Virial Expansion for a strongly correlated Fermi gas

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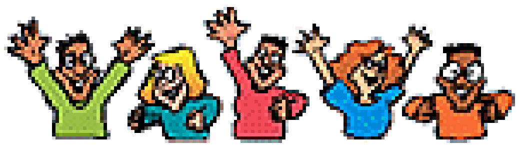
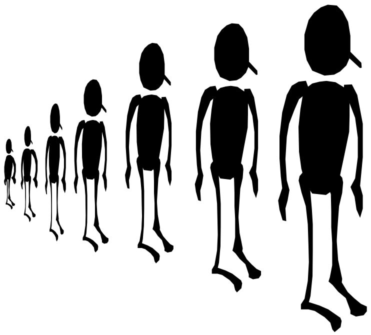
Hawthorn, January.

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.



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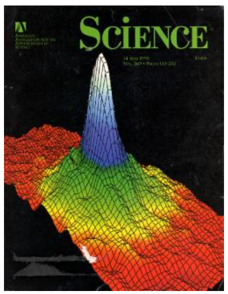
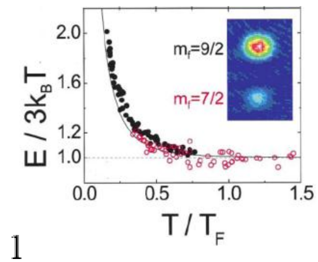
Quantum statistics

2001 Nobel Prize



Quantum Degeneracy

1999

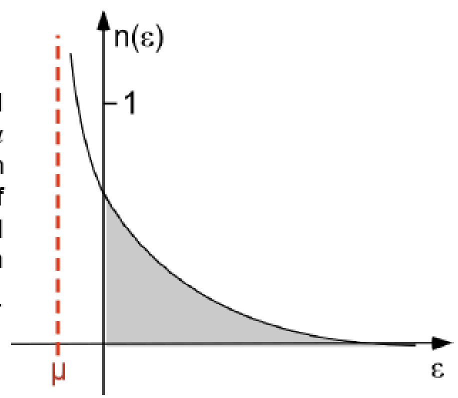


Quantum statistics

Bose-Einstein distribution

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

The chemical potential μ follows from the norm of $n(\varepsilon)$ and depends on *T* and *N*.

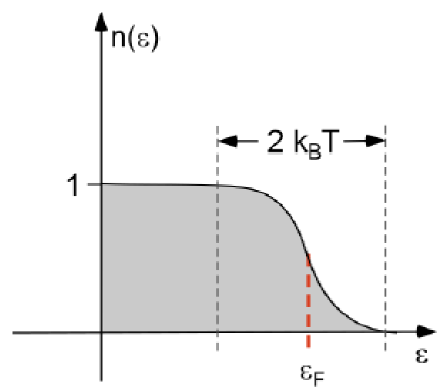


For T→0: $\mu \to \varepsilon_0$ (ground state energy)

macroscopic population of the ground state

Fermi-Dirac distribution

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



For T→0: $\mu \to \varepsilon_F$ (fermi energy)

$$n(\varepsilon) \to \Theta(\varepsilon - \mu) = \begin{cases} 1 & for \quad \varepsilon < \mu \\ 0 & for \quad \varepsilon > \mu \end{cases}$$

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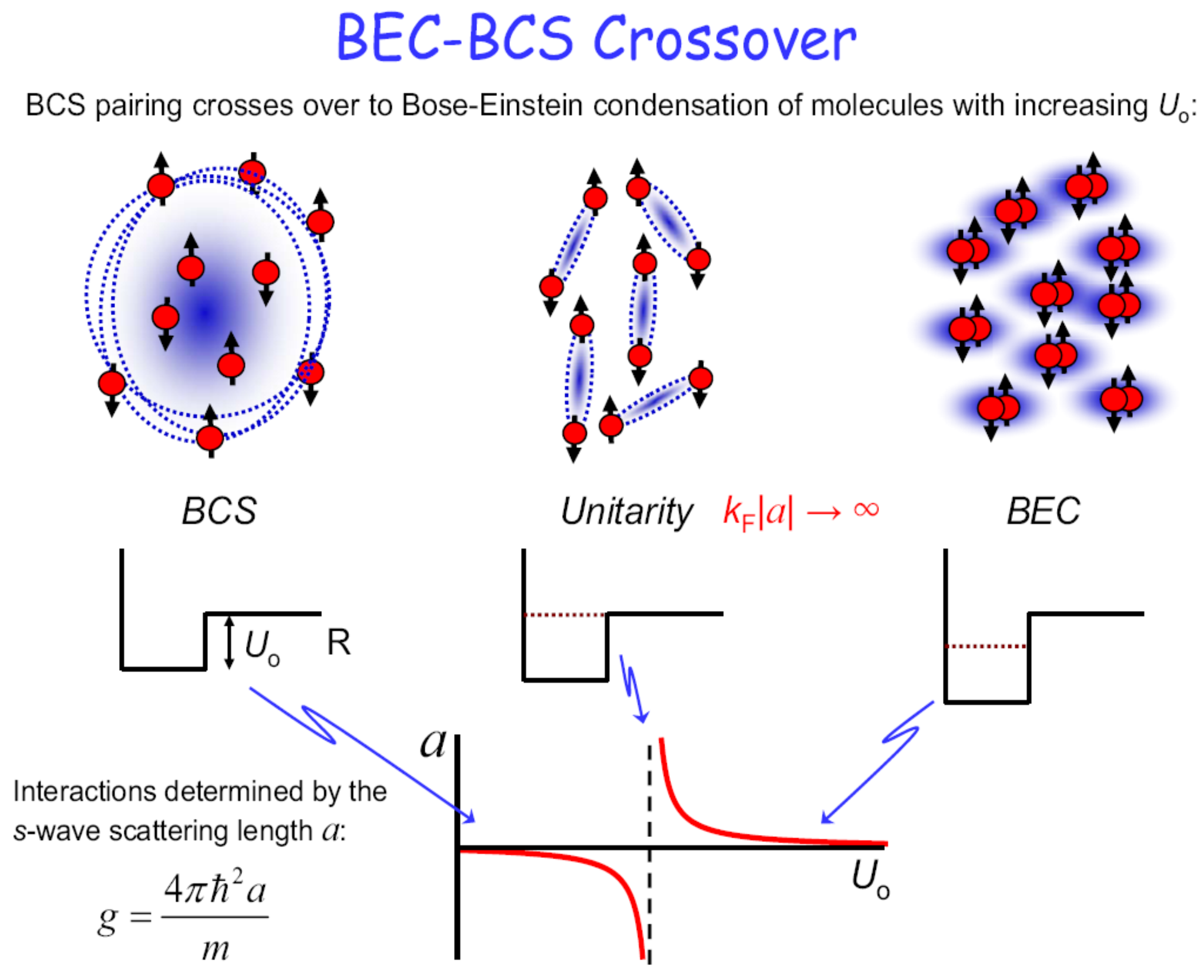
BCS-BEC Crossover

