「量子クラスターで読み解く物質の階層構造」キックオフシンポジウム

ファインマン・ダイアグラム展開に基づく量子モンテカルロ法による冷却フェルミ原子系の高精度数値計算

Takahiro Ohgoe

Department of Applied Physics, The Univ. of Tokyo

Nov. 20, 2018

Collaborators:

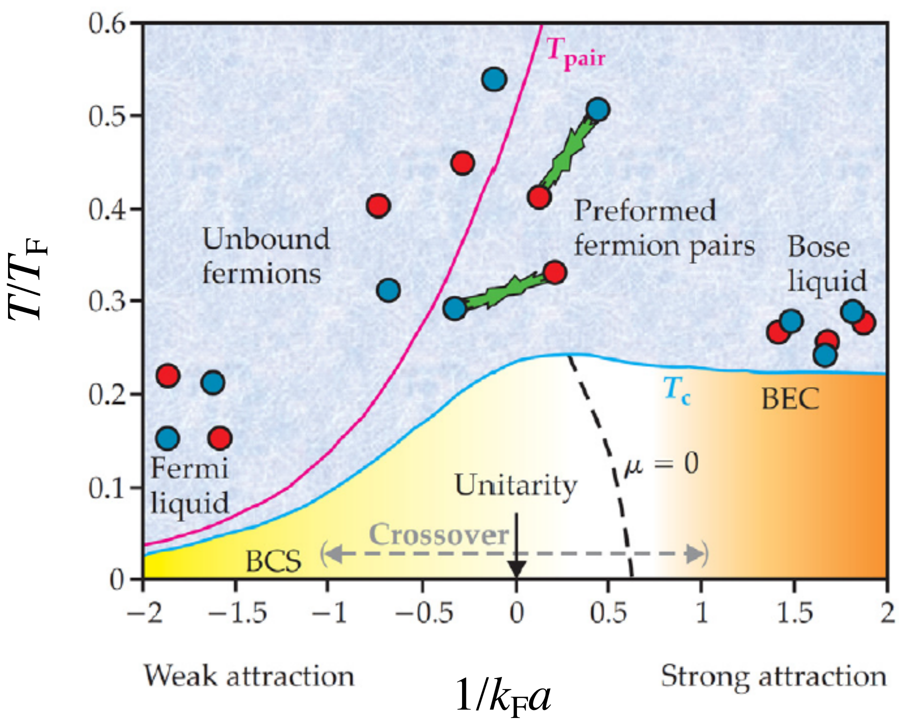
Riccardo Rossi (Flatiron Institute)
Kris Van Houcke, Felix Werner (ENS Paris)
Boris Svistunov, Nikolay Prokof’ev (University of Massachusetts, Amherst)
Evgeny Kozik (King’s College, London)

Two component dilute Fermi gas

"Dilute" gas: Effective range of the interaction r_e
<< Interparticle spacing $n^{-1/3}(\sim k_F^{-1})$

→ **At low temperatures,**
the interaction is characterized by the s-wave scattering length a.

C. A. R. Sa de Melo, Phys. Today **61** 45–51 (2008)



Features

- Universal properties
- BEC-BCS crossover
- Highly controllable cold atom experiments
- Pseudogap?

Feynman-diagrams approach

Conventional Feynman-diagrams approach

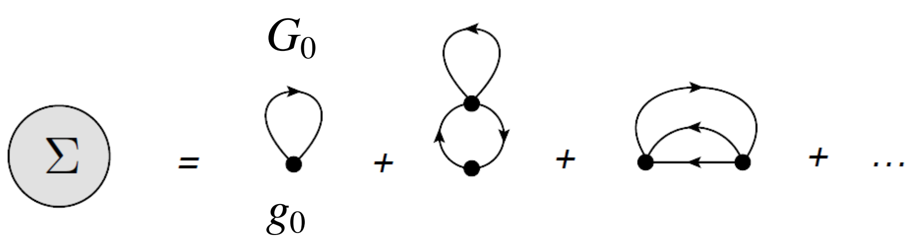
- Widely used in various field of physics.
  However, only particular types of diagrams are usually considered.

