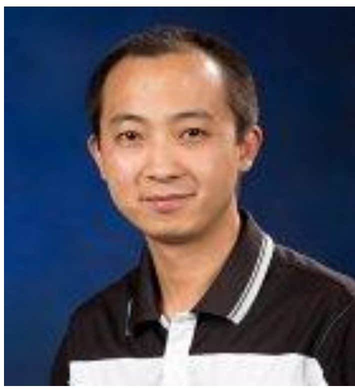
Strongly Interacting Ultracold Fermi gas in the quasirepulsive regime



Lianyi He *Xu-Guang Huang* *Hui Hu*

Xia-Ji Liu

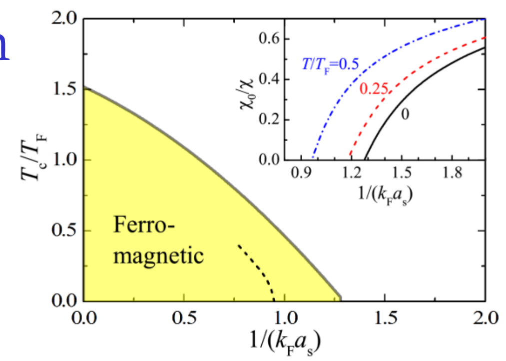
CQOS, Swinburne University

KITP, December 2016

Universality Few-Body System Program

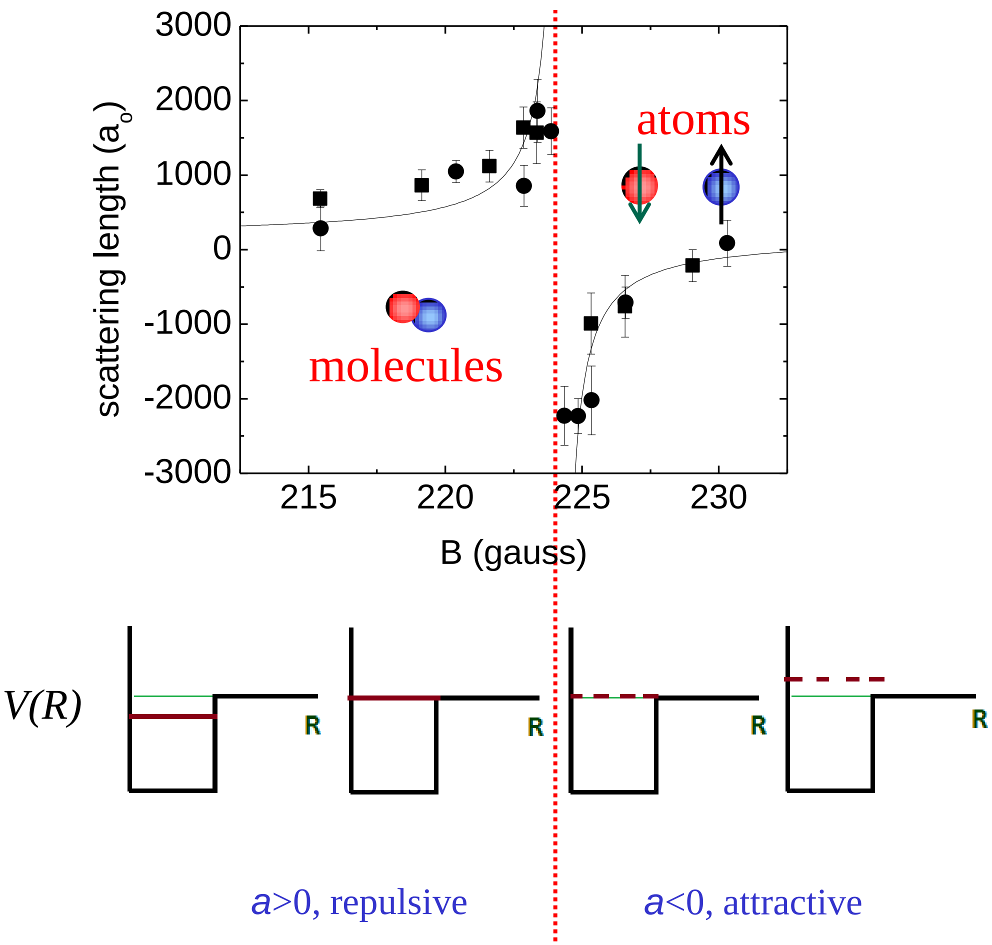
Outline

1. Introduction
2. Stoner ferromagnetic phase transition
3. Definition of upper branch
4. Large-N expansion and dimensional ε expansion
5. Strongly interacting Fermi gas in repulsive regime
6. Conclusion



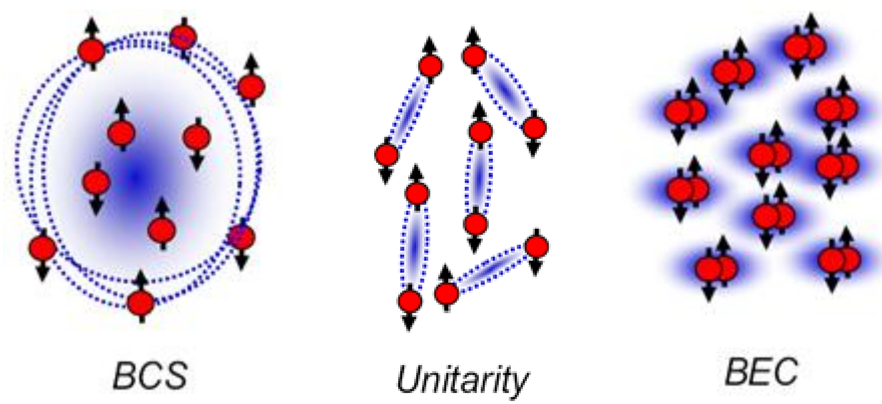
Ultracold Fermion Collision (S-Wave)