BCS Theory

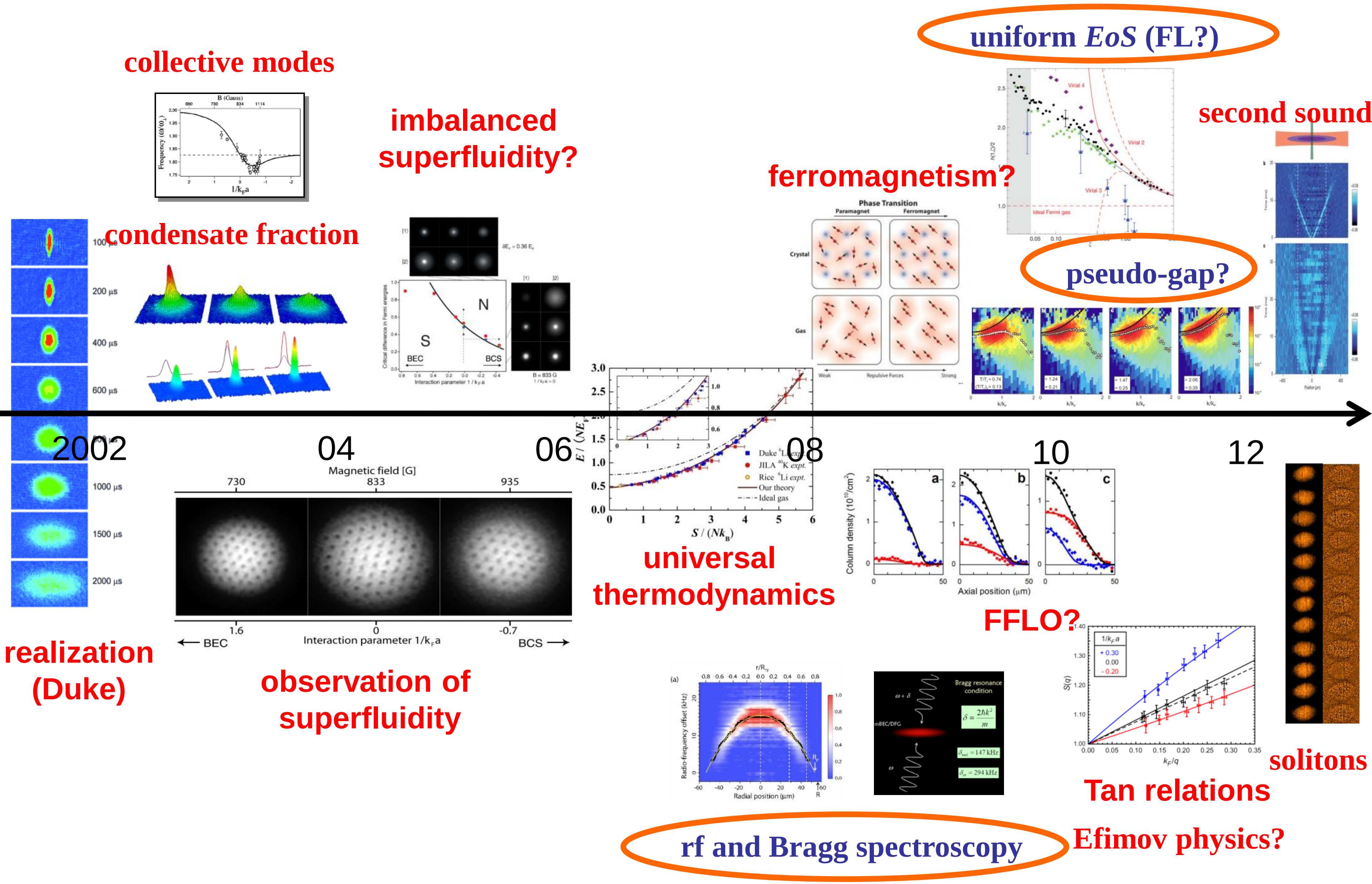


Gross-Pitaevskii equation

BCS fermionic superfluidity → *BEC of molecules*

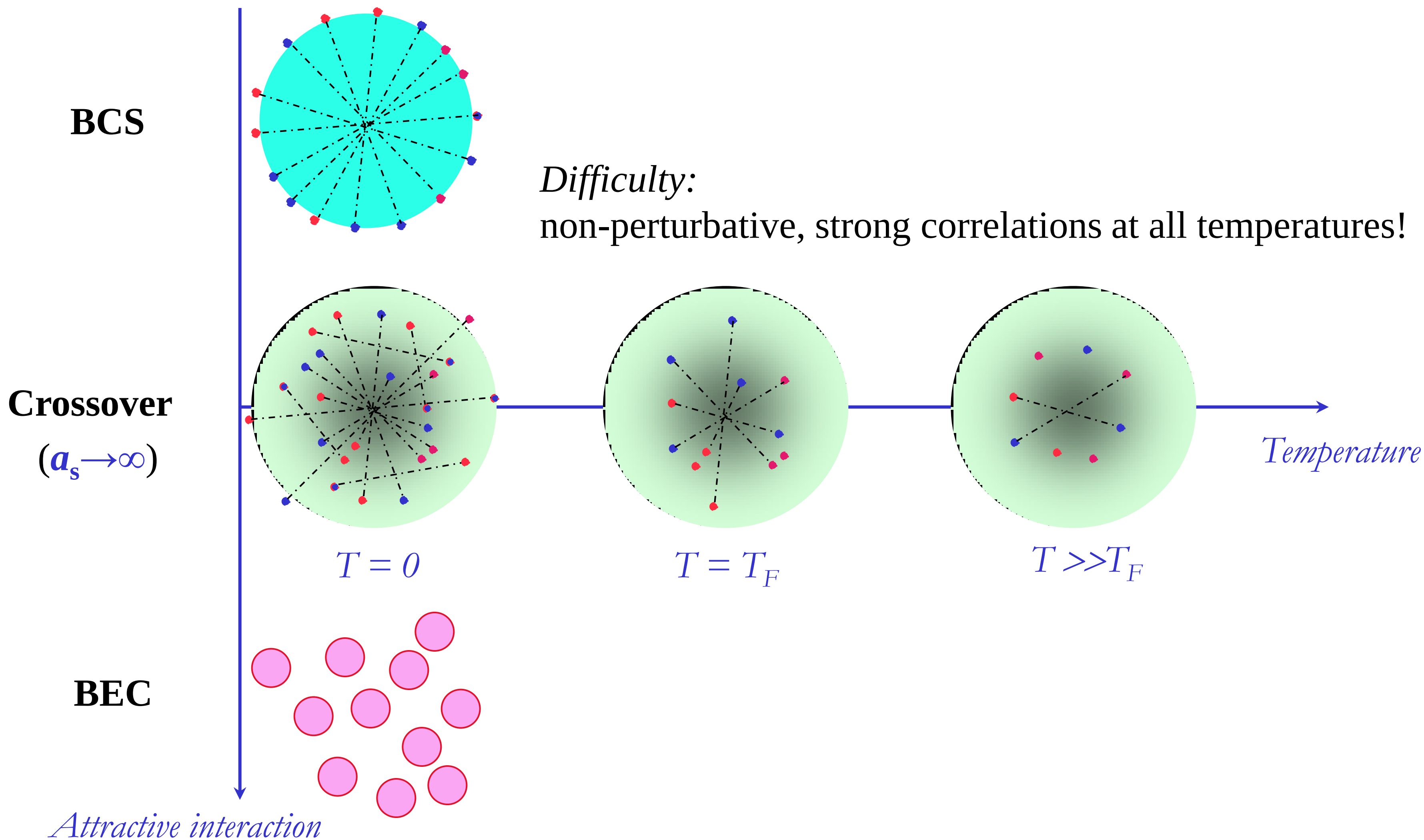
Interaction strength tunable via Feshbach resonances