  e.g. Hartree-Fock, *T*-matrix approx., RPA, FLEX

To go beyond

Diagrammatic Monte Carlo method

- Unbiased sampling of the Feynman diagrams



No finite size effects **We have to go to high orders**

Bold diagrammatic Monte Carlo

To efficiently include many Feynman diagrams, we consider the expansion in terms of **renormalized** Green's functions and interactions (G and Γ).

$$\Sigma(g_0) \Rightarrow \Sigma[G,\Gamma]$$

Bold diagrammatic Monte Carlo method (BDMC)

Previous approach

[Van Houcke et al. (Nat. Phys. 2012)]

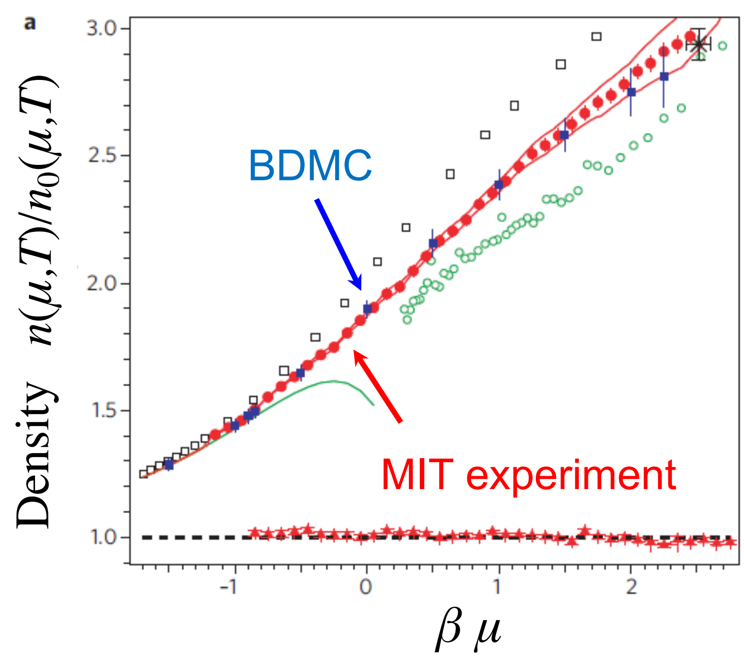
- Convergence radius is assumed to be finite.

Recent new approach

[Rossi, Ohgoe, Van Houcke, Werner (PRL 2018)]

- Convergence radius is zero (divergent series). Combined with the Borel resummation method, we obtained the accurate results.

BDMC vs Experiments (2012)



Continuum limit of lattice model

Lattice model with quadratic dispersion relation

$$\hat{H} = \sum_{\sigma} \int_{BZ} \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{k^2}{2} \hat{\psi}^{\dagger}_{\mathbf{k},\sigma} \hat{\psi}_{\mathbf{k},\sigma} + g_0\, b^3 \sum_{\mathbf{r}\in b\,\mathbb{Z}^3} (\hat{\psi}^{\dagger}_{\uparrow}\hat{\psi}_{\uparrow}\hat{\psi}^{\dagger}_{\downarrow}\hat{\psi}_{\downarrow})(\mathbf{r})$$

$r_e \sim b$

(lattice spacing)

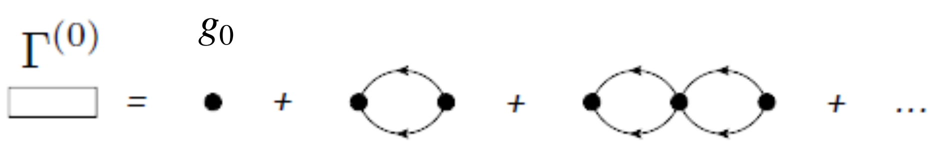
Relation between g_0 and a :

$$\frac{1}{g_0} = \frac{1}{4\pi a} - \int_{\mathcal{B}} \frac{d^3k}{(2\pi)^3} \frac{1}{k^2}$$

Continuum limit

$$g_0 \underset{b\to 0^+}{=} 0^-$$

To eliminate the ultraviolet divergence, we introduce the ladder summation (T-matrix)

