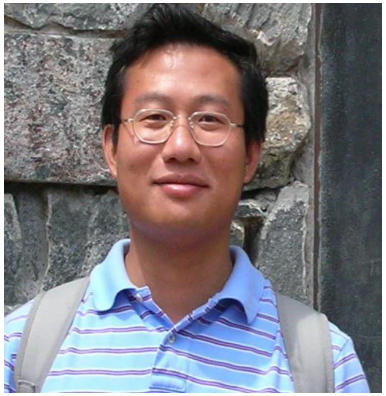
Virial Expansion for a strongly correlated Fermi gas

Xia-Ji Liu

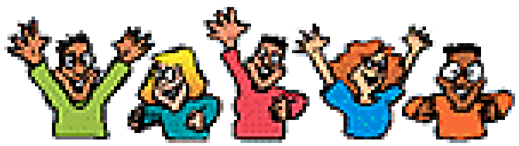
CQOS, Swinburne University

KITP, November 2016

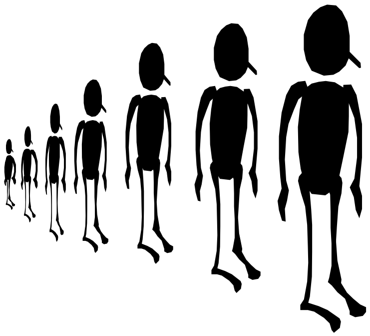
Universality Few-Body System Program

There are two kinds of particles in the world: fermions and bosons

Fermions: half-integral spin electrons, protons, neutrons, 2H, 6Li,… are forbidden by the Pauli exclusion principle to have more than two of the same type in the same state. They are the "loners" of the quantum world. If electrons were not fermions, we would not have chemistry. Fermion obey the rules of Fermi-Dirac statistics.



Bosons: integral spin photons, 1H, 7Li, 23Na, 87Rb, 133Cs,… love to be in the same state. They are the joiners of the quantum world. If photons were not bosons, we would not have lasers. Bosons obey the rules of Bose-Einstein statistics.



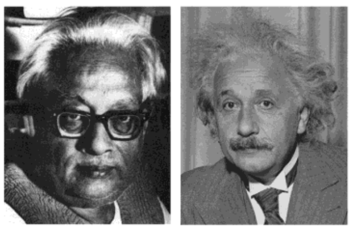
SWINBURNE UNIVERSITY OF TECHNOLOGY

Bose-Einstein Condensation & Quantum Degeneracy

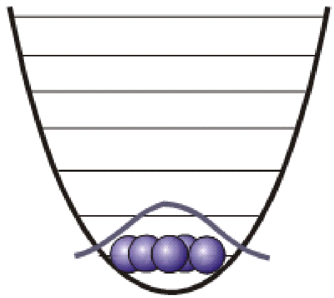
Boson: integer spin

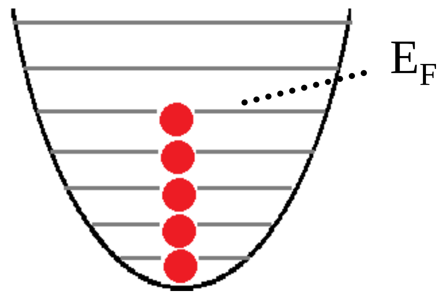
Fermion: half-integer spin

Bose-Einstein condensation * 1925



Satyendra Nath Bose　Albert Einstein





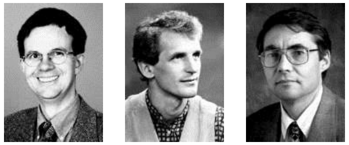
Fermi-Dirac Distribution *1926

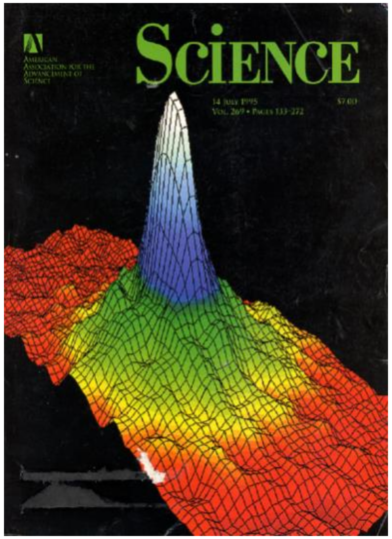
Paul Dirac　Enrico Fermi

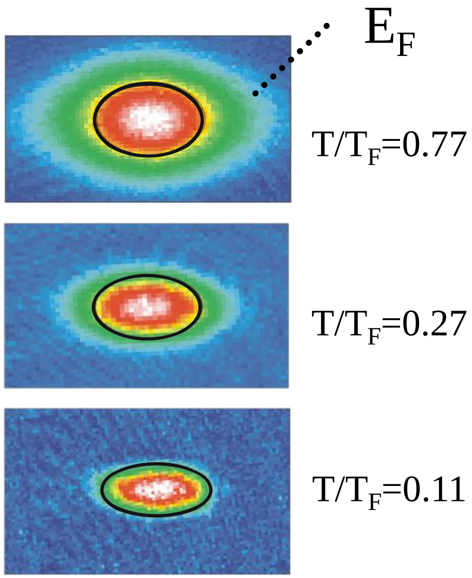
Bose-Einstein distribution

$$n(\varepsilon) = \frac{1}{e^{\beta(\varepsilon-\mu)} - 1}$$

2001 Nobel Prize: BEC







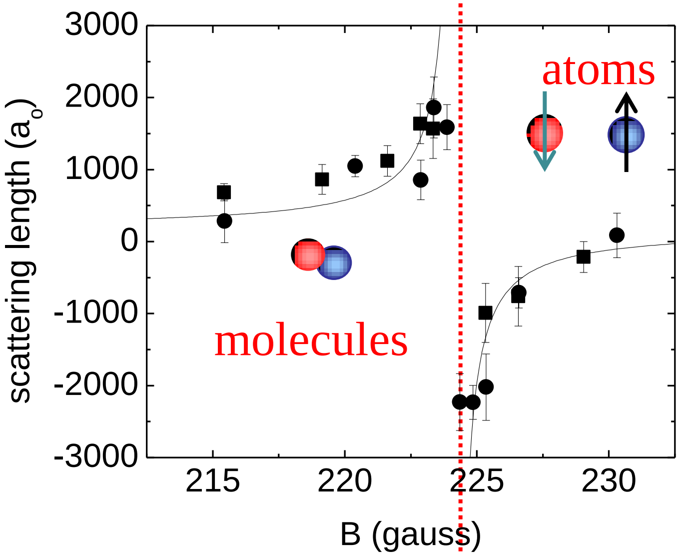
Fermi-Dirac distribution

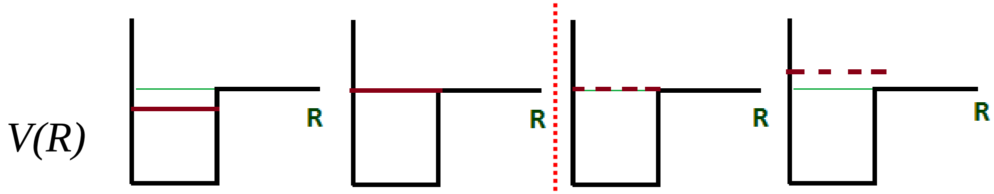
$$n(\varepsilon) = \frac{1}{e^{\beta(\varepsilon-\mu)} + 1} \qquad \beta = \frac{1}{k_B T}$$

D. Jin 1999

Ultracold Fermion Collision (S-Wave)