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?**

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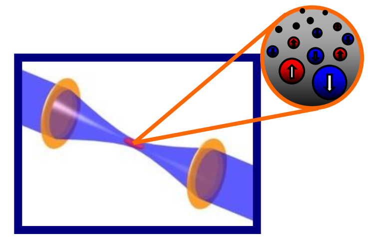
Quantum Monte Carlo? **Virial expansion**

Few-body solutions

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

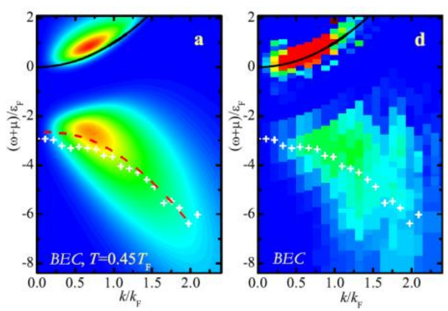
Outline



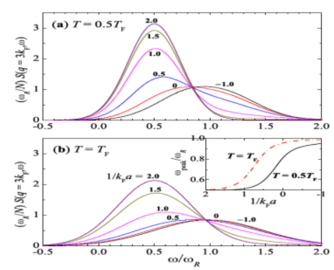
- **Virial expansion: A traditional but "new" method**
- **Few-particle exact solutions as the input to virial expansion**
- **Virial expansion: Applications**

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

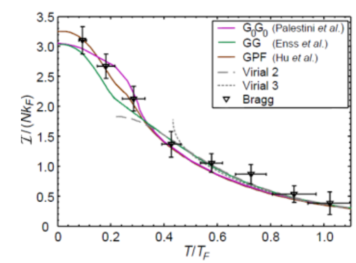
Equation of State



SP Spectral Function



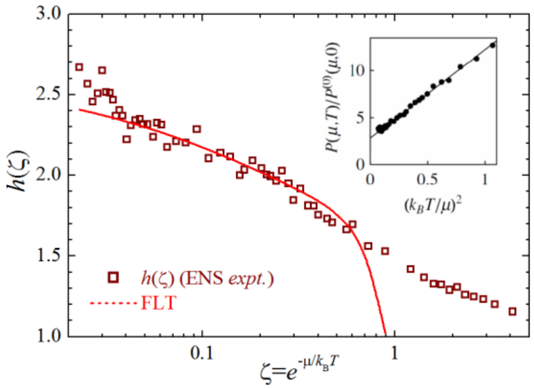
Dynamic Structure Factor

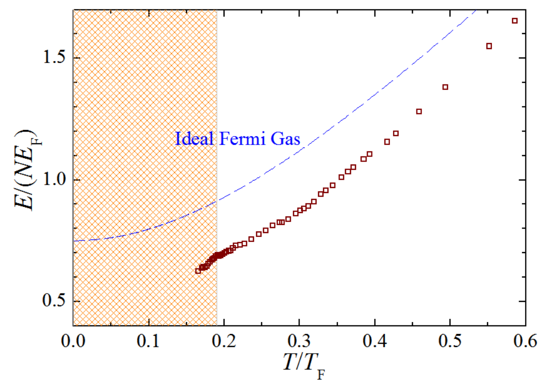


Tan's Contact

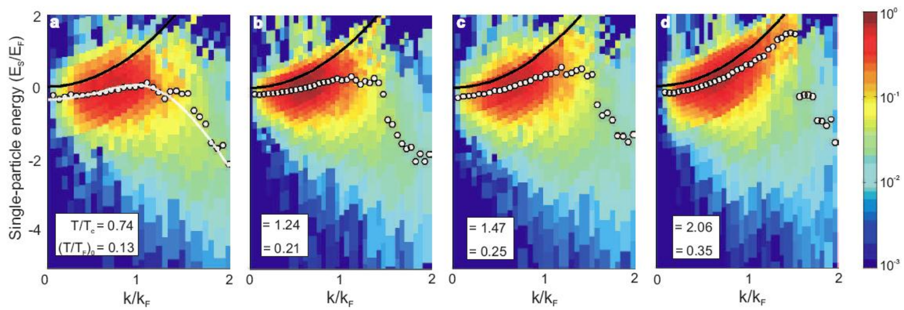
- **Conclusions and outlooks**

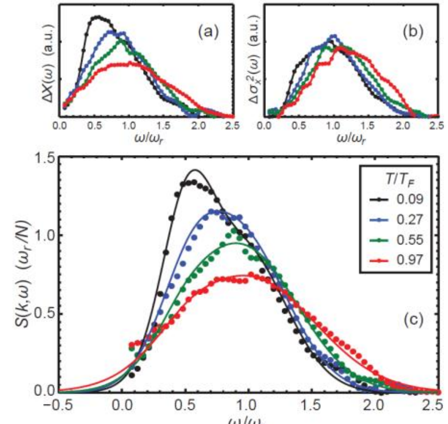
How to understand these experimental results?





unitary equation of state (static)

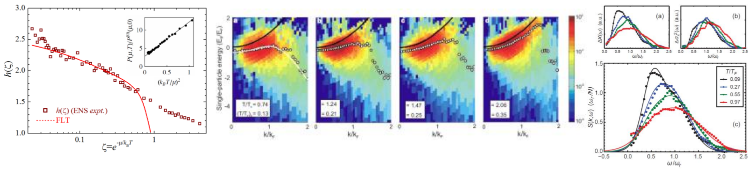




unitary single-particle spectral function　　unitary dynamic structure factor

It is a central, grand challenge to theorists, due to the lack of small interaction parameter!

BEC-BCS crossover: (theoretical challenge)



☺MB physics
at high T:
Virial expansion

Bridge?