Magnetic-field Feshbach resonance

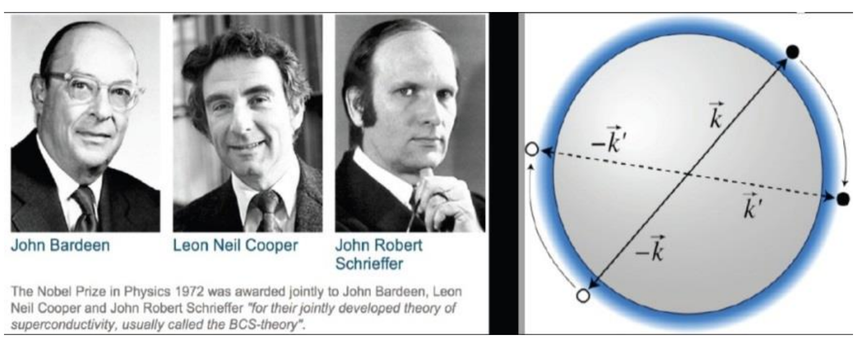


Unitary limit

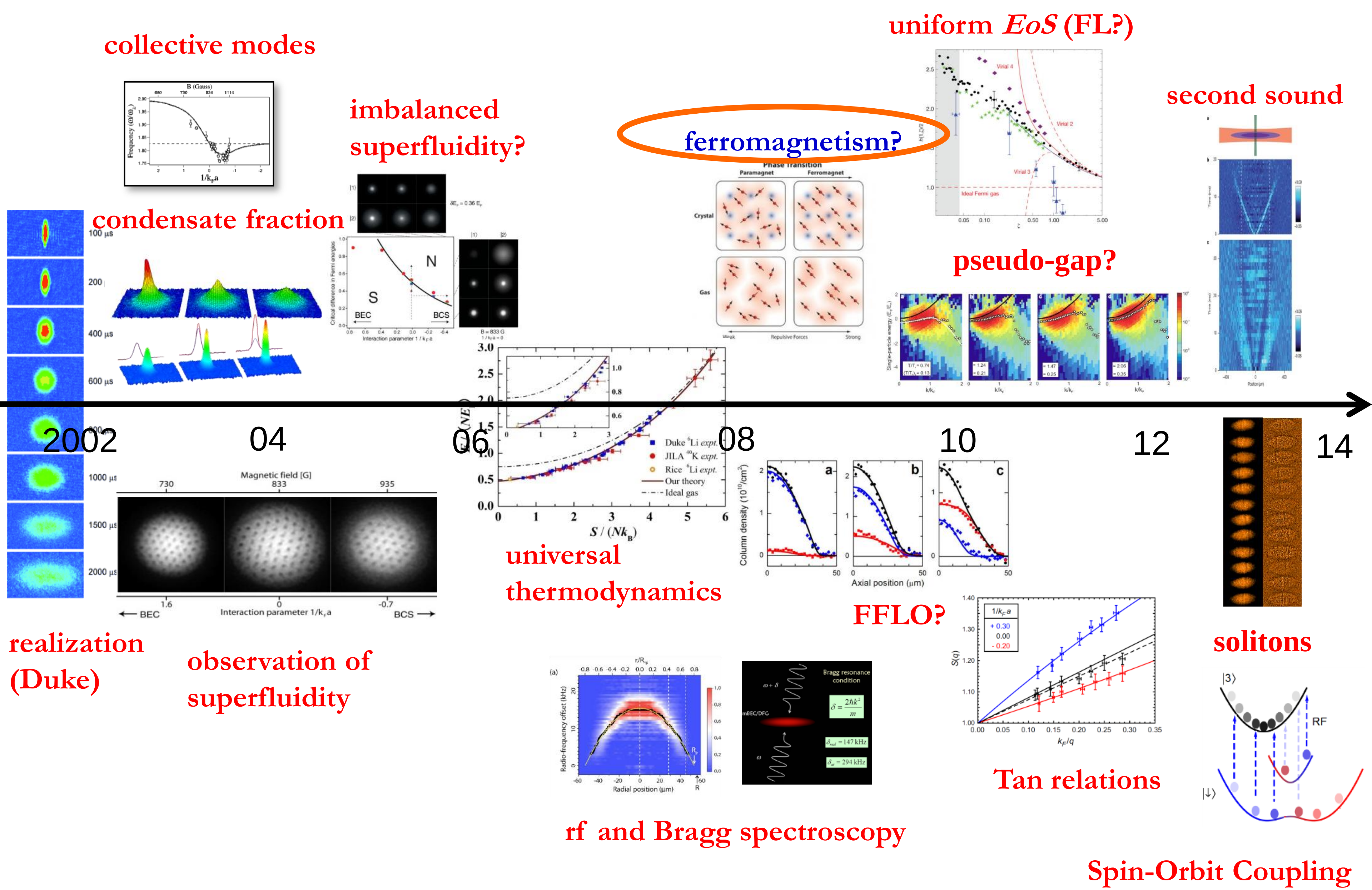
BEC-BCS crossover



BCS fermionic superfluidity → *BEC of molecules*



Global progress (experiment)



Global progress (theory)

1D exact solutions

Large-*N*, ε-expansion, RG?