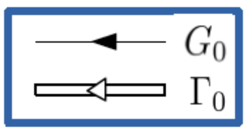


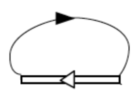
$$\frac{1}{\Gamma^{(0)}(\mathbf{p},\Omega_n)} = \frac{1}{4\pi a} - \int \frac{d\mathbf{k}}{(2\pi)^3} \left[\frac{1}{k^2} + \frac{1 - n^{(0)}_{\uparrow}(\mathbf{p}/2+\mathbf{k}) - n^{(0)}_{\downarrow}(\mathbf{p}/2-\mathbf{k})}{i\Omega_n + 2\mu - p^2/4 - k^2} \right]$$

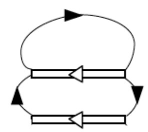
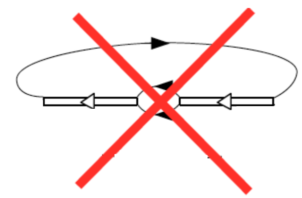
Feynman diagram series

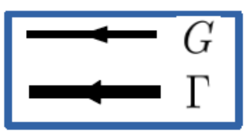
$$Q_{N_{\max}} = \sum_{N=0}^{N_{\max}} a_N \qquad a_N = \sum_{\text{topologies } \mathcal{T}} \int dX_1 \ldots dX_N \; \mathcal{D}(\mathcal{T}; X_1 \ldots X_N)$$

Ladder scheme or Bold scheme (Q = Self energy Σ)



$a_1 =$ 

$a_2 =$  $+$ 



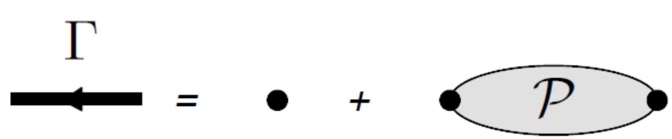
$a_1 =$ 

$a_2 = 0$

Self-consistent calculations are performed for G and Γ.

Γ : pair-propagator

$$\Gamma(\mathbf{r},\tau) = g_0 \delta(\tau) \frac{\delta_{\mathbf{r},\mathbf{0}}}{b^3} - g_0^2 \langle T(\psi_\downarrow \psi_\uparrow)(\mathbf{r},\tau)(\psi_\uparrow^\dagger \psi_\downarrow^\dagger)(\mathbf{0},0)\rangle$$



Large-order asymptotics

Asymptotic estimation of a_N [Lipatov, Sov. Phys. JETP 1977]

Idea : Functional integral representation + Saddle point method

e.g. φ^4 theory

$$Z(g) = \int \mathcal{D}\phi \exp(-S_0\{\phi\} - gS_{\mathrm{int}}\{\phi\})$$

The order *n*-th expansion coefficient (Goursat's formula)

$$Z_N = \frac{1}{2\pi i}\oint_C \frac{dg}{g^{N+1}} \int \mathcal{D}\phi \exp(-S_0\{\phi\} - gS_{\mathrm{int}}\{\phi\})$$

$$= \frac{1}{2\pi i}\oint_C dg \int \mathcal{D}\phi \exp(-S_0\{\phi\} - gS_{\mathrm{int}}\{\phi\} - (N+1)\ln g)$$

Saddle point method (in terms of *g* and *φ*)

$$\overset{N\to\infty}{\sim} S\{\phi_c\}^{-N} N! \qquad \phi_c \text{ : instanton which satisfies } S'\{\phi_c\} = 0$$

Case of the unitary Fermi gas

In our case, we introduce a *coupling constant* z by $\Gamma \to z\Gamma$.

Then, we consider

$$Q(z) = \boxed{\int \mathcal{D}\varphi}\, e^{-S^{(z)}} \, .$$

Its Taylor series is $\boxed{\sum_{N=0}^{\infty} a_N\, z^N}$.

We finally evaluate $Q(z=1) = Q_{\rm phys}$.