Magnetic-field Feshbach resonance



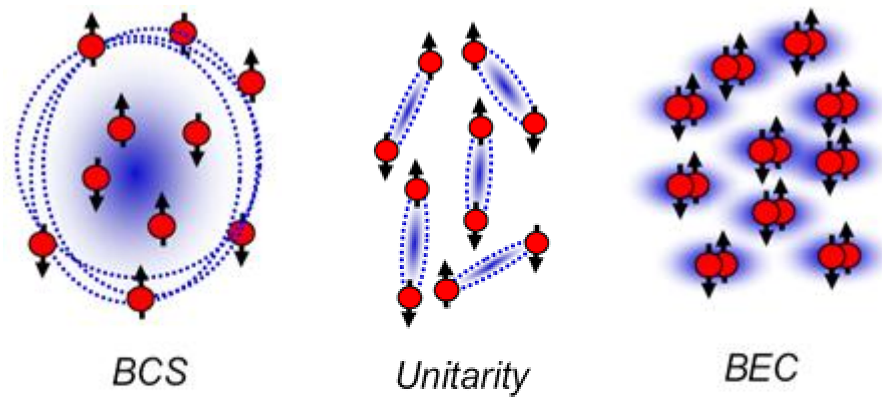


a>0, repulsive

a<0, attractive

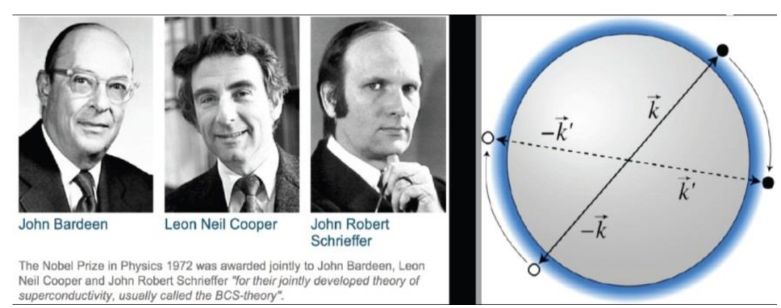
Unitary limit

BEC-BCS crossover

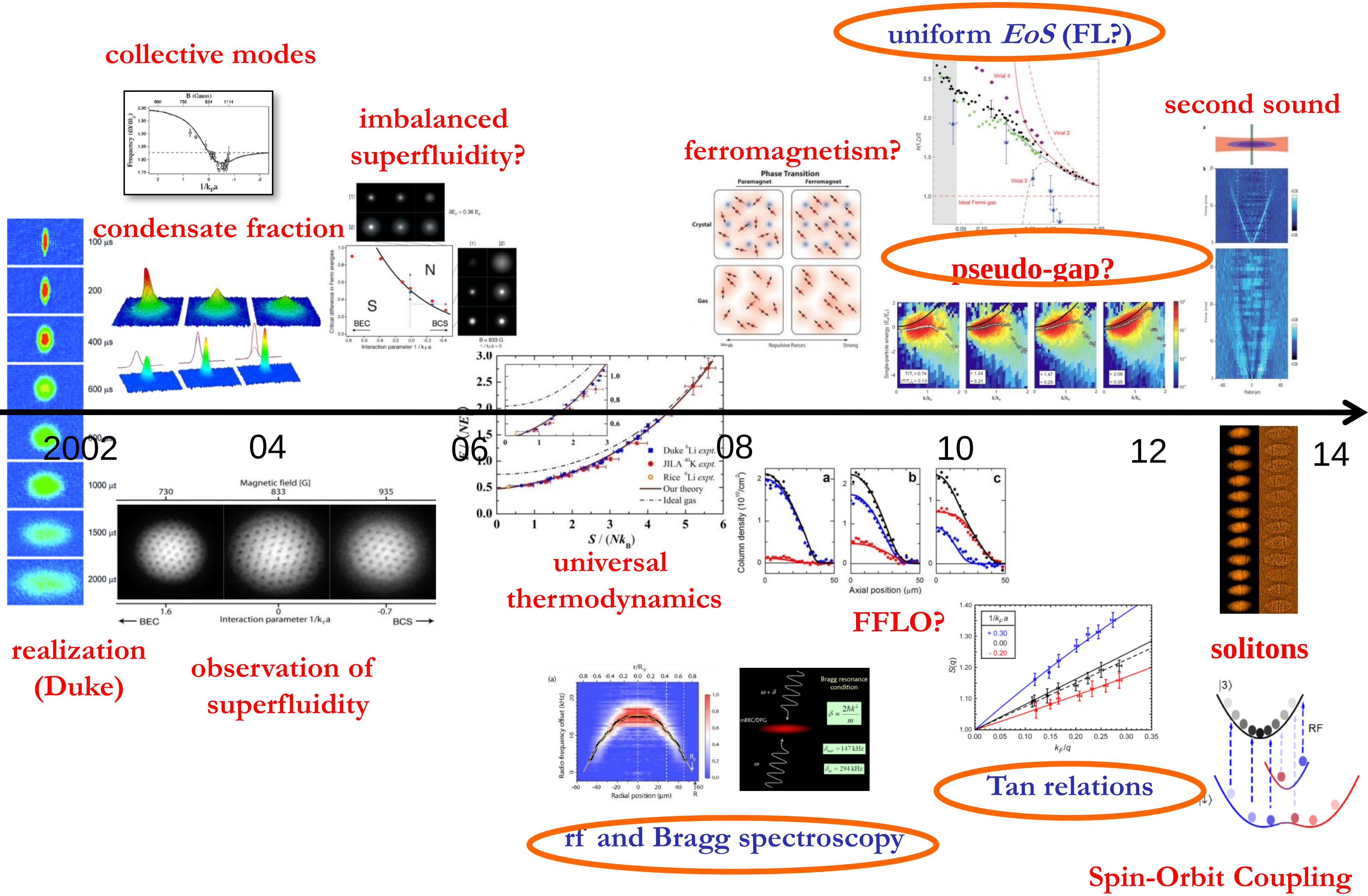


BCS fermionic superfluidity

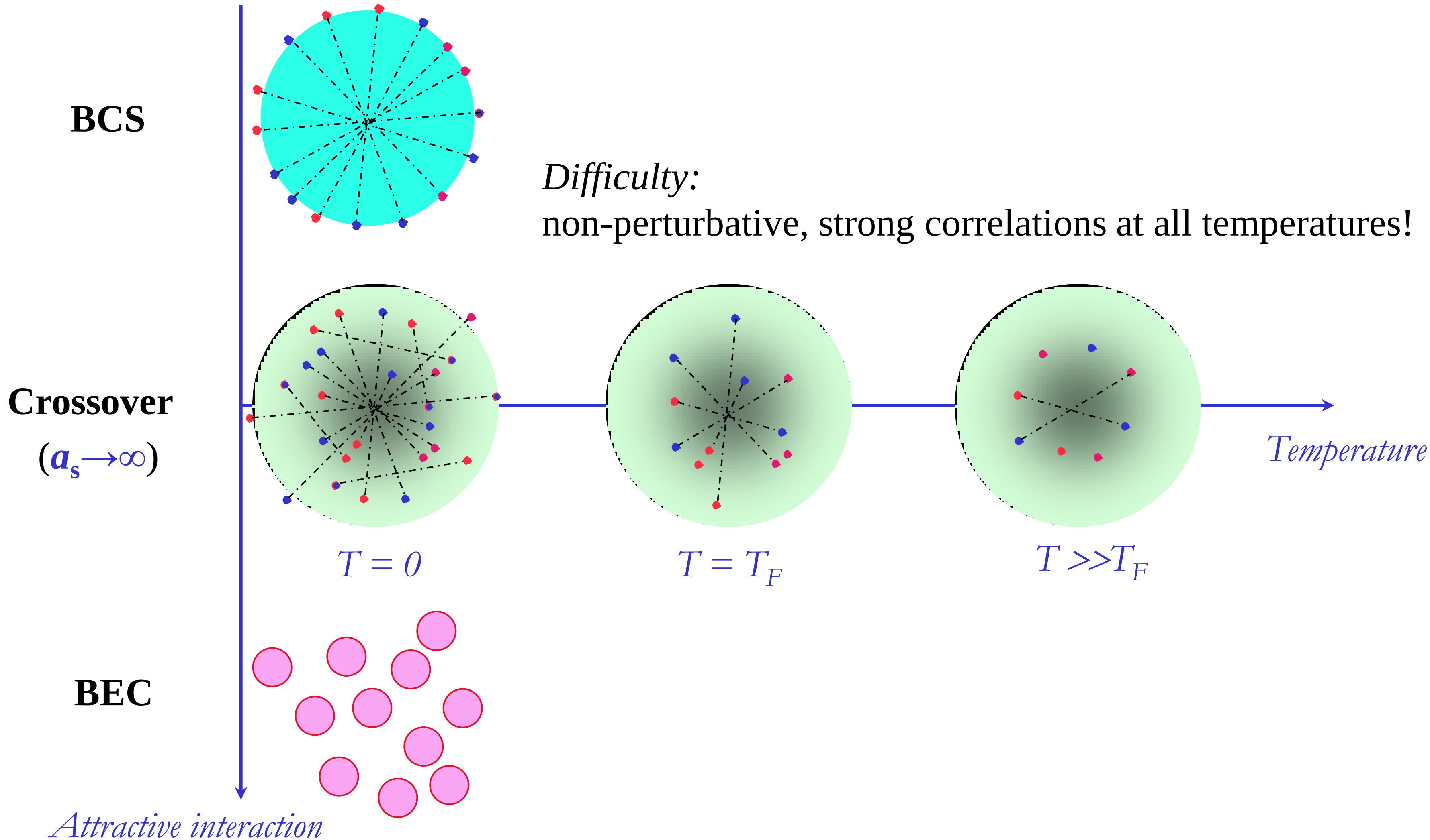
BEC of molecules



Global progress (experiment)



Challenging many-body problem



Difficulty:
non-perturbative, strong correlations at all temperatures!