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

2002 04 06 08 10 12

Quantum Monte Carlo? **Virial expansion**

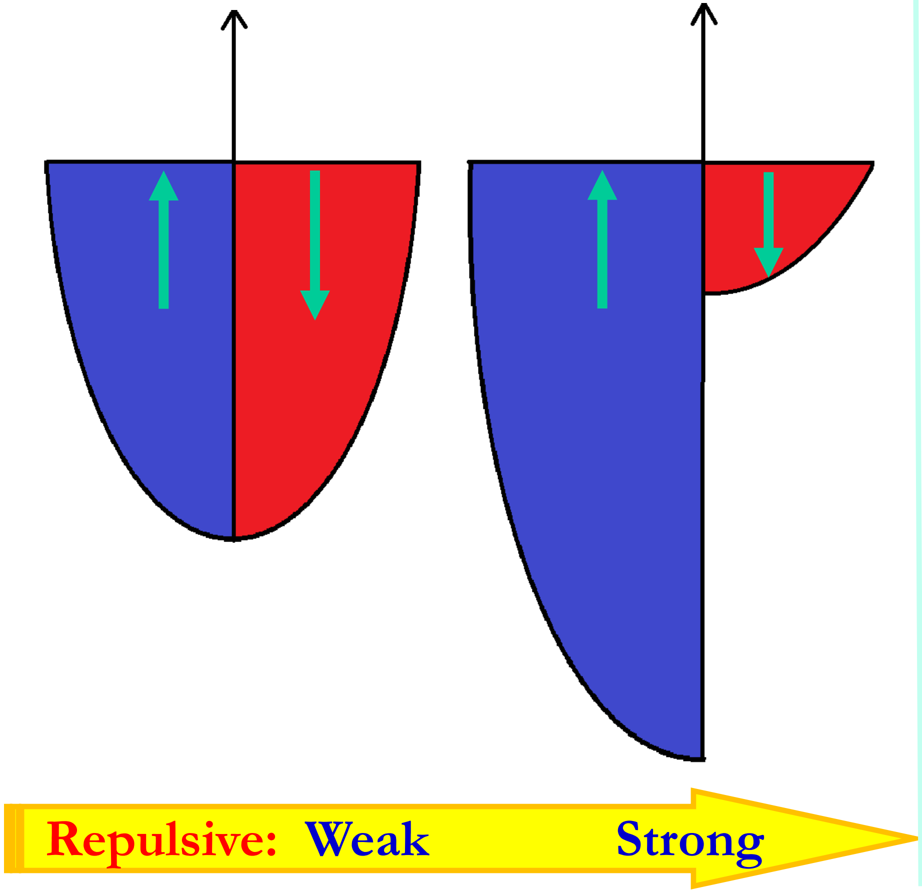
Few-body solutions

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

Question: Stoner Ferromagnetic Phase Transition ?

Phase transition for a repulsive Fermi gas (U>0)?

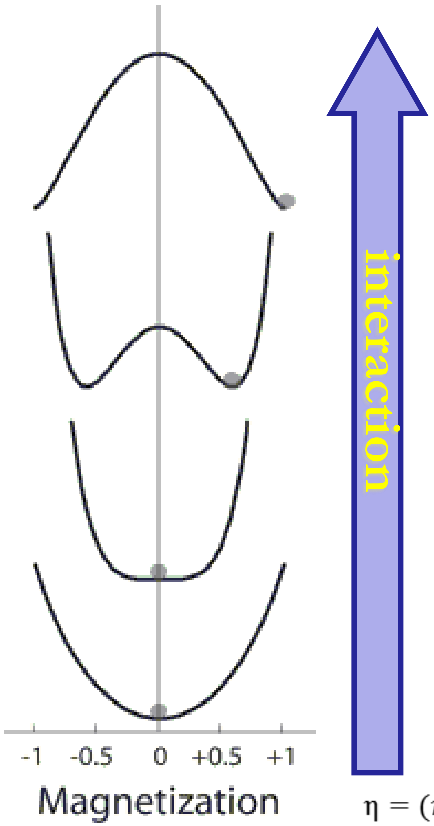
Spontaneous spin polarization decreases interaction energy but increases kinetic energy of electrons



$$H = \int d^3x\{\psi_\sigma{}^+\left(\frac{\nabla^2}{2m}\right)\psi_\sigma + U_0\Psi^+{}_\uparrow\Psi^+{}_\downarrow\Psi_\downarrow\Psi_\uparrow\}$$

Mean Field Model: $\eta = (n_1 - n_2)/(n_1 + n_2)$

$$E = E_F 2Vn\{\frac{3}{10}\left[(1+\eta)^{\frac{5}{3}} + (1-\eta)^{\frac{5}{3}}\right] + \frac{2}{3\pi}k_F a(1+\eta)(1-\eta)\}$$