Few-particle solutions

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

☺MB physics
at short-range:
Tan relations

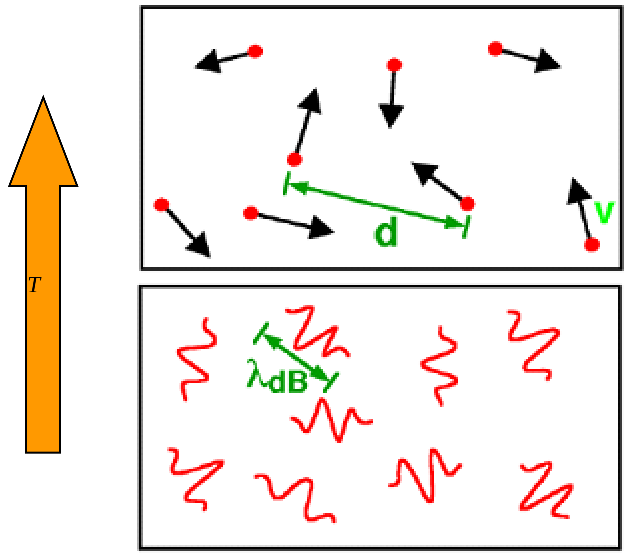
Blume, Daily, Stecher, Greene;
Busch, Englert, Rzazewski, Wilkens;
Werner, Castin;
Kestner, Duan;
Julienne, Bohn, Tiesinga;
……

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



High Temperature

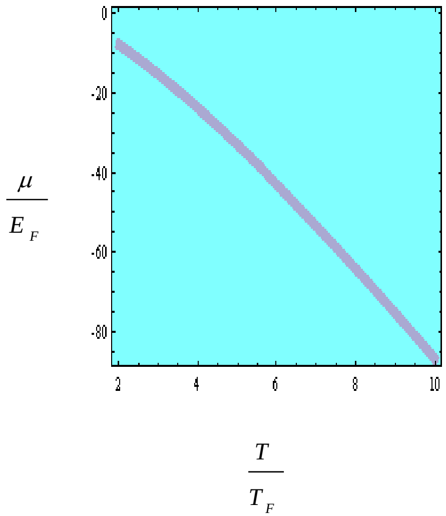
"Billiard balls"

Low Temperature

"Wave packets"

Thermal fluctuation

ABC of virial expansion (VE)



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

$$\mu \to -\infty$$

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

ABC of virial expansion (VE)

Thermodynamic potential

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

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

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

$$Z_G = 1 + zQ_1 + z^2 Q_2 + z^3 Q_3 \cdots$$

N-cluster partition function:

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

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

$$|x| \le 1$$

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

Virial Coefficients

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

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?

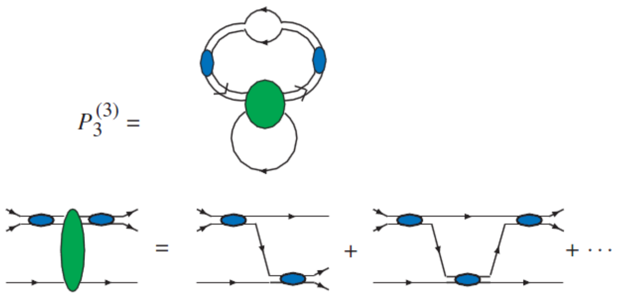
For a homogeneous system, where the energy level is continuous, it seems impossible to calculate directly virial coefficient using *N*-cluster partition function, *i.e.*, $b_3 = (Q_3 - Q_1Q_2 + \frac{1}{3}Q_1^3), \ldots$

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)] :

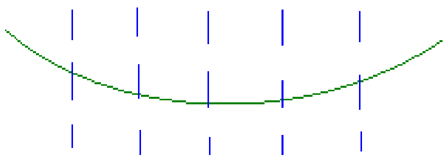


leads to, $\Delta b_3(\text{Rupak}) \approx 1.05$ (incorrect ☹)

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)],**



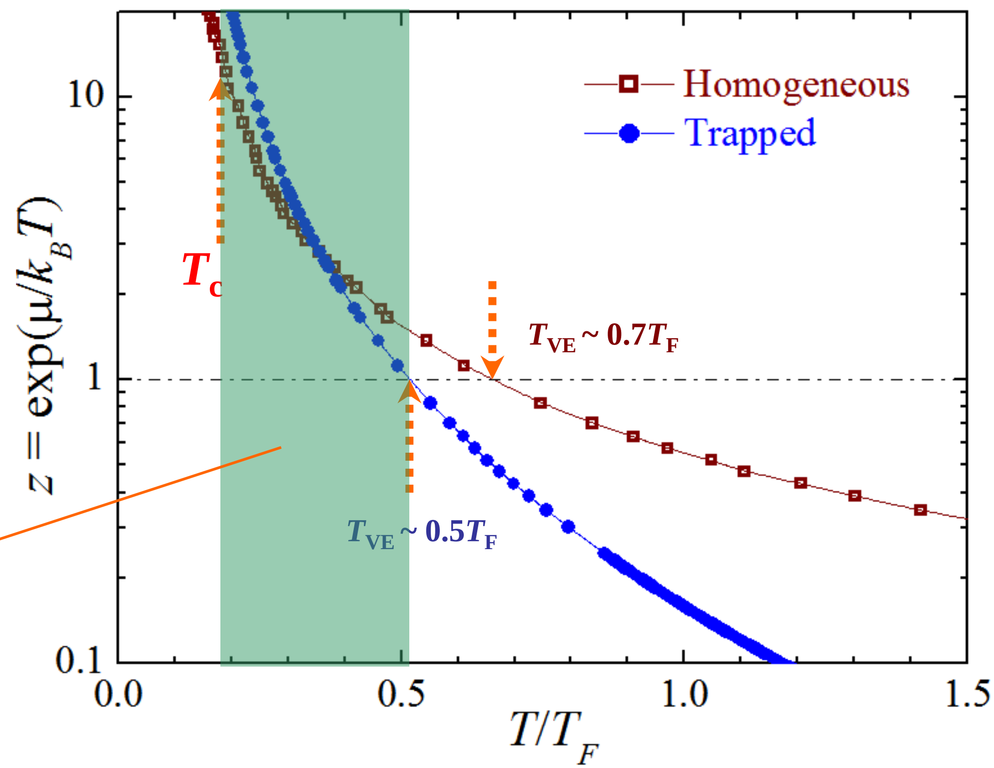
LDA

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

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

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

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

$$= A_1 + z(A_2 - A_1Q_1) + \cdots,$$

virial expansion functions:

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

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

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

Quantum virial expansion of DSF

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

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

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

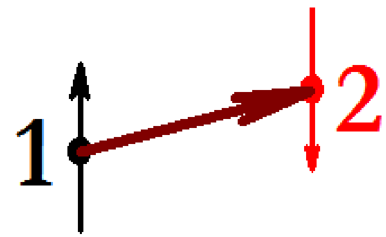
Finally, we use $$S_{\sigma\sigma'}\left(\mathbf{r},\mathbf{r}';\omega\right) = -\frac{\mathrm{Im}\,\chi_{\sigma\sigma'}\left(\mathbf{r},\mathbf{r}';i\omega_n\rightarrow\omega+i0^+\right)}{\pi(1-e^{-\beta\omega})}$$

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

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

The solution:

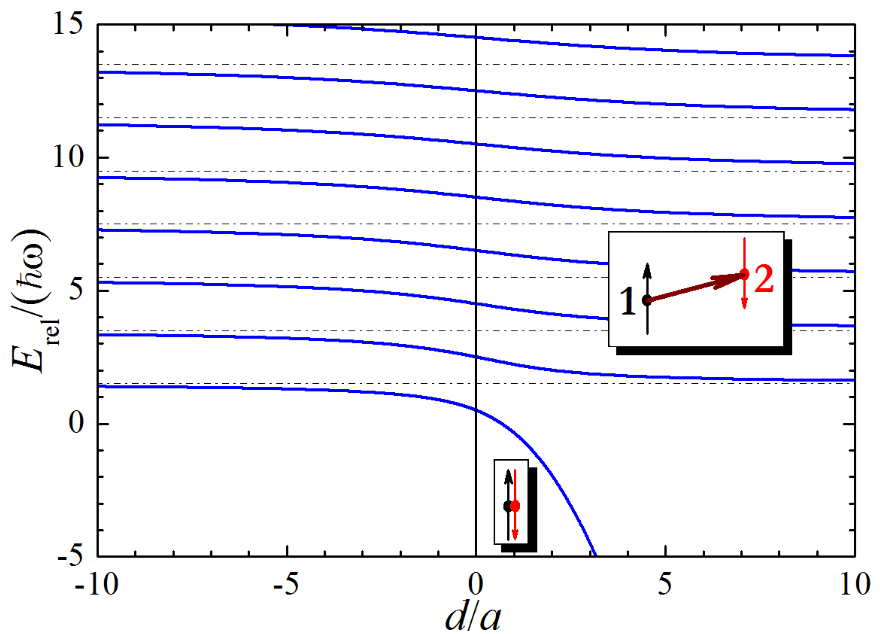
$$\psi^{\mathrm{rel}}_{2b}(r;\nu) = \Gamma(-\nu)U\left(-\nu, \frac{3}{2}, \frac{r^2}{d^2}\right)\exp\left(-\frac{r^2}{2d^2}\right)$$

U is the second Kummer function

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

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

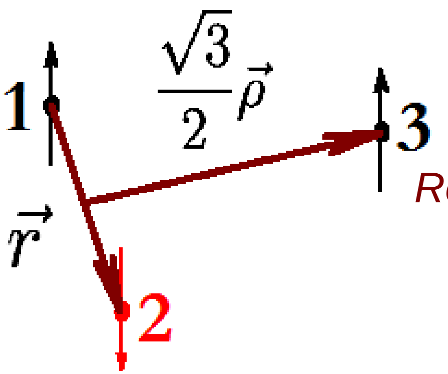
Two-particle problem in harmonic traps



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

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

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

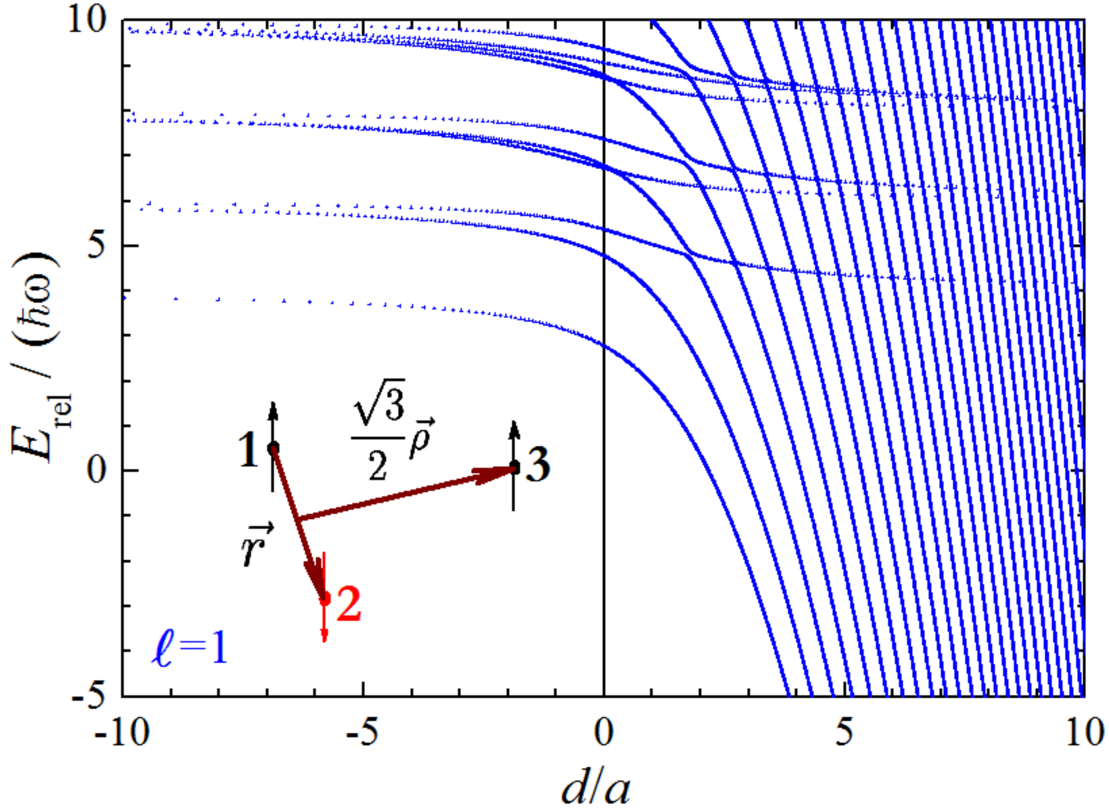
(***P***$_{13}$: particle exchange operator)