For fermionic theory, we utilize the Hubbard-Stratonovich transformation and integrate out the fermions. [Parisi, Itzykson, Zuber, Balian]

$$Q(z) = \int \mathcal{D}\eta \underbrace{\int \mathcal{D}\varphi\; e^{-S^{(z)}[\eta,\varphi]}}_{e^{-S_B^{(z)}[\eta]}}$$

Apply the Lipatov's method

$$a_N \underset{N\to\infty}{\sim} (N/5)!\; A^{-N} \;\cos\left(\frac{4\pi}{5}N\right)$$

Convergence radius is zero

Borel resummation method

Borel resummation method

− **Mathematical procedure to reproduce the non-perturbative quantity $Q(z=1)$ from the divergent series.**

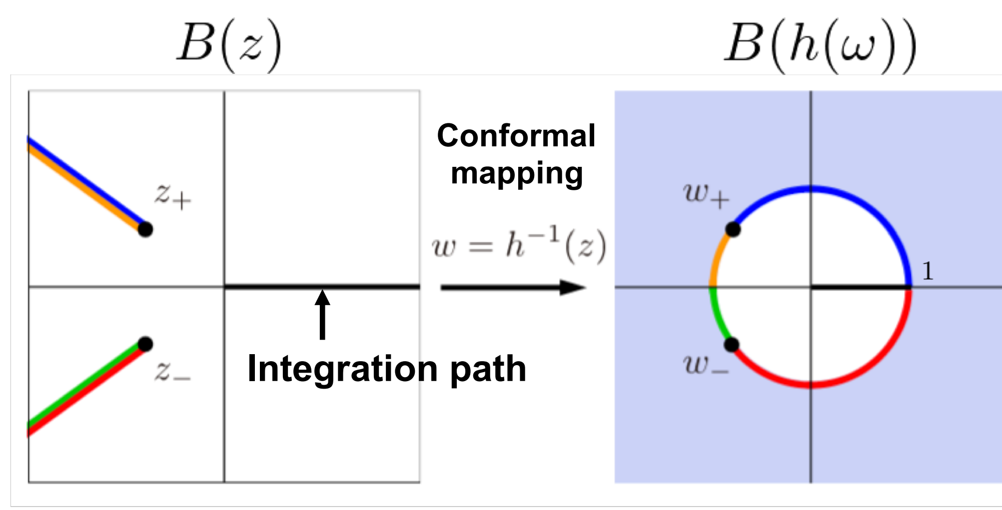
- Borel transform : $B(z) := \sum_{N=0}^{\infty} \frac{a_N}{(N/5)!} z^N \qquad |z| < A$
- Inverse Borel transform : $Q(1) = \int_0^\infty dz\, z^4\, e^{-z^5} B(z)$

Nevanlinna theorem (1919)