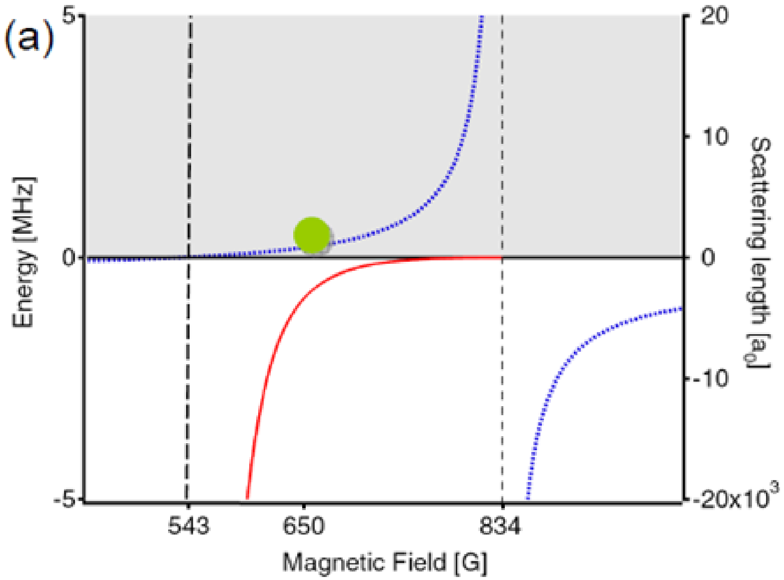


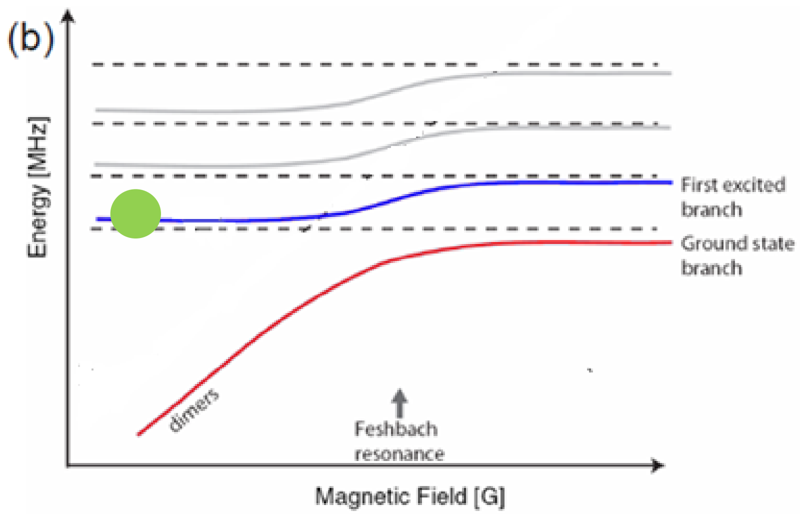
$$k_F a = \frac{\pi}{2}$$

U to W shape

$\eta = (n_1 - n_2)/(n_1 + n_2)$

Question: How to realize a repulsive Fermi gas?





Feshbach resonance in 6Li between the two lowest hyperfine states. The red line shows the molecular binding energy, and the blue lines show the scattering length.

The blue line below the Feshbach resonance represents the excited state where the interaction is repulsive.

Experimentally, severe atom loss!!!

Stoner Ferromagnetic Phase Transition

Experiment	Results
MIT **Ketterle group** (Science 2009)	ruled out by spin-density fluctuation measurement (PRL 2012)
Innsbruck **Grimm group** (Nature 2012)	repulsive polaron suggestion at a narrow FR
Cambridge **Köhl group** (Nature 2012)	repulsive polaron suggestion at low-dimensions
Theory: Phase Transition at T=0	$\mathbf{k_F a_s}$
First order perturbation theory by Stoner 1937	$\pi/2$
Second order perturbation theory (2nd PT) (PRL 95, 230403)	**1.054**
Quantum Monte Carlo (PRL 103, 207201; 105, 030405; PNAS 108, 51); Variational calculation (PRA 83, 053635); **Non-perturbative ladder approximation (PRA 85, 043624);**	**0.8-0.9**

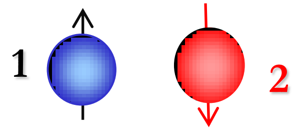
Stoner Ferromagnetic Phase Transition

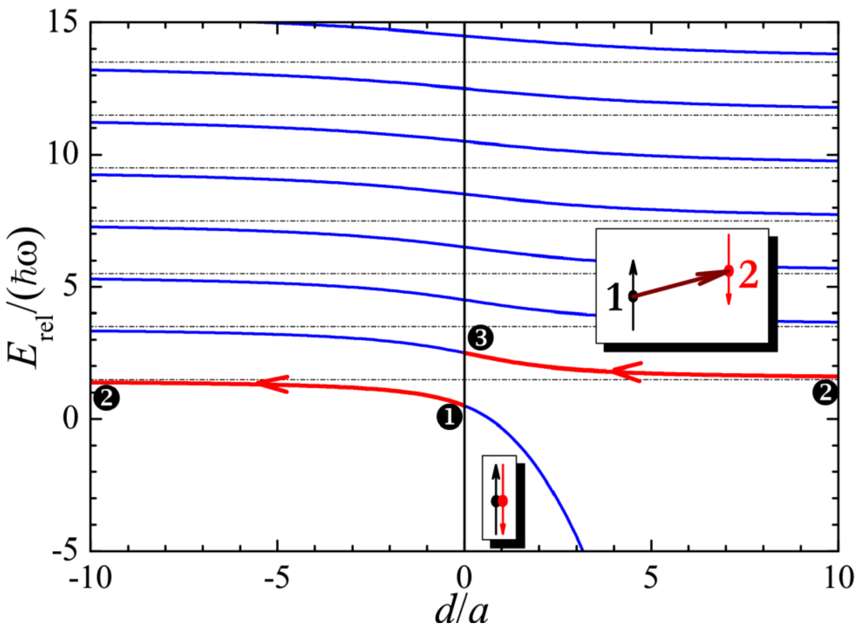
Phase transition for a strongly interacting Fermi gas?

No theoretical description at finite temperature, apart from the 2^{nd} PT and the polaron limit.

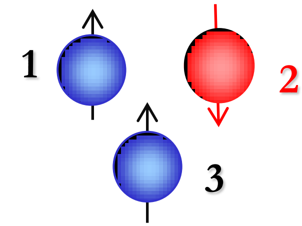
A grand experimental & theoretical challenge!!!