Global progress (theory)

1D exact solutions

Mean field

Large-*N*, ε-expansion, RG?

***T*-matrix approximation?** **Tan relations!** **Operator product expansion?**

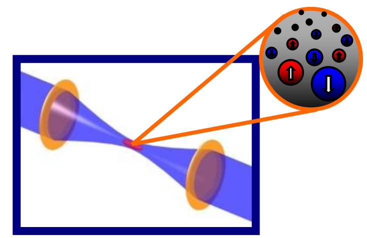
2002 04 06 08 10 12

Quantum Monte Carlo? **Virial expansion**

Few-body solutions

Color: Black (tried, experienced), blue (to be tried), red (interested)

Outline



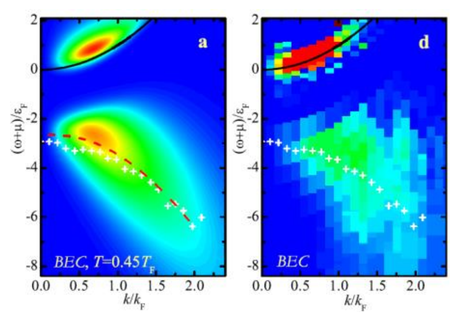
- Virial expansion: A traditional but "new" method

- Few-particle exact solutions as the input to virial expansion

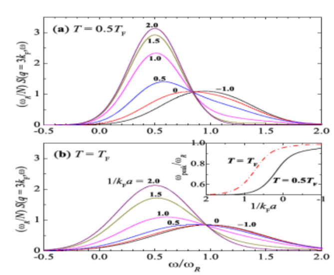
- Virial expansion: Applications

$$\boxed{b_3 = (Q_3 - Q_1 Q_2 + \frac{1}{3} Q_1^3), \ldots}$$

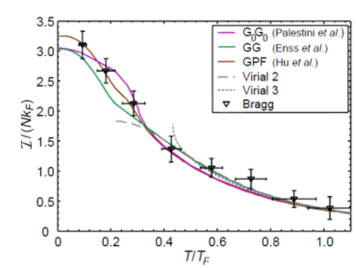
Equation of State



SP Spectral Function



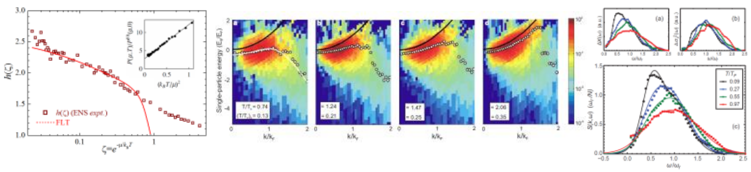
Dynamic Structure Factor



Tan's Contact

- Conclusions and outlooks

BEC-BCS crossover: (theoretical challenge)



☺MB physics
at high T:
Virial expansion

Few-particle
solutions

Bridge?

Many-Body physics:
☹ *No* small interaction
parameter!

☺MB physics
at short-range:
Tan relations

Blume, Daily, Stecher, Greene;
Busch, Englert, Rzazewski, Wilkens;
Werner, Castin;
Kestner, Duan;
Julienne, Bohn, Tiesinga;
……

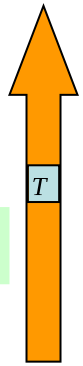
$i.e., \Delta S(q,\omega) \approx W(q,\omega) C$

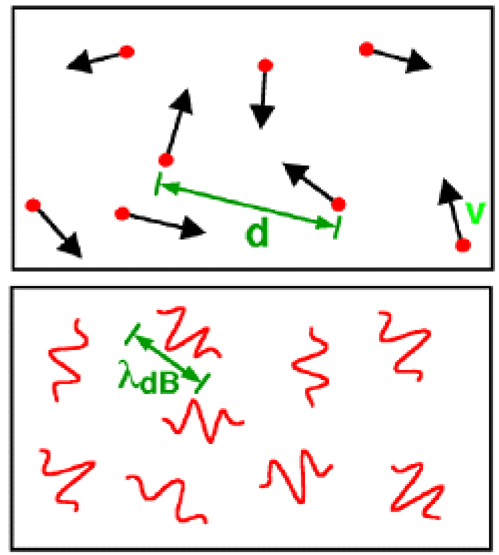
Virial expansion:
A traditional but “new” method

ABC of virial expansion (VE)

Classical Particles

Thermal fluctuation





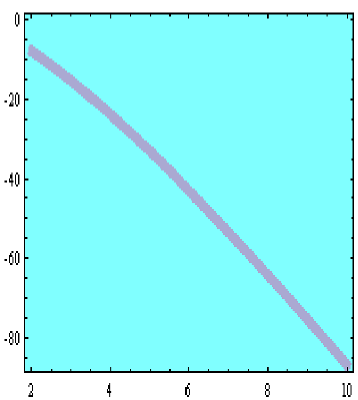
High Temperature

"Billiard balls"

Low Temperature

"Wave packets"

$\frac{\mu}{E_F}$



$\frac{T}{T_F}$

$$\mu(T, N) = -k_B T \ln\left[6\left(\frac{k_B T}{E_F}\right)^3\right]$$

$$\mu \rightarrow -\infty$$

The fugacity $z = \exp\left(\mu / k_B T\right) << 1$

ABC of virial expansion (VE)

Thermodynamic potential

$$\Omega(T, V, \mu) = -k_B T \ln Z_G$$

$$Z_G = Tr\left(e^{-\beta(H_0 - \mu N)}\right)$$

$$Z_G = \sum_N \sum_j e^{-\beta(E_j - \mu N)}$$

$$Z_G = 1 + \underbrace{zQ_1 + z^2 Q_2 + z^3 Q_3 \cdots}_{x}$$

z: *The fugacity*

***N*-cluster partition function:**

$$Q_N = Tr_N[\exp(-\beta H_N)]$$

$$\boxed{\ln(1+x) = x - \frac{x^2}{2} + \frac{x^3}{3} + \cdots}$$

$$|x| < 1$$

$$\Omega = -k_B T Q_1 \left(z + b_2 z^2 + b_3 z^3 + \cdots + b_n z^n + \cdots\right)$$

Virial Coefficients

$$b_2 = (Q_2 - \frac{1}{2}Q_1^2)/Q_1, \qquad b_3 = (Q_3 - Q_1 Q_2 + \frac{1}{3}Q_1^3), \qquad b_4 = \ldots$$

To obtain b_n, just solve a "n-body" problem and find out the energy levels !

b_2: T.-L. Ho & E. J. Mueller, *PRL* **92**, 160404 (2005).
b_3: Liu, HH & Drummond, *PRL* **102**, 160401 (2009); *PRA* **82**, 023619 (2010).

ABC of virial expansion (VE)

Numerically, we calculate $\boxed{\Delta b_n = b_n - b_n^{(1)}}$ **for a trapped gas!**

***n*-th virial coefficient of a non-interacting Fermi gas**

What's new here?

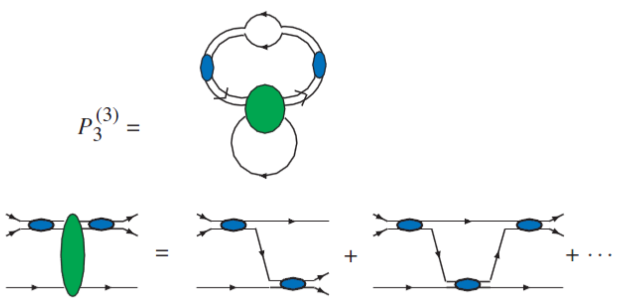
For a homogeneous system, where the energy level is continuous, it seems impossible to calculate directly virial coefficient using N-cluster partition function, *i.e.*, $b_3 = (Q_3 - Q_1 Q_2 + \frac{1}{3} Q_1^3), \ldots$

For the second virial coefficient, Beth & Uhlenbeck (1937):

$$\frac{\Delta b_2}{\sqrt{2}} = \sum_i \mathrm{e}^{-E_b^i/(k_B T)} + \frac{1}{\pi}\int_0^\infty \mathrm{d}k \frac{\mathrm{d}\delta_0}{\mathrm{d}k} \mathrm{e}^{-\lambda^2 k^2/(2\pi)}$$

δ_0: s-wave phase shift;
λ: de Broglie wavelength.

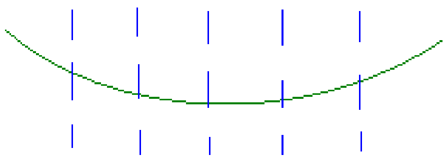
For the third coefficient, complicated diagrammatic calculations [Rupak, *PRL* **98**, 090403 (2007)] :



leads to, $\Delta b_3(\mathrm{Rupak}) \approx 1.05$ (incorrect ☹)

The harmonic trap helps! The discrete energy level helps to calculate the *N*-cluster partition function.