Conformal mapping
$\int_0^\infty dz = \int_0^1 dw$

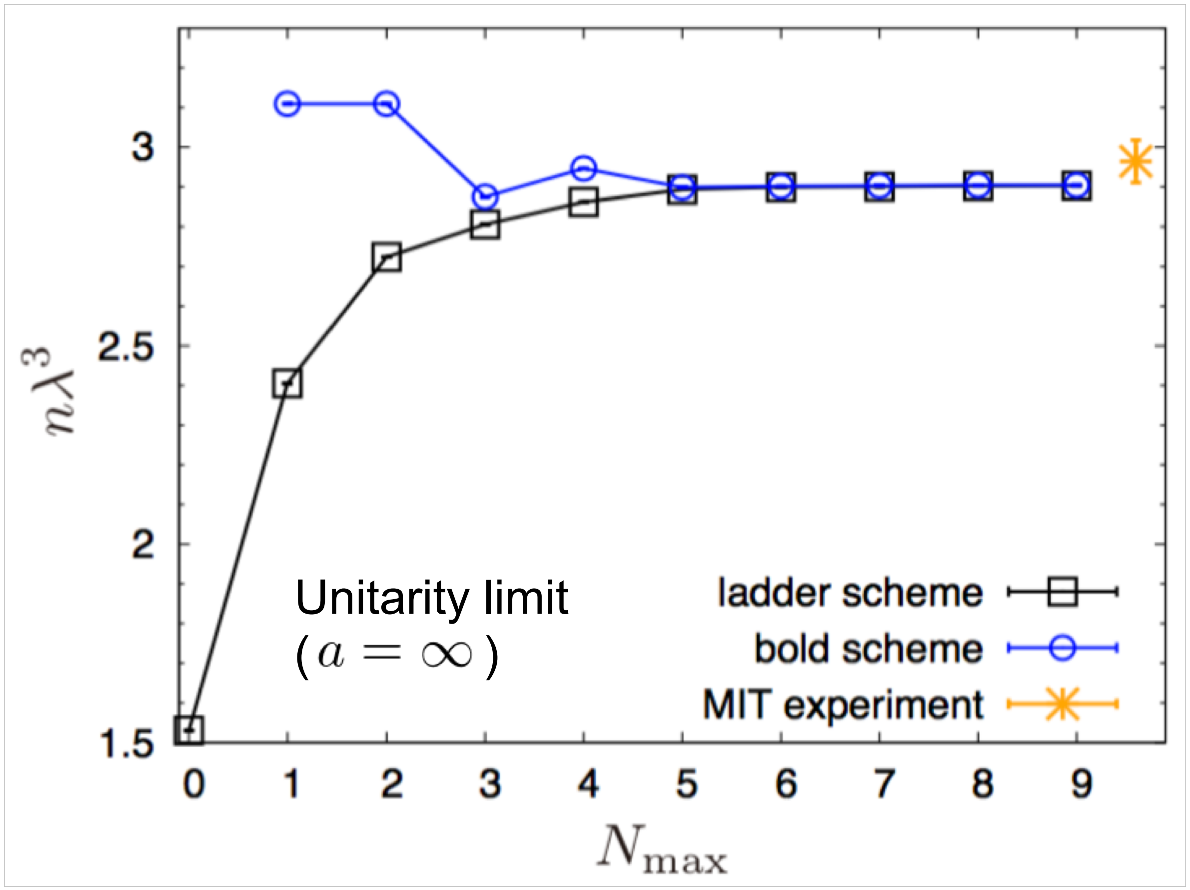
[Le Guillou and Zinn-Justin, PRL 1977]

$z_\pm = A \exp(\pm i4\pi/5)$



Results by Diagrammatic MC

$$\mu = 0 \qquad \left(\frac{T}{T_F} \approx 0.6 \right)$$

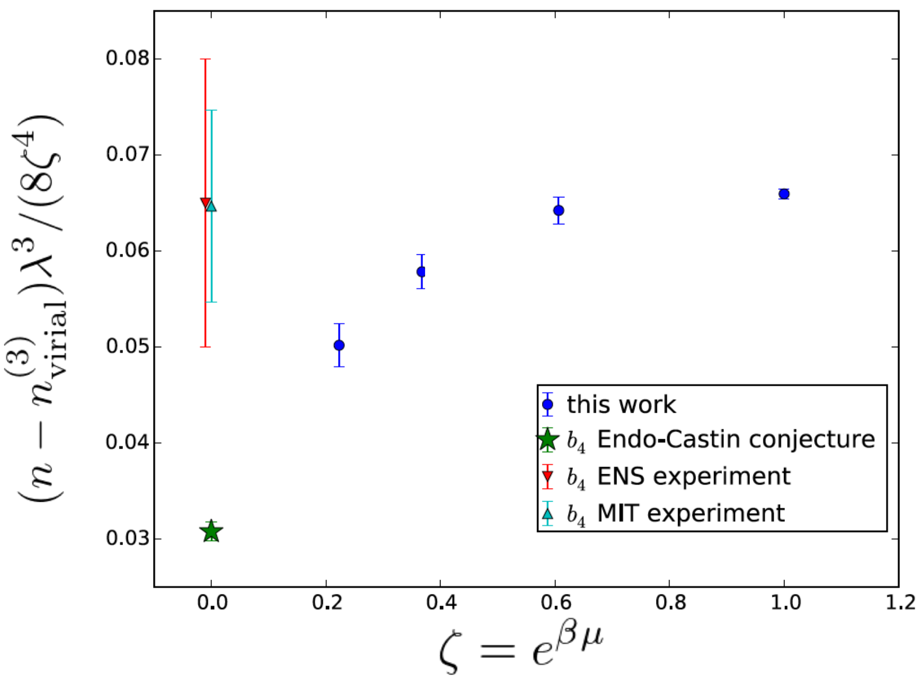


$$\lambda = \sqrt{2\pi\hbar^2\beta/m}$$

Highly accurate results with error of 0.2%.