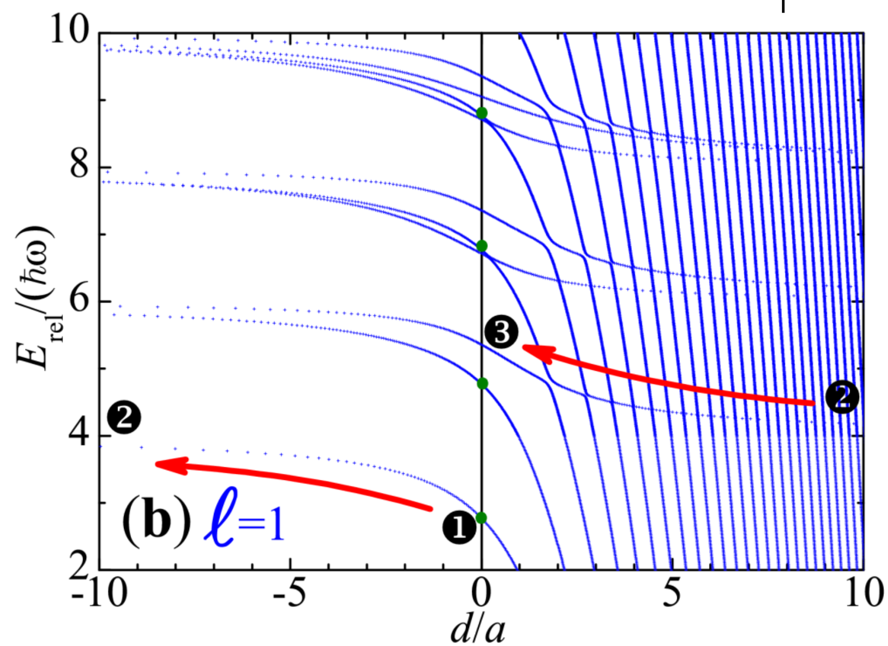
Two Particles





Three Particles





$$H = H_{cm} + H_{rel}$$

Phys. Rev. Lett. 102, 160401 (2009)

The concept of upper branch is well-defined for a two-particle system, however, an unambiguous definition of upper branch is yet to be established

Upper Branch: previous works

The first work for upper branch investigated by Engelbrecht and Randeria in 1990 (PRL)

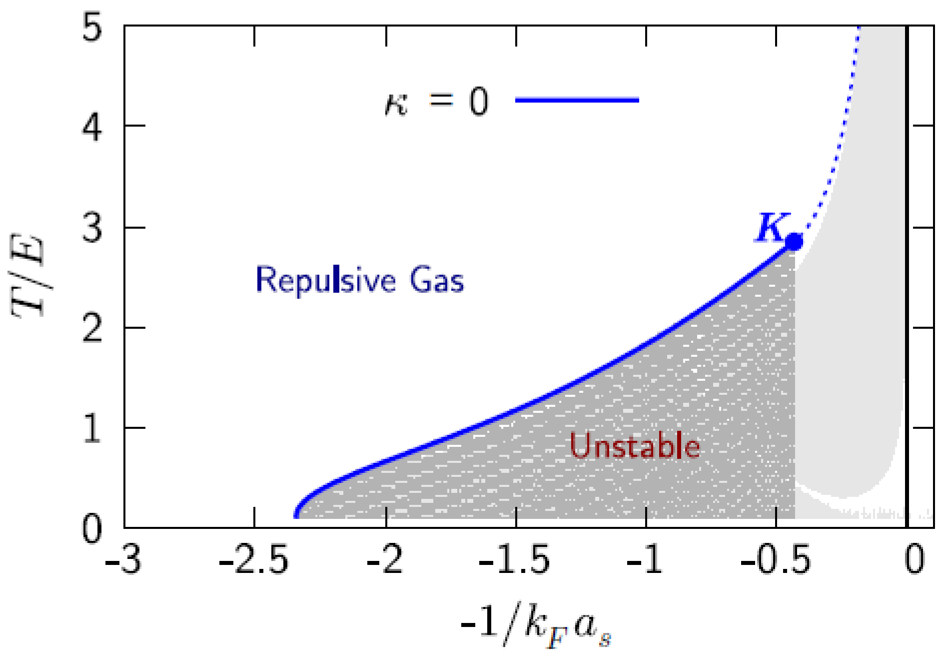
Important clarification by Shenoy and Ho (PRL2011):
the excluded molecular pole approximation (EMPA), i.e., excluding the contribution from the molecular states

PRL 107, 210401 (2011) PHYSICAL REVIEW LETTERS week ending 18 NOVEMBER 2011

Nature and Properties of a Repulsive Fermi Gas in the Upper Branch of the Energy Spectrum

Vijay B. Shenoy[1,*] and Tin-Lun Ho[2,†]
[1]Centre for Condensed Matter Theory, Indian Institute of Science, Bangalore 560 012, India
[2]Department of Physics, Ohio State University, Columbus, Ohio 43210, USA
(Received 15 June 2011; published 14 November 2011)

We generalize the Noziéres-Schmitt-Rink method to study the repulsive Fermi gas in the absence of molecule formation, i.e., in the so-called "upper branch." We find that the system remains stable except close to resonance at sufficiently low temperatures. With increasing scattering length, the energy density of the system attains a maximum at a positive scattering length before resonance. This is shown to arise from Pauli blocking which causes the bound states of fermion pairs of different momenta to disappear at different scattering lengths. At the point of maximum energy, the compressibility of the system is substantially reduced, leading to a sizable uniform density core in a trapped gas. The change in spin susceptibility with increasing scattering length is moderate and does not indicate any magnetic instability. These features should also manifest in Fermi gases with unequal masses and/or spin populations.