How to obtain homogeneous virial coefficient?



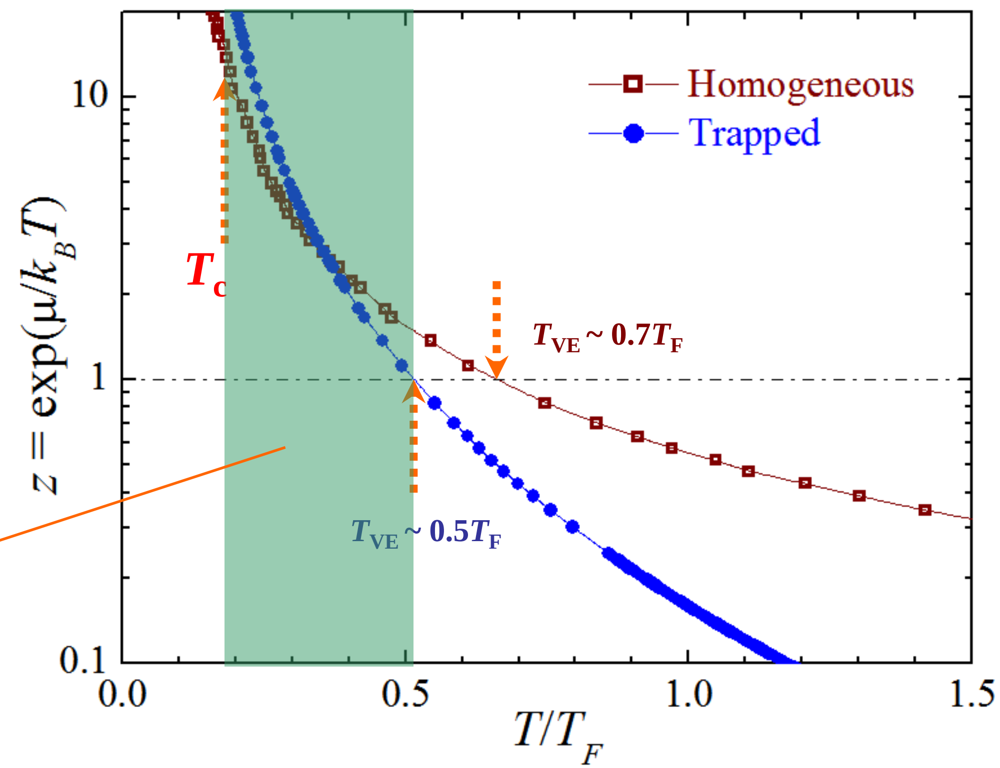
Let us consider the *unitarity* limit and use **LDA** **[μ(r) = μ - *V*(r)],**

$$\Omega_{trap} \propto \sum_{n=1} b_{n,T} z^n \overset{\textbf{LDA}}{\propto} \int d\mathbf{r} \sum_{n=1} b_{n,H} z^n(\mathbf{r}) = \int d\mathbf{r} \sum_{n=1} b_{n,H} z^n \exp[-n\beta V(\mathbf{r})]$$

$$\boxed{b_{n,T}(\mathrm{trap}) = \left[\frac{1}{n^{3/2}}\right] b_{n,H}(\mathrm{homogeneous})}$$

Liu, HH & Drummond, *PRL* **102**, 160401 (2009); *PRA* **82**, 023619 (2010).

Validity of virial expansion? (unitarity case)



Non-trivial re-summation of virial expansion terms? *i.e.*, *Páde* approximation?

Unitary ***z*(*T*)** from the ENS data; *see*, HH, Liu & Drummond, *New. J. Phys.* **12**, 063038 (2010).

Virial expansion of single-particle spectral function

$$G_{\sigma\sigma'}\left(\mathbf{r},\mathbf{r}';\tau\right) = -\exp\left[\mu\tau\right]\frac{1}{\mathcal{Z}}\mathrm{Tr}\left[z^{\mathcal{N}}e^{-\beta\mathcal{H}}e^{\tau\mathcal{H}}\hat{\Psi}_{\sigma}\left(\mathbf{r}\right)e^{-\tau\mathcal{H}}\hat{\Psi}^{+}_{\sigma'}\left(\mathbf{r}'\right)\right]$$

$$= A_1 + z\left(A_2 - A_1 Q_1\right) + \cdots,$$

virial expansion functions:

$$A_N = -\exp\left[\mu\tau\right]\mathrm{Tr}_{N-1}\left[e^{-\beta\mathcal{H}}e^{\tau\mathcal{H}}\hat{\Psi}_{\sigma}\left(\mathbf{r}\right)e^{-\tau\mathcal{H}}\hat{\Psi}^{+}_{\sigma'}\left(\mathbf{r}'\right)\right]$$

To obtain A_n, solve a "*n*-body" problem and the wave functions!

HH, Liu, Drummond & Dong, *PRL* **104**, 240407 (2010).

Sun and Leyronas PRA 92, 053611 (2015) calculated 3rd order spectral function

Quantum virial expansion of DSF

VE for dynamic susceptibility:

$$\chi_{\sigma\sigma'} \equiv -\frac{\mathrm{Tr}\left[e^{-\beta(\mathcal{H}-\mu\mathcal{N})}e^{\mathcal{H}\tau}\hat{n}_{\sigma}(\mathbf{r})\,e^{-\mathcal{H}\tau}\hat{n}_{\sigma'}(\mathbf{r}')\right]}{\mathrm{Tr}e^{-\beta(\mathcal{H}-\mu\mathcal{N})}}$$

$$\chi_{\sigma\sigma'}(\mathbf{r},\mathbf{r}';\tau) = zX_1 + z^2(X_2 - X_1Q_1) + \cdots$$

virial expansion functions: $X_n = -\,\mathrm{Tr}_n[e^{-\beta\mathcal{H}}e^{\tau\mathcal{H}}\hat{n}_{\sigma}(\mathbf{r})e^{-\tau\mathcal{H}}\hat{n}_{\sigma'}(\mathbf{r}')]$

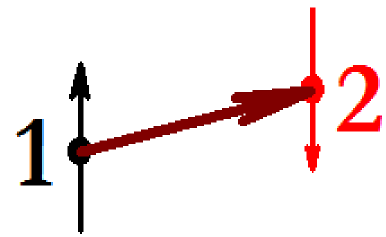
Finally, we use $S_{\sigma\sigma'}(\mathbf{r},\mathbf{r}';\omega) = -\frac{\mathrm{Im}\,\chi_{\sigma\sigma'}(\mathbf{r},\mathbf{r}';i\omega_n \to \omega + i0^+)}{\pi(1-e^{-\beta\omega})}$

HH, Liu, & Drummond, *PRA* **81**, 033630 (2010).

Few-particle exact solutions: As the input to virial expansion

Blume, Daily, Stecher, Greene;
Busch, Englert, Rzazewski, Wilkens;
Werner, Castin;
Kestner, Duan;
Julienne, Bohn, Tiesinga;
……

Two-particle problem in harmonic traps



CM motion: $\left[-\frac{\hbar^2}{2M}\Delta_{\vec{C}} + \frac{1}{2}M\omega^2 C^2\right]\psi_{\rm CM}(\vec{C}) = E_{\rm CM}\psi_{\rm CM}(\vec{C}),\ \boxed{E_{\rm CM} \in (\tfrac{3}{2}+\mathbb{N})\hbar\omega}$

Relative motion: $\left[-\frac{\hbar^2}{2\mu}\nabla^2_{\mathbf{r}} + \frac{1}{2}\mu\omega^2 r^2\right]\psi^{\rm rel}_{2b}(\mathbf{r}) = E_{\rm rel}\psi^{\rm rel}_{2b}(\mathbf{r}),\ \boxed{\psi^{\rm rel}_{2b}(r) \to (1/r - 1/a)}$ **BP** condition

The solution:

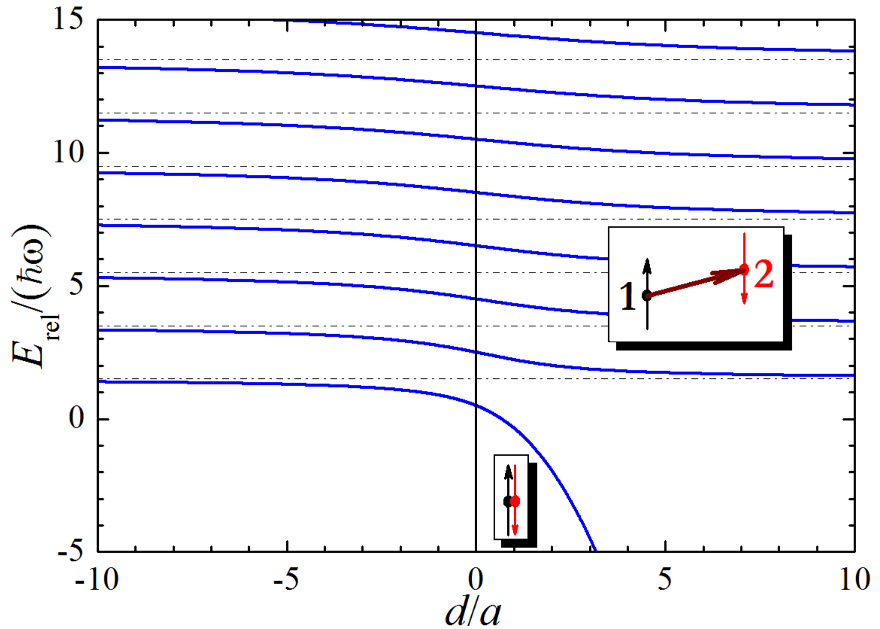
$$\psi^{\rm rel}_{2b}(r;\nu) = \Gamma(-\nu)U\left(-\nu, \frac{3}{2}, \frac{r^2}{d^2}\right)\exp\left(-\frac{r^2}{2d^2}\right)$$

U is the second Kummer function

$E_{\rm rel} = \left(2\nu + \frac{3}{2}\right)\hbar\omega$ is determined from the BP condition

See, Busch *et al.*, *Found. Phys.* (1998)

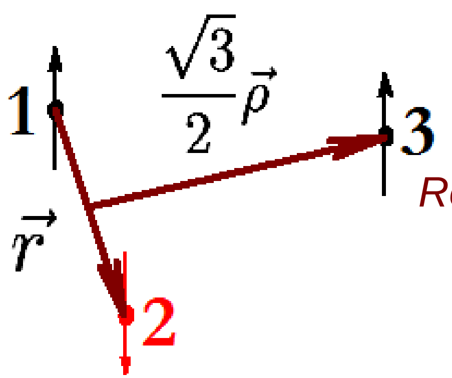
Two-particle problem in harmonic traps



Analytic result is known at unitarity: $E_{\rm rel} = \left(2n + \frac{1}{2}\right)\hbar\omega, \;\; n \in \mathbb{N}.$ [*See*, Busch *et al.*, *Found. Phys.* (1998)]

$$b_2 - b_2^{(1)} = (Q_2 - Q_2^{(1)})/Q_1 = \frac{1}{2}\left[\sum_n \exp(-\beta E_{rel,n}) - \sum_n \exp(-\beta E_{rel,n}^{(1)})\right] = \left(\frac{1}{4}\right)\frac{2\exp(-\beta\hbar\omega/2)}{1+\exp(-\beta\hbar\omega)},$$

Three-particle problem in harmonic traps



CM motion: $\left[-\frac{\hbar^2}{2M}\Delta_{\vec{C}} + \frac{1}{2}M\omega^2C^2\right]\psi_{\mathrm{CM}}(\vec{C}) = E_{\mathrm{CM}}\psi_{\mathrm{CM}}(\vec{C}),\ \boxed{E_{\mathrm{CM}} \in (\tfrac{3}{2}+\mathbb{N})\hbar\omega}$

Relative motion: $\left[-\frac{\hbar^2}{m}\left(\Delta_{\vec{r}} + \Delta_{\vec{\rho}}\right) + \frac{1}{4}m\omega^2(r^2+\rho^2)\right]\psi(\vec{r},\vec{\rho}) = E\,\psi(\vec{r},\vec{\rho})$

BP condition: $\psi(\vec{r},\vec{\rho}) \underset{r\to 0}{=} \left(\frac{1}{r} - \frac{1}{a}\right)A(\vec{\rho}) + O(r)$

In general: $\boxed{\psi(\vec{r},\vec{\rho}) = (\hat{\mathbf{1}} - \hat{\mathbf{P}}_{13})\sum_n a_n \phi_{nl}(\rho)Y_{lm}(\hat{\rho})\Gamma(-\nu_n)U(-\nu_n,\frac{3}{2};r^2)\exp(-\frac{r^2}{2})Y_{00}(\hat{r})}$

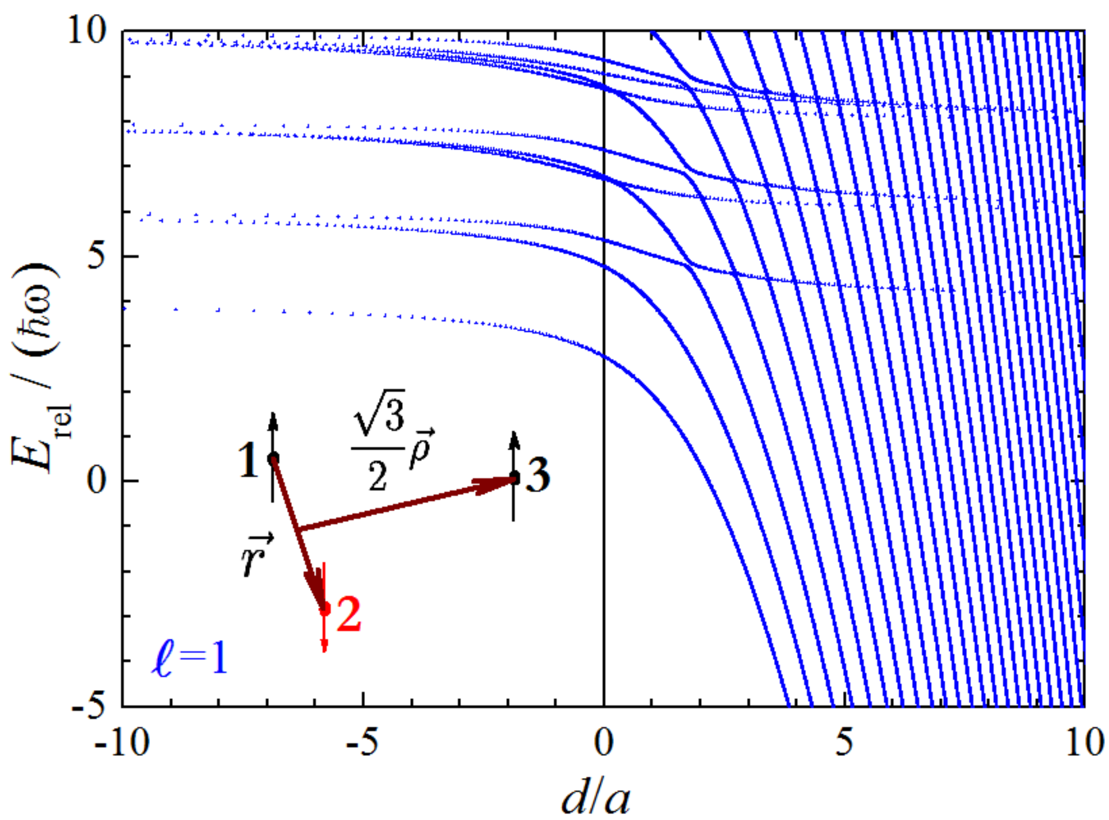
(P_{13}: particle exchange operator)

$$[(2n+l+\frac{3}{2})+(2\nu_n+\frac{3}{2})]\hbar\omega = E_{rel}$$

is determined from the BP condition

Liu, HH & Drummond, *PRA* **82**, 023619 (2010)

Three-particle problem in harmonic traps



Relative energy levels "*E*" as a function of the inverse scattering length (l = 1 section).