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

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):

$$\boxed{E_{rel} = 1 + 2q + s_{ln}}$$

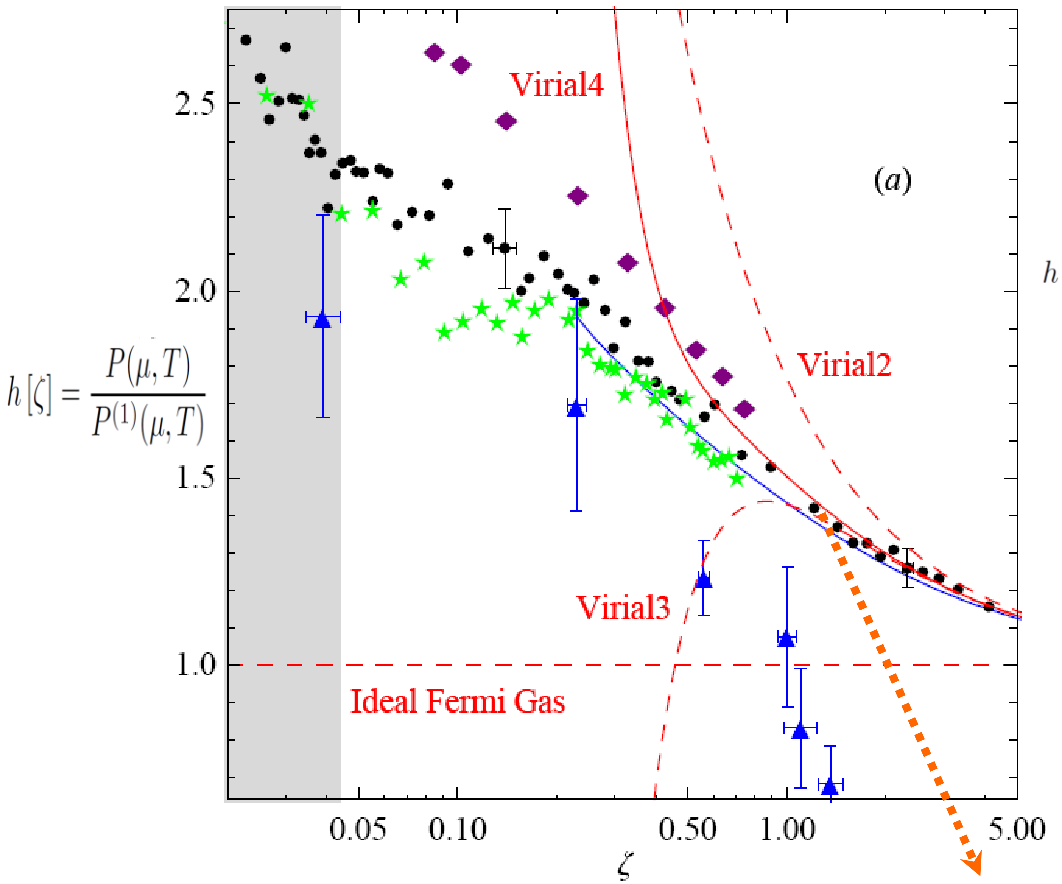
$$b_3 - b_3^{(1)} = \frac{Q_3 - Q_3^{(1)}}{Q_1} - (Q_2 - Q_2^{(1)}) = \frac{e^{-\beta\hbar\omega}}{1-e^{-2\beta\hbar\omega}} \sum_{l,n} (2l+1)\left[\exp(-\beta\hbar\omega s_{ln}) - \exp(-\beta\hbar\omega s_{ln}^{(1)})\right],$$

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].

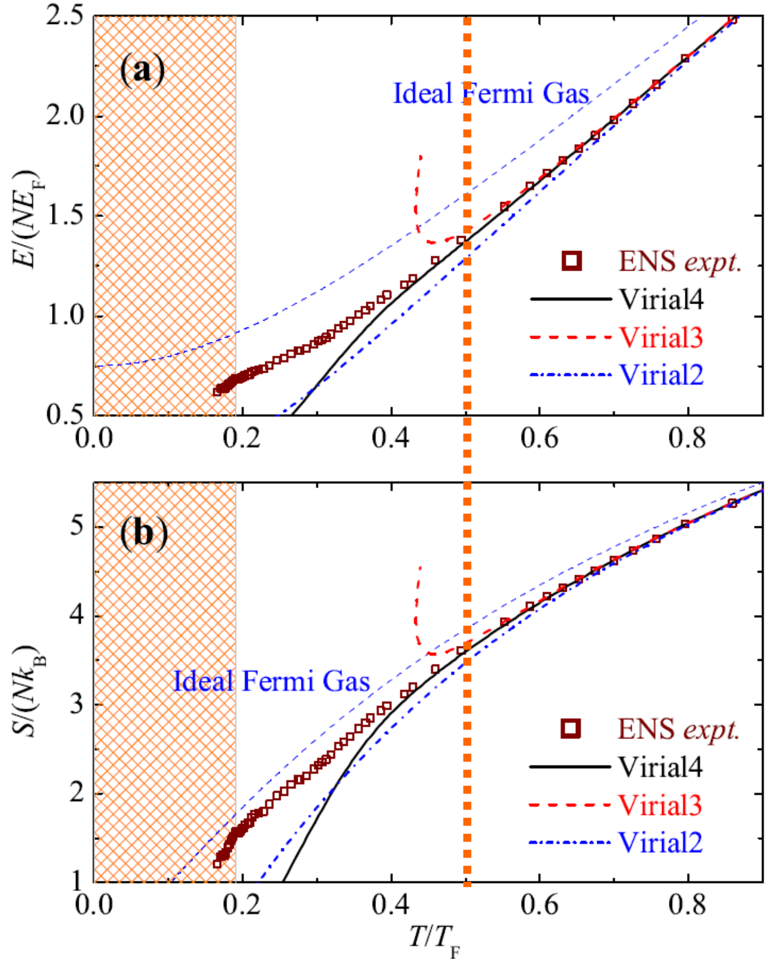
Nascimbène *et al.*, *Nature*, 25 February 2010.

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

√ $\Delta b_3(\text{Liu } et\ al.) \approx -0.35510298$ (*PRL* 2009)

X $\Delta b_3(\text{Rupak}) \approx 1.05$ (*PRL* 2007)