4th Virial Coefficient

Virial expansion (powers of fugacity $\zeta = e^{\beta\mu}$) : $n^{(J)}_{\text{virial}}\lambda^3 = 2\sum_{j=0}^{J} j b_j \zeta^j$



$$(n - n^{(3)}_{\text{virial}})\lambda^3/(8\zeta^4) \to b_4$$
$$(\zeta \to 0)$$

Our data reveals the behavior at small ζ which the experiments could not.
Our results reconcile the experiments and the Endo & Castin conjecture [J. Phys. 2016].

Tan's contact

Contact $\boxed{C \equiv \lim_{k\to\infty} k^4 n_\sigma(\boldsymbol{k})}$

S. Tan, Ann. Phys. **323** 2971 (2008)
S. Tan, Ann. Phys. **323** 2952 (2008)

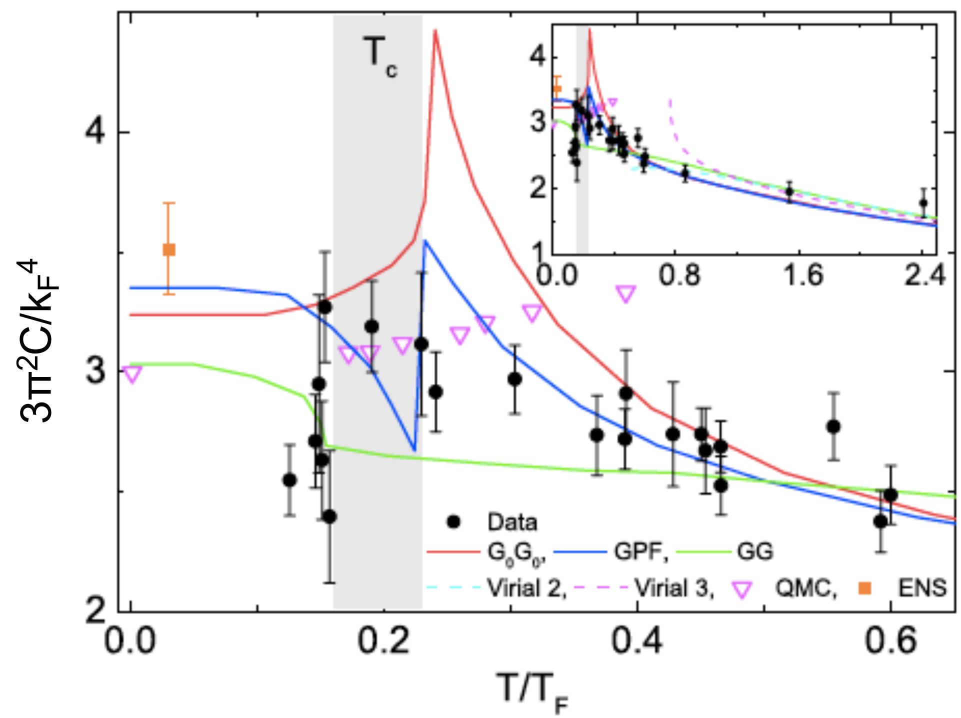
Universal relations

- $C = g_0^2 \langle \psi_\uparrow^\dagger \psi_\downarrow^\dagger \psi_\downarrow \psi_\uparrow(\mathbf{0})\rangle$
  $= -\Gamma(\mathbf{0}, 0-)$