Two key features:

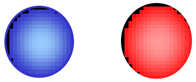
(1)A switch from the upper branch to ground branch (negative Tan's contact);

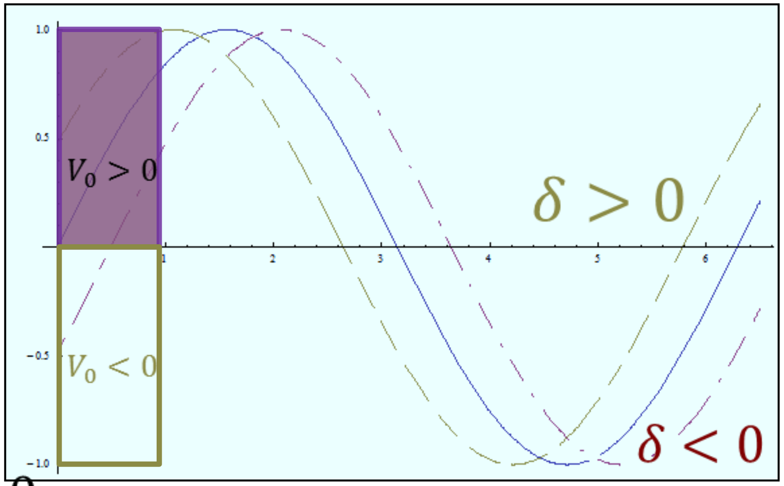
(2)The large unstable area at low temperatures.

Definition of the Upper Branch

Knowledge from a two-particle system

Scattering problem:





(**1**) bound state as pole $\delta \to \pi$

$$\delta_{2\mathrm{B}}(k) = \pi - \arctan(ka_s) \quad \text{for } a_s > 0$$
$$\delta_{2\mathrm{B}}(k) = \quad - \arctan(ka_s) \quad a_s < 0$$

(**2**) Naively, Phase shift: repulsive $\delta < 0$

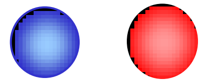
attractive $\delta > 0$

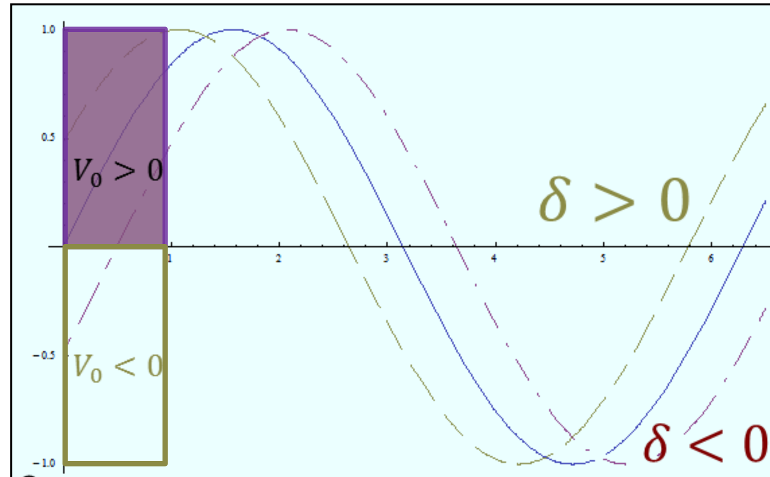
(**3**) Therefore, for the **upper branch**, phase π difference !!!

$$\delta_{2\mathrm{B}}(k) = - \arctan(ka_s) \quad a_s > 0$$

Definition of the Upper Branch

Knowledge from a two-particle system

Scattering problem: 



Phase shift: repulsive $\delta < 0$

attractive $\delta > 0$

bound state as pole $\delta \to \pi$

$$\delta_{2\mathrm{B}}(k) = \pi - \arctan(k a_s) \quad \text{for } a_s > 0$$
$$\delta_{2\mathrm{B}}(k) = \quad - \arctan(k a_s) \quad a_s < 0$$

phase shift δ in many body system *Nozières and Schmitt-Rink*, JLTP **59**, 195 (1985)

$$\delta_{\mathrm{att}}(q,\omega) \equiv -\arg[-\Gamma^{-1}(\mathbf{q}, i\nu_l \to \omega + i0^+)]$$

Γ is vertex function

repulsive phase shift differs from attractive phase shift by a constant shift π

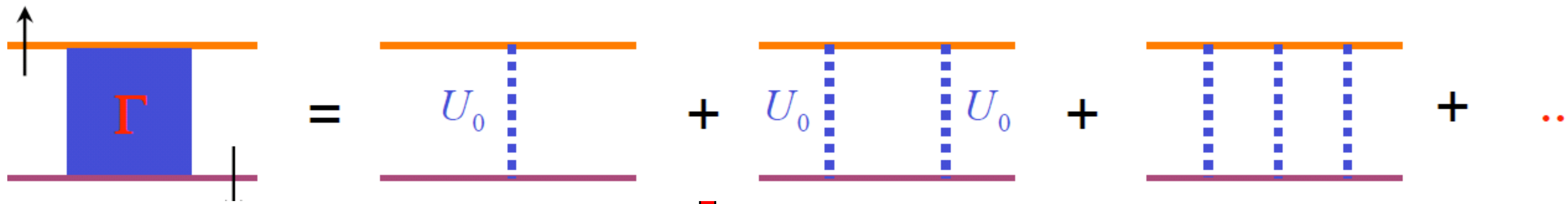
$$\delta_{\mathrm{rep}}(\mathbf{q},\omega) = [\delta_{\mathrm{att}}(\mathbf{q},\omega) - \pi]\,\Theta\,[\omega - \omega_b(\mathbf{q})]$$

ω_b: the existence of a two-body bound state

This means that the **π** *shift coming from the bound state should be subtracted*

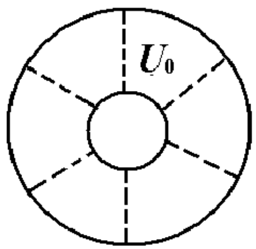
Nozieres & Schmitt-Rink theory

T-matrix



For *Nozieres & Schmitt-Rink* (NSR) thermodynamic potential: (above critical temperature)