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



Here,

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

$\Delta b_3 \approx -0.35510298$

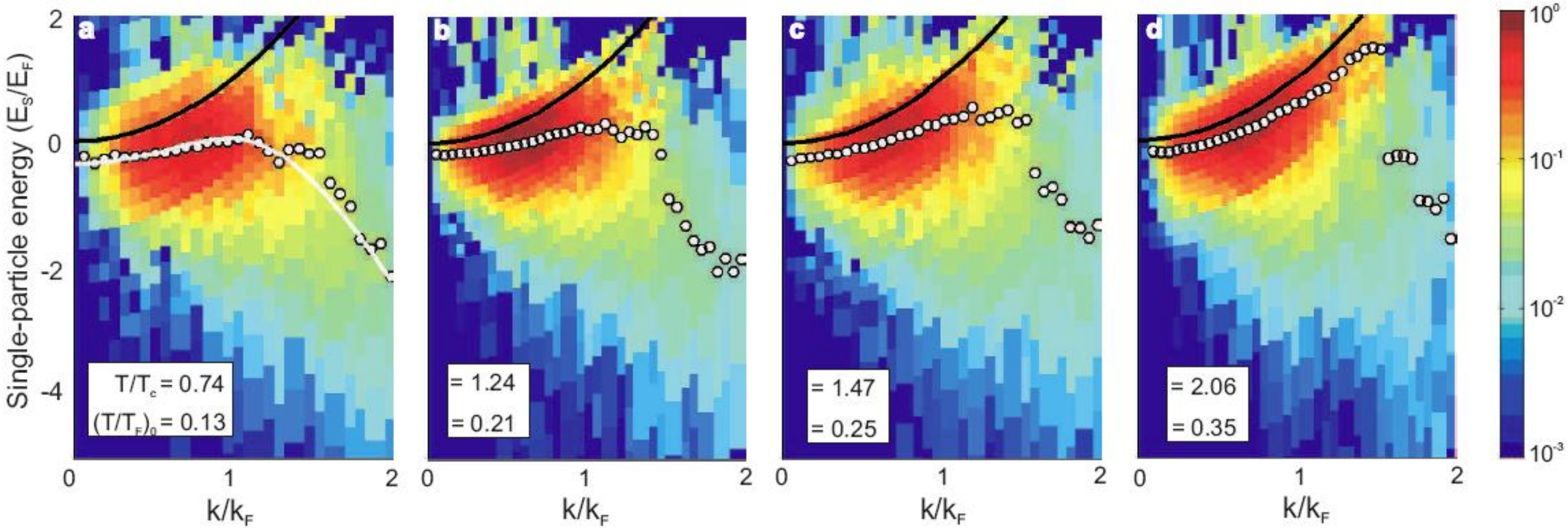
$\Delta b_4(\text{ENS}) \approx 0.096(15)$

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

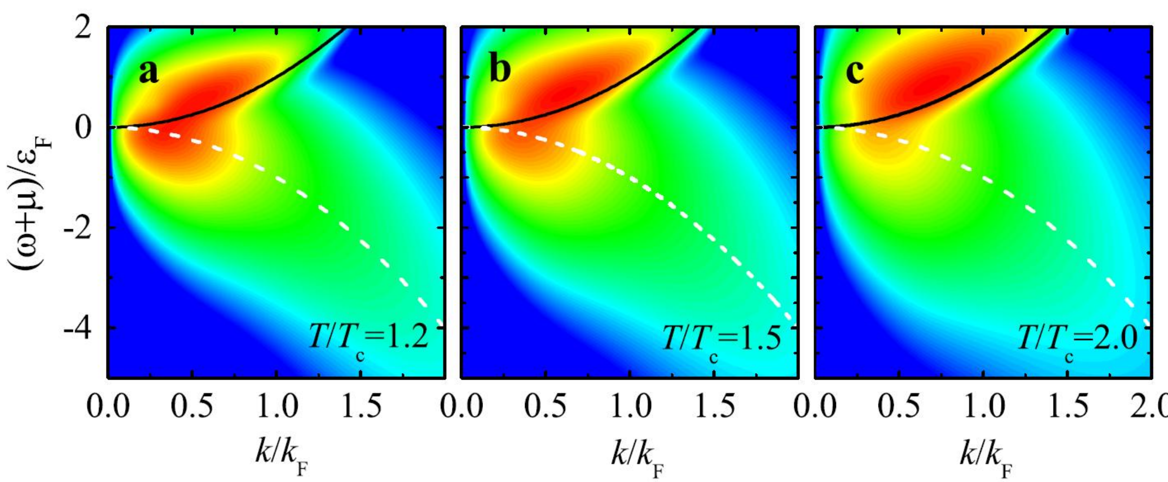
Theory data:
HH *et al.*, *New J. Phys.* **12**, 063038 (2010).

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).



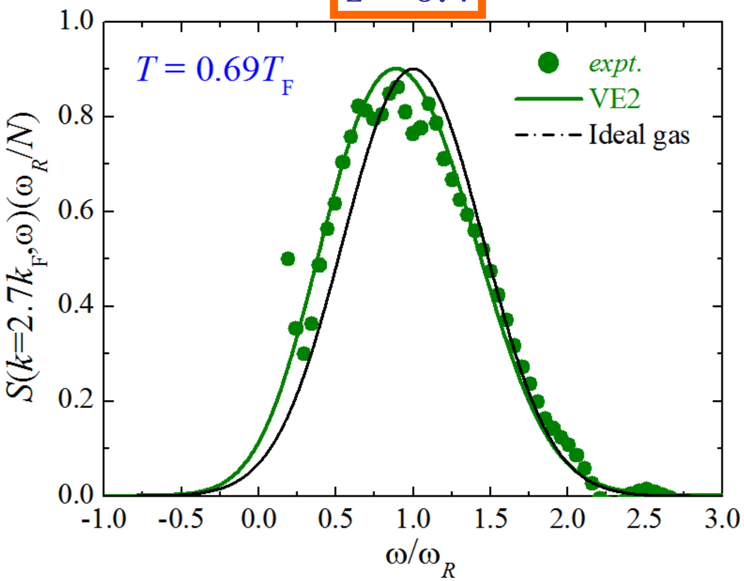
$z \sim 10$

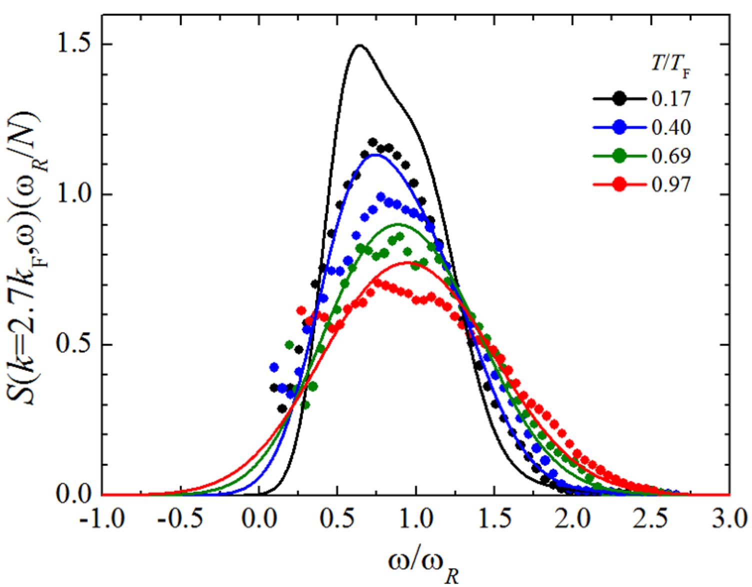
Theory: HH *et al.*, *PRL* **104**, 240407 (2010).