Three-particle problem at unitarity

$$R = \sqrt{\frac{r^2+\rho^2}{2}}, \quad \vec{\Omega} = (\alpha, \hat{r}, \hat{\rho})$$

$$\alpha = \arctan\left(\frac{r}{\rho}\right)$$

Separable wavefunctions !

$$\psi(R,\vec{\Omega}) = \frac{F(R)}{R^2}(1-\hat{P}_{13})\frac{\varphi(\alpha)}{\sin(2\alpha)} Y_l^m(\hat{\rho})$$

(P_{13}: *particle exchange operator*)

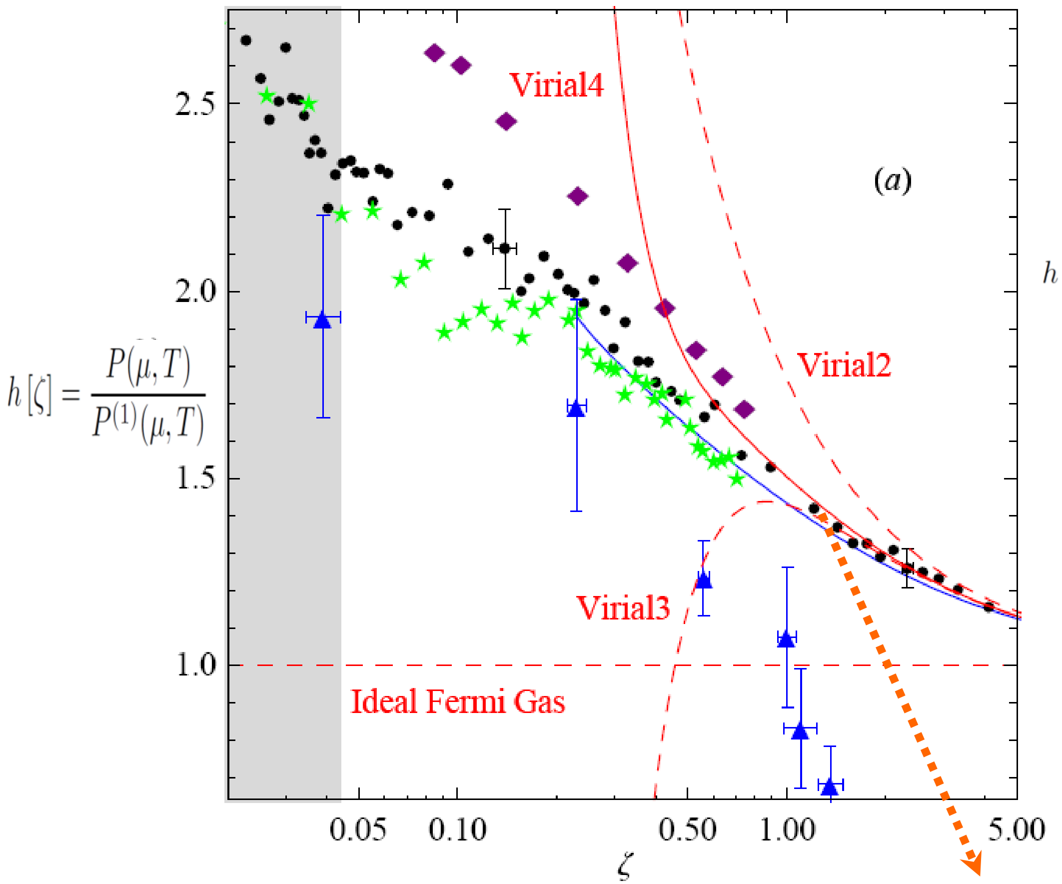
See, Werner & Castin, *PRL* (2006): $\boxed{E_{rel} = 1 + 2q + s_{\mathrm{ln}}}$

$$b_3 - b_3^{(1)} = \frac{Q_3 - Q_3^{(1)}}{Q_1} - (Q_2 - Q_2^{(1)}) = \frac{e^{-\beta\hbar\omega}}{1-e^{-2\beta\hbar\omega}} \sum_{l,n} (2l+1)\left[\exp(-\beta\hbar\omega s_{\mathrm{ln}}) - \exp(-\beta\hbar\omega s_{\mathrm{ln}}^{(1)})\right],$$

Numerically, $b_3 - b_3^{(1)} = -\mathbf{0.06833960} + \mathbf{0.038867}\left(\frac{\hbar\omega}{k_B T}\right)^2 - \mathbf{0.0135}\left(\frac{\hbar\omega}{k_B T}\right)^4 + \ldots,$

Virial expansion: Applications

Virial coefficient at unitarity (uniform case)



We now comment the main features of the equation of state. At high temperature, the EOS can be expanded in powers of ζ^{-1} as a virial expansion [11]:

$$h[\zeta]=\frac{P(\mu,T)}{P^{(1)}(\mu,T)}=\frac{\sum_{k=1}^{\infty}\left((-1)^{k+1}k^{-5/2}+b_k\right)\zeta^{-k}}{\sum_{k=1}^{\infty}(-1)^{k+1}k^{-5/2}\zeta^{-k}},$$

where b_k is the k^{th} virial coefficient. Since we have $b_2 = 1/\sqrt{2}$ in the measurement scheme described above, our data provides for the first time the experimental values of b_3 and b_4. $b_3 = -0.35(2)$ is in excellent agreement with the recent calculation $b_3 = -0.291 - 3^{-5/2} = -0.355$ from [11] but not with $b_3 = 1.05$ from [12]. $b_4 = 0.096(15)$ involves the 4-fermion problem at unitarity and could interestingly be computed along the lines of [11].

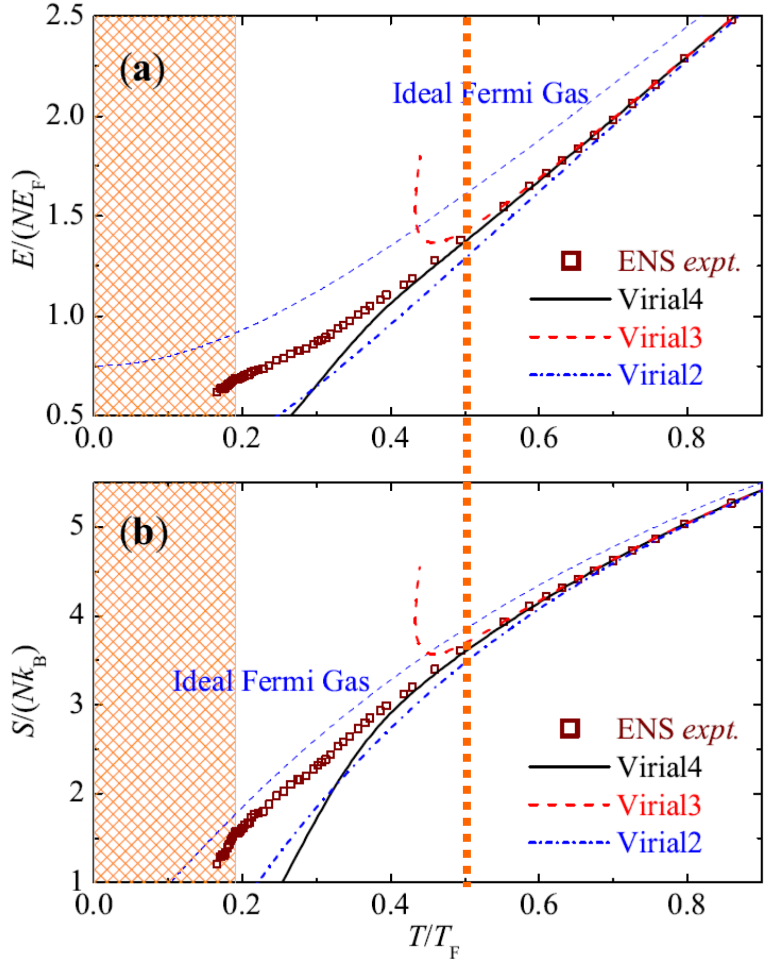
Nascimbène *et al.*, *Nature,* 25 February 2010.

$\Delta b_2 = 1/\sqrt{2}$ (known 70s ago)

√ Δb_3(Liu *et al.*) ≈ −0.35510298 (*PRL* 2009)

X Δb_3(Rupak) ≈ 1.05 (*PRL* 2007)

Unitary *EoS* at high *T*: trapped case



Here,

$$\Delta b_2 = 1/\sqrt{2}$$

$$\Delta b_3 \approx -0.35510298$$

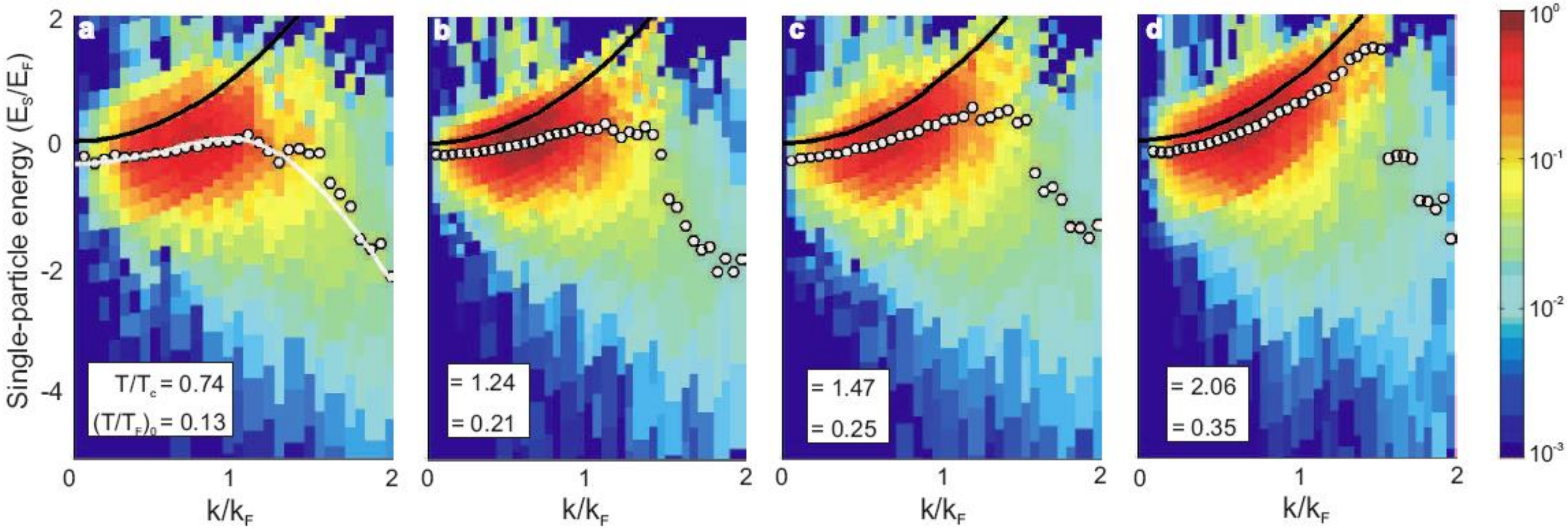
$$\Delta b_4(\mathrm{ENS}) \approx 0.096(15)$$