- $$\frac{dE}{d(1/a)} = -\frac{\hbar^2}{4\pi m} C$$

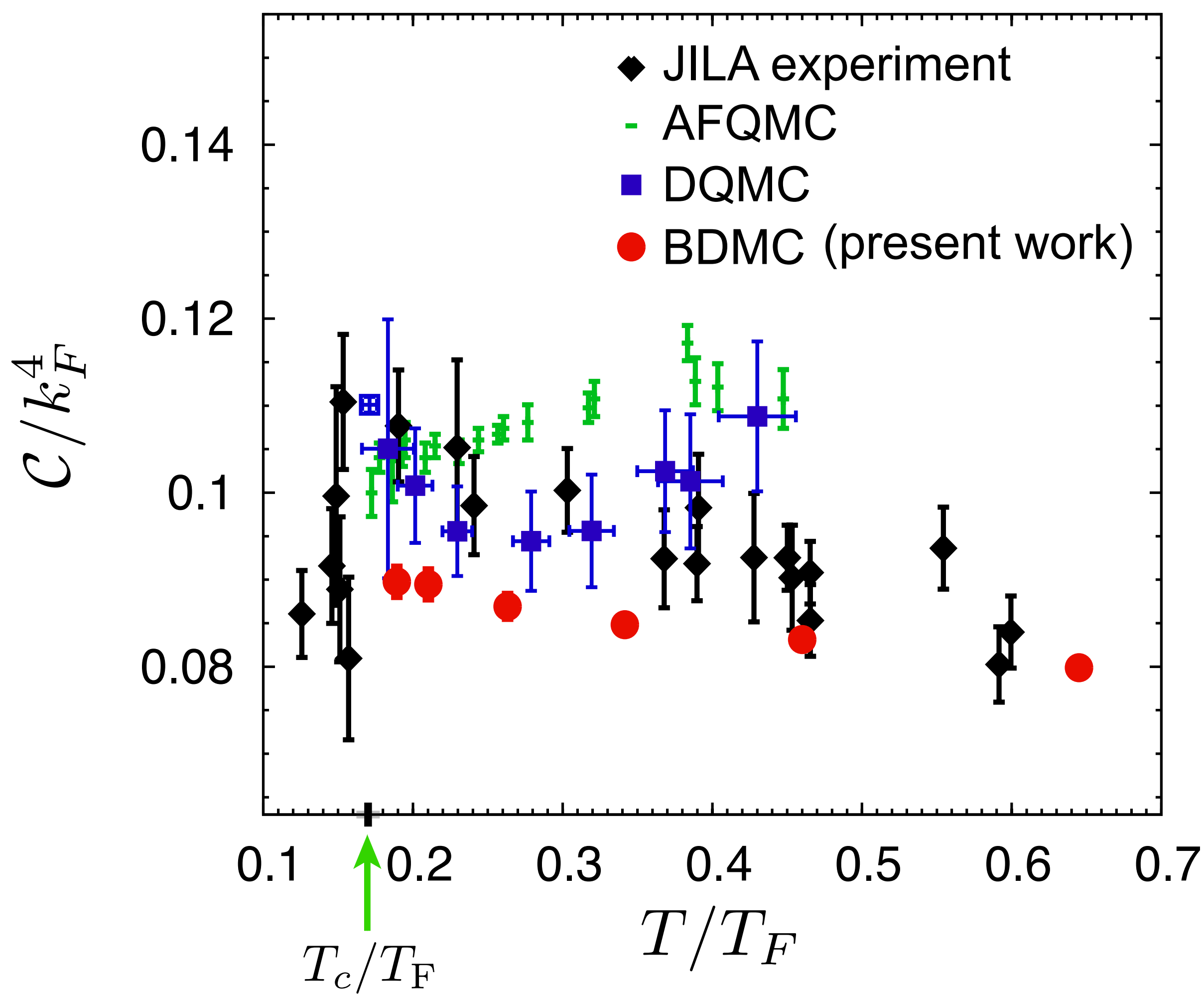
etc.

Sagi et al., PRL 2012 (JILA)



The results are **not** consistent with each other.

Situation of Tan's contact in 2018



Summary

Theory of the unitary Fermi gas (continuum limit)

- Feynman diagram series have zero convergence radius.

  We have overcome the problem by the Borel resummation method.

- By the bold diagrammatic MC, we obtain highly-accurate results of density and Tan’s contact.

[1] R. Rossi, T. Ohgoe, K. Van Houcke and F. Werner, PRL **121** 130405 (2018)

[2] R. Rossi, T. Ohgoe, *et al*, PRL **121** 130406 (2018)

Future issues

Spectral function, imbalanced gas, superfuid phase, …