Trapped dynamic structure factor (second order only)

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

$z \sim 0.4$





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: $\left[\frac{\partial \Omega}{\partial a_s^{-1}}\right]_{T,\mu} = -\frac{\hbar^2}{4\pi m}\mathcal{I}$

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

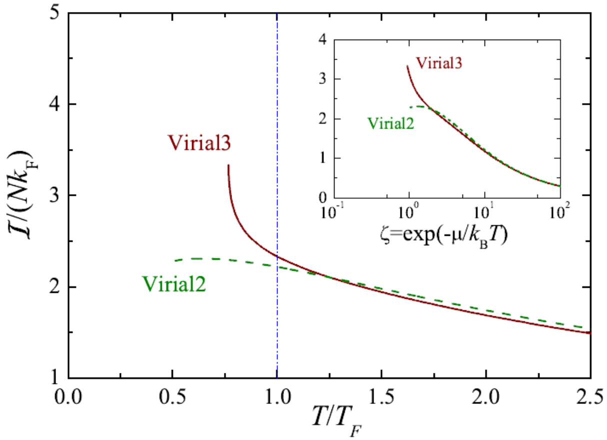
$$\Omega = \Omega^{(1)} - \frac{2k_BT}{\lambda_{dB}^3}\left[\Delta b_2 z^2 + \Delta b_3 z^3 + \cdots\right]$$

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

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

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

$\mathcal{I}_{\text{virial}}$

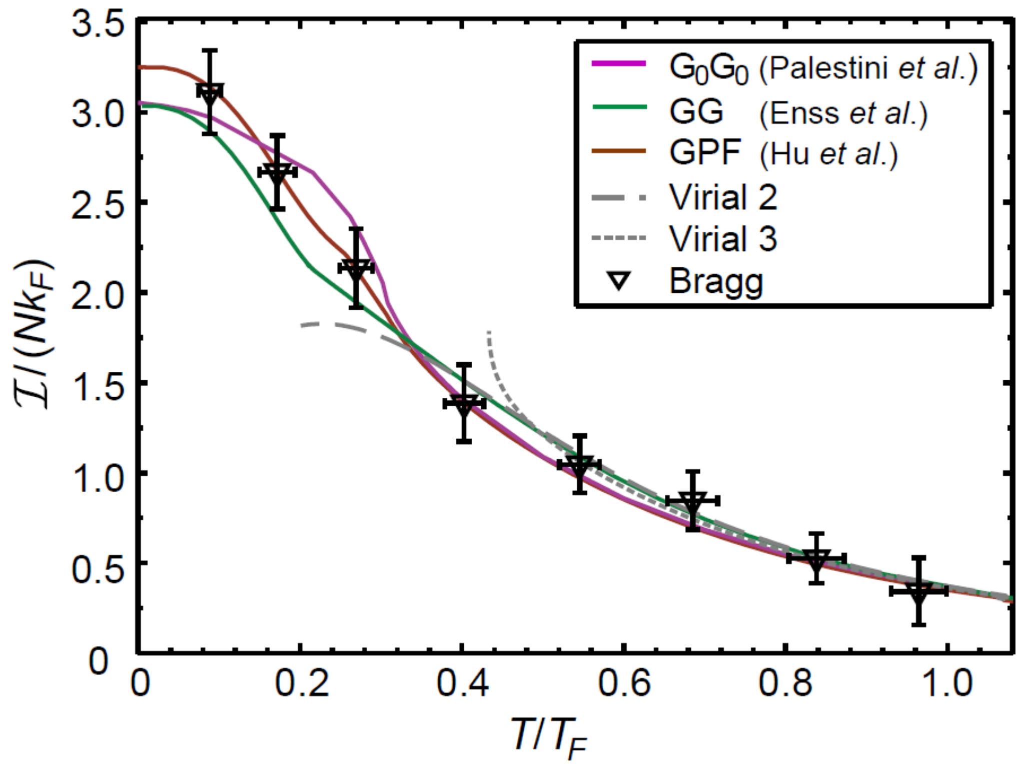


Note that,

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

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

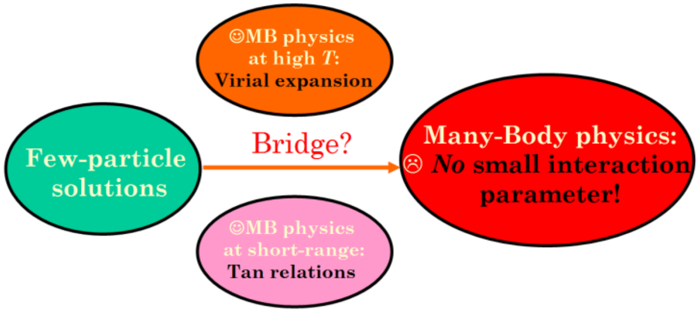
Trapped contact at unitarity (theory vs experiment)



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

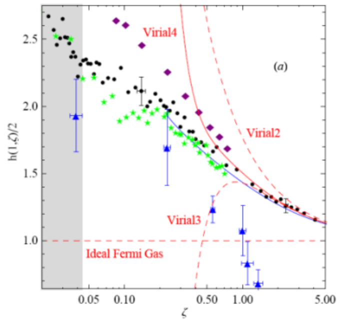
Theory: HH, Liu & Drummond, *NJP* (2011).

Taking home messages

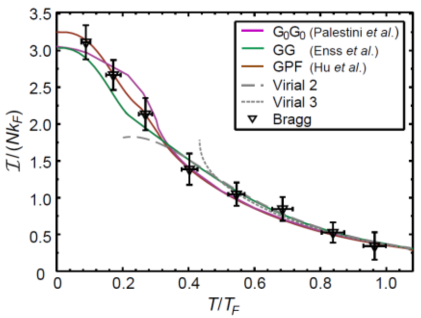


i.e., $\Delta S(q,\omega) \approx W(q,\omega)C$

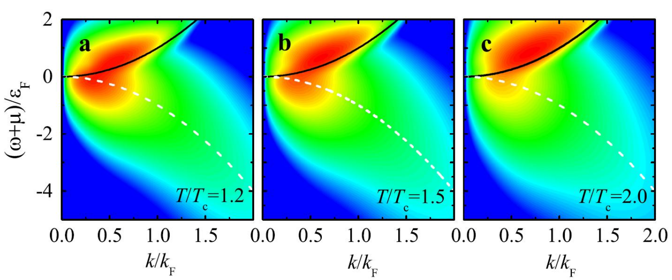
Virial expansion solves completely the large-T strong-correlated problem!



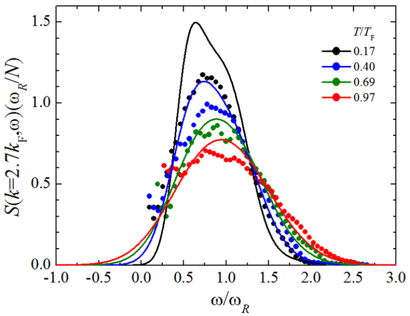
EoS



Tan's contact



SP Spectral Function



DSF

Outlooks (improved virial expansion)

- **4th order virial coefficient: experiment** $\Delta b_4 \approx 0.096$ **and theory** $\Delta b_4 \approx -0.016$

- **Can we improve** $A(k,\omega)$ **and** $S(k,\omega)$ **to the 3rd and 4th order?**

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

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