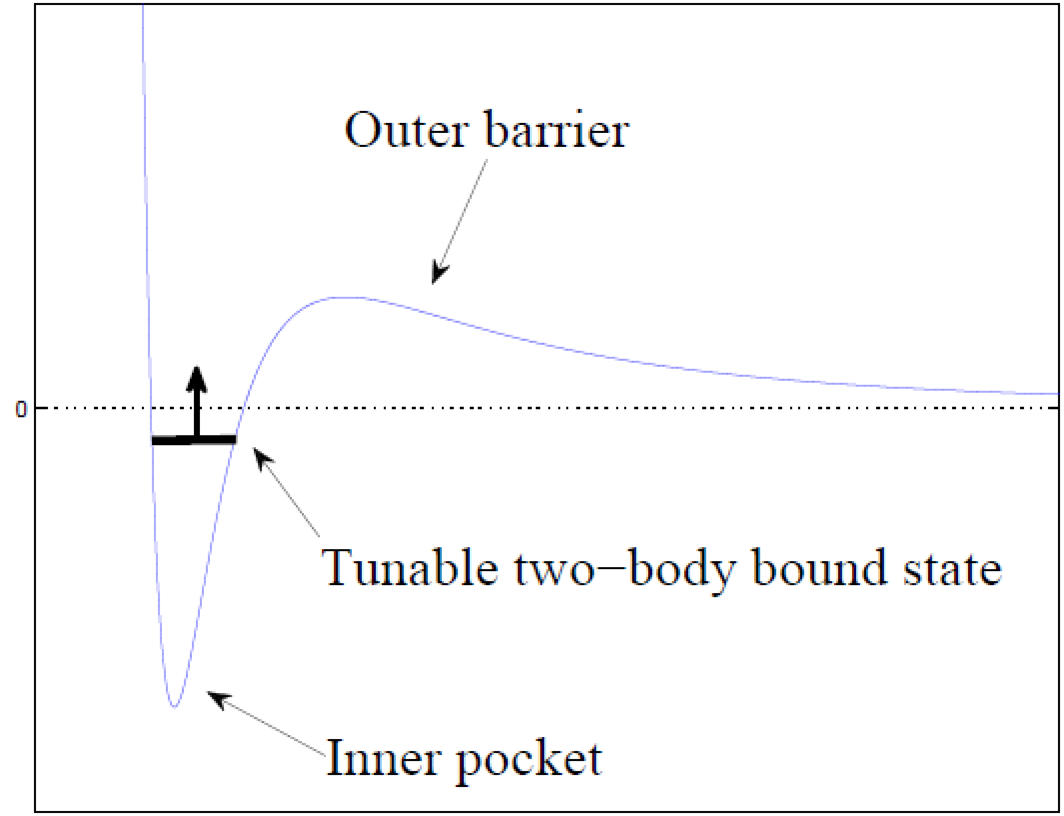
EXTERNAL FIELD MANIPULATION

Use external DC and AC fields to tune dipole-dipole potential

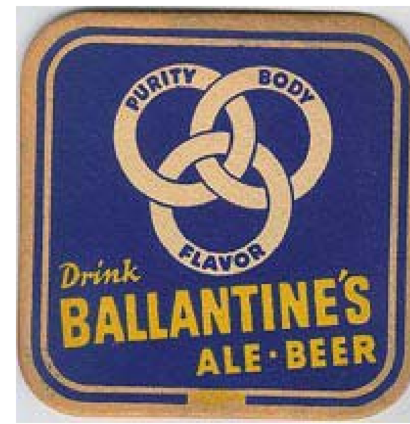


A. Micheli *et al.*, Phys. Rev. A **76,** 043604 (2007)

NEW GROUND STATE

Assume no two-body bound state

For three bosonic polar molecules there will be a bound **three-body** state
A Borromean system!



Two-component fermionic molecules are more complicated due to the Pauli principle

The many-body physics should be controlled by the three-body bound state. A **trion** quantum gas!

S.-J. Huang *et al.*, Phys. Rev. A **85**, 055601 (2012)

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Thank you for your attention