Expt. data:
Calculated from $h(\zeta)$ of ENS's *Unitarity EoS*

Theory data:
HH *et al.*, *New J. Phys.* **12**, 063038 (2010).

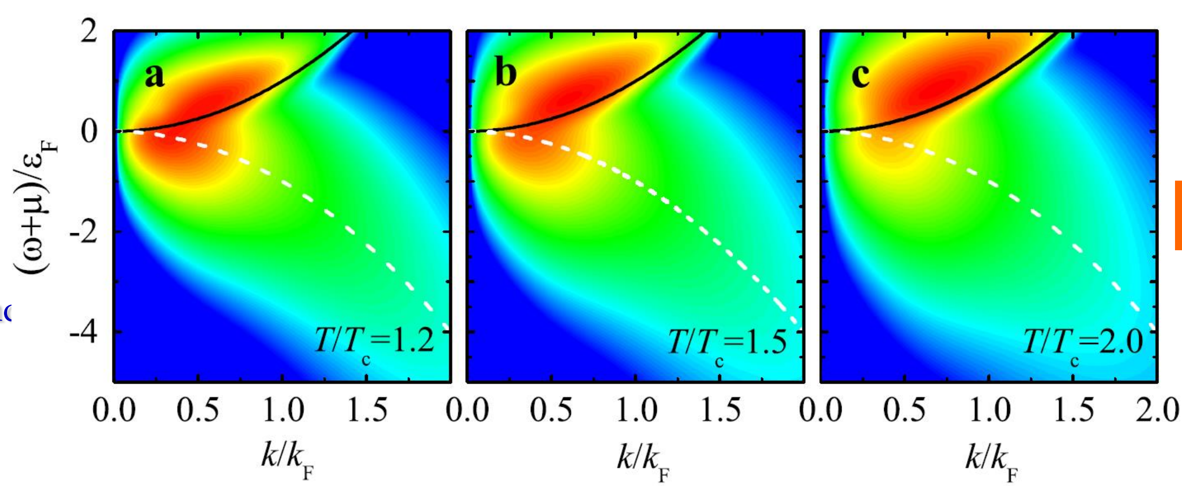
Trapped spectral function (second order only)

$$A(k,\omega) = A^{(1)}(k,\omega) + z^2 A_2(k,\omega) + \cdots$$



Expt.: JILA,
Nature Physics (2010).

Theory: HH Liu, Drummond
PRL **104**, 240407 (2010).



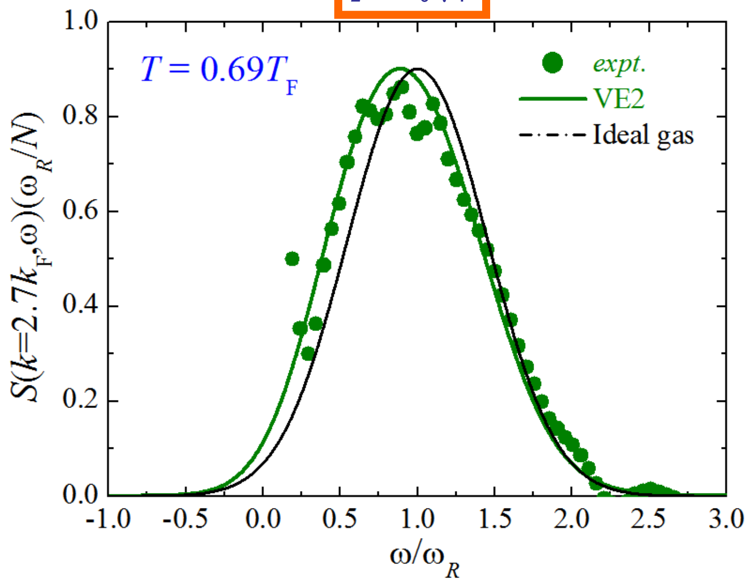
$z \sim 10$

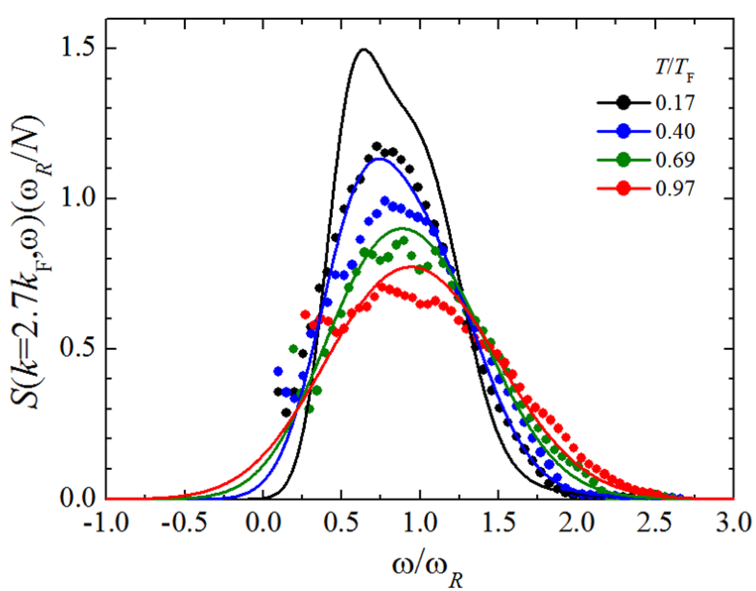
Trapped dynamic structure factor (second order only)

$$S(k,\omega)=S^{(1)}(k,\omega)+z^2S_2(k,\omega)+\cdots$$

$\boxed{z\sim 0.4}$

Low T





Expt.: Kuhnle, Hoinka, Dyke, HH, Hannaford & Vale, *PRL*, **106** 170402 (2011).

Theory: HH, Liu, & Drummond, *PRA* **81**, 033630 (2010).

VE applications (Tan's contact)

The finite-T contact may be calculated using adiabatic relation: $\left[\frac{\partial \Omega}{\partial a_s^{-1}}\right]_{T,\mu} = -\frac{\hbar^2}{4\pi m} I$

(**high-*T* regime**) Recall that the virial expansion for thermodynamic potential,

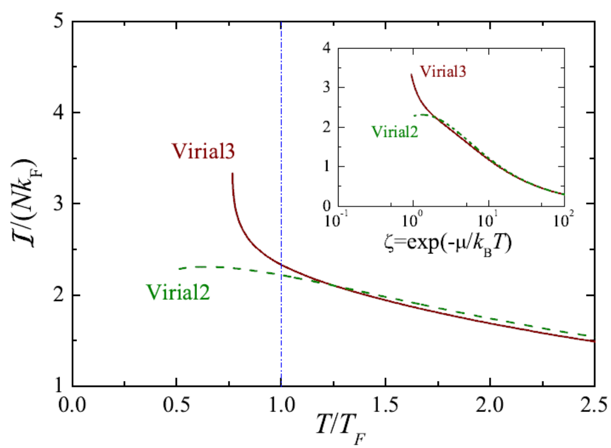
$$\Omega = \Omega^{(1)} - \frac{2k_BT}{\lambda_{dB}^3}\left[\Delta b_2 z^2 + \Delta b_3 z^3 + \cdots\right]$$

Using the adiabatic relation, it is easy to see that,

$$I_{\text{virial}} = \frac{4\pi m}{\hbar^2}\frac{2k_BT}{\lambda_{dB}^2}\left[\underbrace{\frac{\partial \Delta b_2}{\partial(\lambda_{dB}/a_s)}}_{c_2} z^2 + \underbrace{\frac{\partial \Delta b_3}{\partial(\lambda_{dB}/a_s)}}_{c_3} z^3 + \cdots\right]$$