$\delta\Omega = \; \ldots +$



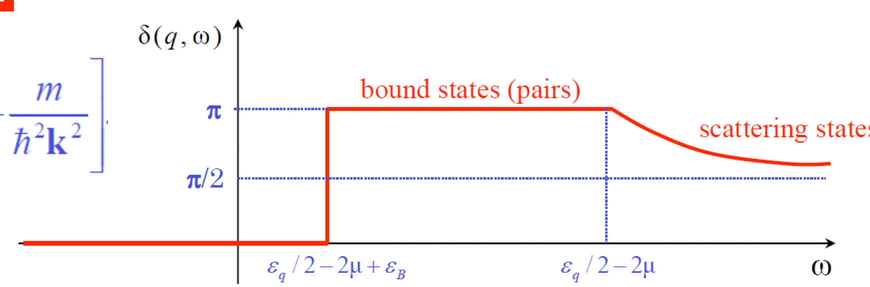
$+ \ldots = \delta\Omega$ (free bosons)

$$\Omega - \Omega^{(1)} = -V \int \frac{d\mathbf{q}}{(2\pi)^3} \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{d\omega}{e^{\beta\omega}-1} \delta(\mathbf{q}, \omega).$$

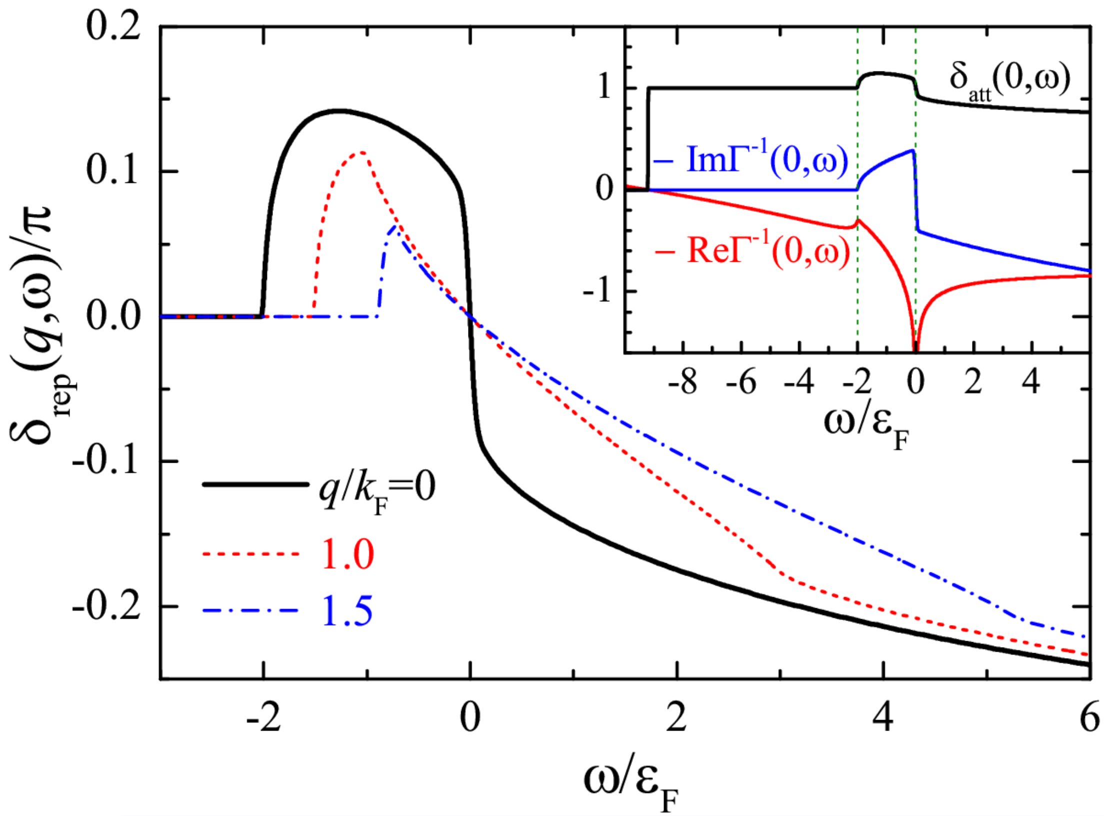
$$\delta(q,\omega) \equiv -\arg[-\Gamma^{-1}(\mathbf{q}, i\nu_l \to \omega + i0^+)]$$

$$\Gamma^{-1}(\mathbf{q}, \omega + i0^+) = \frac{m}{4\pi\hbar^2 a} + \int \frac{d\mathbf{k}}{(2\pi)^3} \left[\frac{f(\xi_{\mathbf{q}/2+\mathbf{k}}) + f(\xi_{\mathbf{q}/2-\mathbf{k}}) - 1}{\omega + i0^+ - \xi_{\mathbf{q}/2+\mathbf{k}} - \xi_{\mathbf{q}/2-\mathbf{k}}} - \frac{m}{\hbar^2 \mathbf{k}^2} \right].$$

$$n - n^{(1)} = \int \frac{d\mathbf{q}}{(2\pi)^3} \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{d\omega}{e^{\beta\omega}-1} \frac{\partial \delta(q,\omega)}{\partial \mu}$$



Phase Shift in the Upper Branch



$k_F a = 0.5$

$$\delta_{\text{rep}}\left(\mathbf{q},\omega\right) = \left[\delta_{\text{att}}\left(\mathbf{q},\omega\right) - \pi\right]\Theta\left[\omega - \omega_s\left(\mathbf{q}\right)\right]$$

Note: apart from the bound state, the contribution to the phase shift from the scattering state also decreases by π. Previous EMPA prescription: Shenoy and Ho, PRL 107, 210401 (2011)