At the unitarity limit, we find that, $c_2=1/\pi$ and $c_3 \approx -0.141$. **☺ to be used as a benchmark!**

I_{virial}

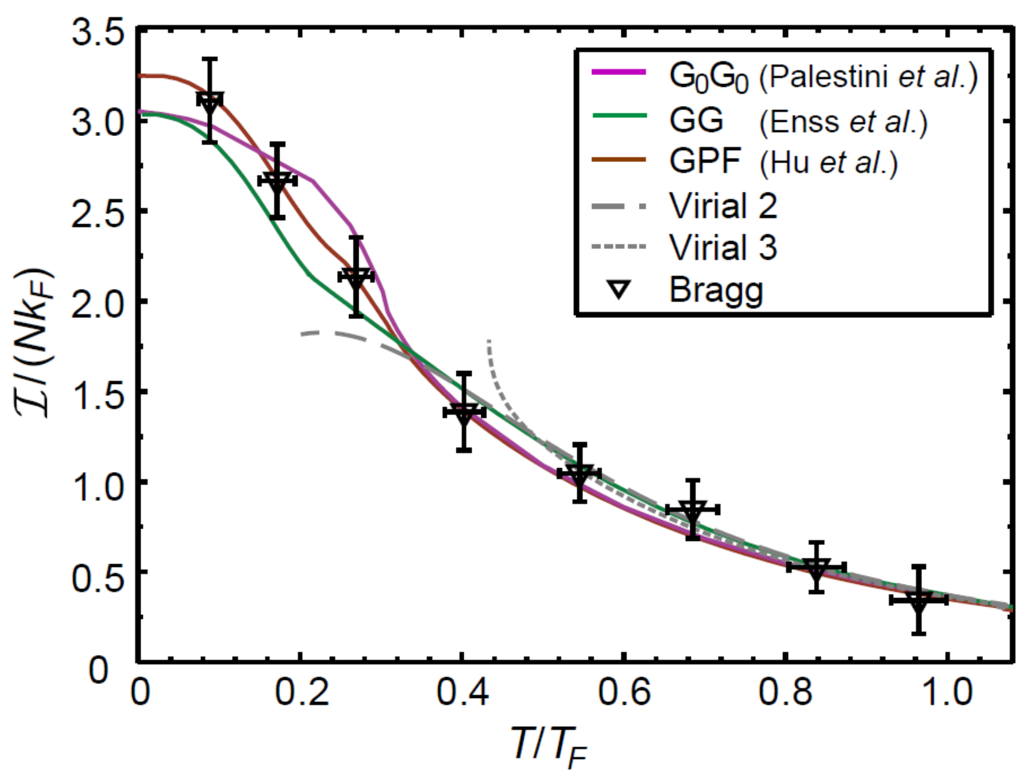


Note that,

$c_n(\text{trap}) = (1/n^{3/2})\, c_n(\text{homo})$

Hu, Liu & Drummond, *NJP* **13**, 035007(2011).

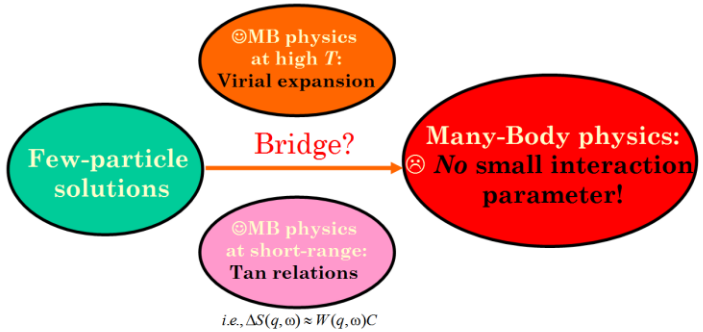
Trapped contact at unitarity (theory vs experiment)



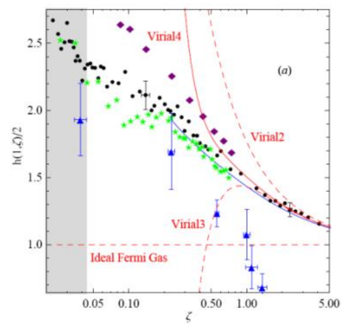
Expt.: Kuhnle, Hoinka, Dyke, HH, Hannaford & Vale, *PRL*, **106** 170402 (2011).

Theory: HH, Liu & Drummond, *NJP* (2011).

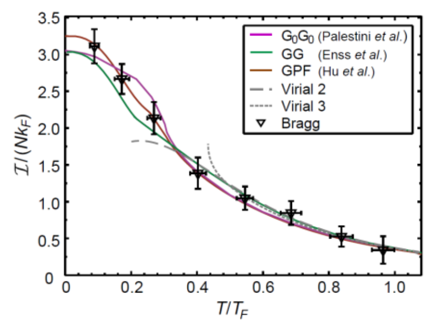
Taking home messages



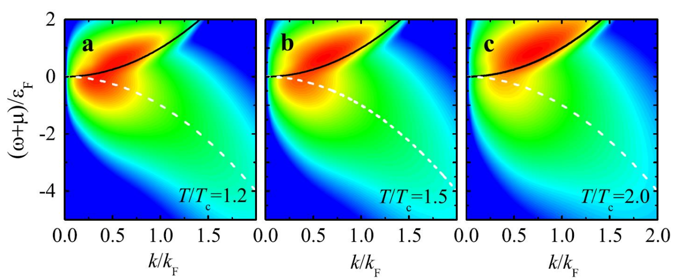
Virial expansion solves completely the large-T strong-correlated problem!



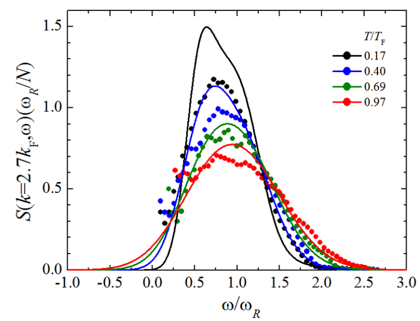
EoS



Tan's contact



SP Spectral Function



DSF

Outlooks (improved virial expansion)

- **High order virial coefficient: 4th order coefficient Exp. VS Theory.**
  5th order virial coefficient
  … …

- **Can we improve *S*(*k*,ω) to the 3rd and 4th order?**

  i.e., **based on the 3- and 4-body solutions by**
  Daily & Blume;
  Stecher & Greene;
  Werner & Castin;
  ……

- **Can we improve *A*(*k*,ω) to the 4th order?**

- **Efimov physics or *triplet* pairing response in *A*(*k*,ω) and *S*(*k*,ω) ?**

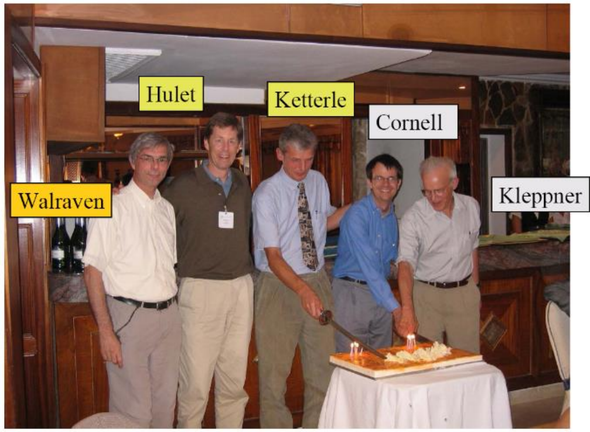
Latest progress on the fourth virial coefficient

Δb_4	Reference	Comment
0.096(15)	Nascimbene, Navon, Jiang, Chevy & Salomon, *Nature* **463**, 1057 (2010).	**ENS experiment**
0.096(10)	Ku, Sommer, Cheuk & Zwierlein, *Science* **335**, 563 (2012).	**MIT experiment**
–0.016(4)	Rakshit, Daily & Blume, *PRA* **85**, 033634 (2012).	sum-over-states approach
0.06	Ngampruetikorn, Parish & Levinsen, *PRA* **91**, 013606 (2015).	diagrammatic approach (a subset of 4-body diagrams)
0.062	Endo & Castin, Journal of Physics A: **49**, 265301 (2016).	3-body inspired conjecture
0.078 (18)	Yan & Blume, *PRL* **116**, 230401 (2016).	**Path-Integral Monte-Carlo**

Bosons
Fermions
Mixtures

Trapping potential:
Single trap
Lattice
Random potential

Playground of Cold Atoms



BEC Workshop, San Feliu, Spain, Sept. 10 -15, 2005

Spatial dimension:
1D, 2D, 3D

Interaction:
Strong/weak
Isotropic/anisotropic
Short-rangle/long-range

External fields:
Light, magnetic/electric field