1) No branch switch and there is no violation of Tan's adiabatic theorem.
2) Applied to arbitrary coupling strength and low-*T* regime within a large-*N* expansion

Phase Shift in the Upper Branch

$$\delta_{\mathrm{rep}}(\mathbf{q},\omega) = \left[\delta_{\mathrm{att}}(\mathbf{q},\omega) - \pi\right]\Theta\left[\omega - \omega_s(\mathbf{q})\right]$$

Proof: from the viewpoint of virial expansion $z = e^{\beta\mu} \ll 1$

$$\Omega^{(2)} = \sum_{n=2}^{\infty} \Omega_n^{(2)} = -\frac{2T}{\lambda_{\mathrm{dB}}^3} \sum_{n=2}^{\infty} b_n^{(2)} z^n$$

$$\Omega - \Omega^{(1)} = -V \int \frac{d\mathbf{q}}{(2\pi)^3} \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{d\omega}{e^{\beta\omega}-1} \delta(\mathbf{q},\omega)$$

$$\delta(q,\omega) \equiv -\arg\left[-\Gamma^{-1}(\mathbf{q}, i\nu_l \to \omega + i0^+)\right]$$

$$b\left(E + \frac{\mathbf{q}^2}{4m} - 2\mu\right) = \sum_{n=1}^{\infty} z^{2n} e^{-n\beta\left(E + \frac{\mathbf{q}^2}{4m}\right)}$$

$$f(\varepsilon - \mu) = \sum_{n=1}^{\infty} z^n (-1)^{n-1} e^{-n\beta\varepsilon}$$

$$\delta(E,\mathbf{q}) = \delta_{2\mathrm{B}}(E) + \sum_{n=1}^{\infty} z^n \phi_n(E,q)$$

$$\Gamma^{-1}(q,\omega + i0^+) = \frac{m}{4\pi\hbar^2 a} + \int \frac{d\mathbf{k}}{(2\pi)^3}\left[\frac{f(\xi_{\frac{q}{2}+k}) + f(\xi_{\frac{q}{2}-k}) - 1}{\omega + i0^+ - \xi_{\frac{q}{2}+k} - \xi_{\frac{q}{2}-k}} - \frac{m}{\hbar^2 \mathbf{k}^2}\right]$$

$$E = \omega + 2\mu - \frac{\mathbf{q}^2}{4m}$$

By resuming only the scattering contribution to all order in z, we obtain precisely the repulsive phase shift prescription, following the EMPA idea by Shenoy and Ho.

Large-N Expansion Theory

The method is based on the introduction of an artificial small parameter $\frac{1}{N}$,
with N the number of distinct "spin" ½ fermion flavors with Sp(2N) symmetry

$$\mathcal{H} = \sum_{\sigma=\uparrow,\downarrow} \int d^3\mathbf{r}\,\psi_\sigma^\dagger(\mathbf{r})\left(-\frac{\nabla_\mathbf{r}^2}{2m} - \mu_\sigma\right)\psi_\sigma(\mathbf{r}) + \lambda \int d^3\mathbf{r}\,\psi_\uparrow^\dagger(\mathbf{r})\psi_\downarrow^\dagger(\mathbf{r})\psi_\downarrow(\mathbf{r})\psi_\uparrow(\mathbf{r}),$$

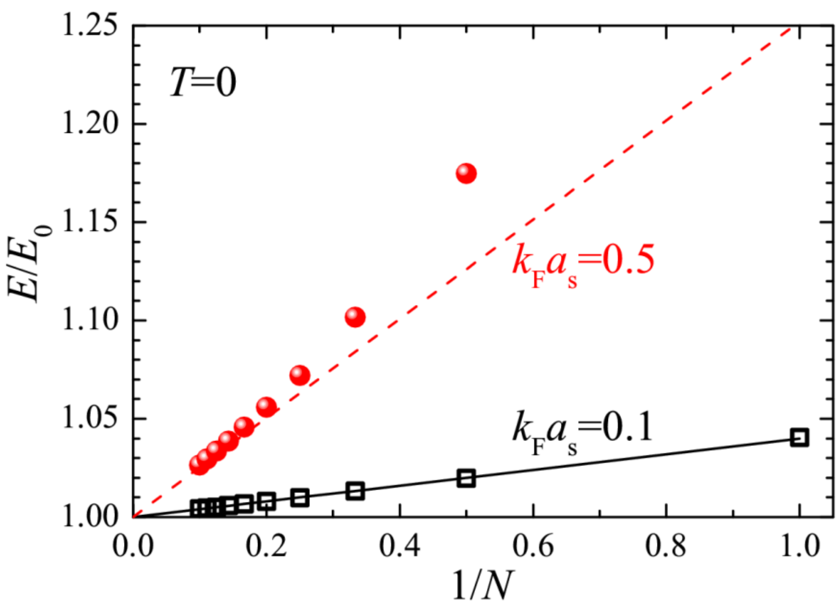
$$\mathcal{H} = \sum_{i=1}^{N}\sum_{\sigma=\uparrow,\downarrow} \int d^3\mathbf{r}\,\psi_{i\sigma}^\dagger(\mathbf{r})\left(-\frac{\nabla_\mathbf{r}^2}{2m} - \mu\right)\psi_{i\sigma}(\mathbf{r}) + \frac{\lambda}{N}\sum_{i,j=1}^{N} \int d^3\mathbf{r}\,\psi_{i\uparrow}^\dagger(\mathbf{r})\psi_{i\downarrow}^\dagger(\mathbf{r})\psi_{j\downarrow}(\mathbf{r})\psi_{j\uparrow}(\mathbf{r}),$$

$N \to \infty$ is the solution of the BCS mean-field theory

There is no phase transition with decreasing N

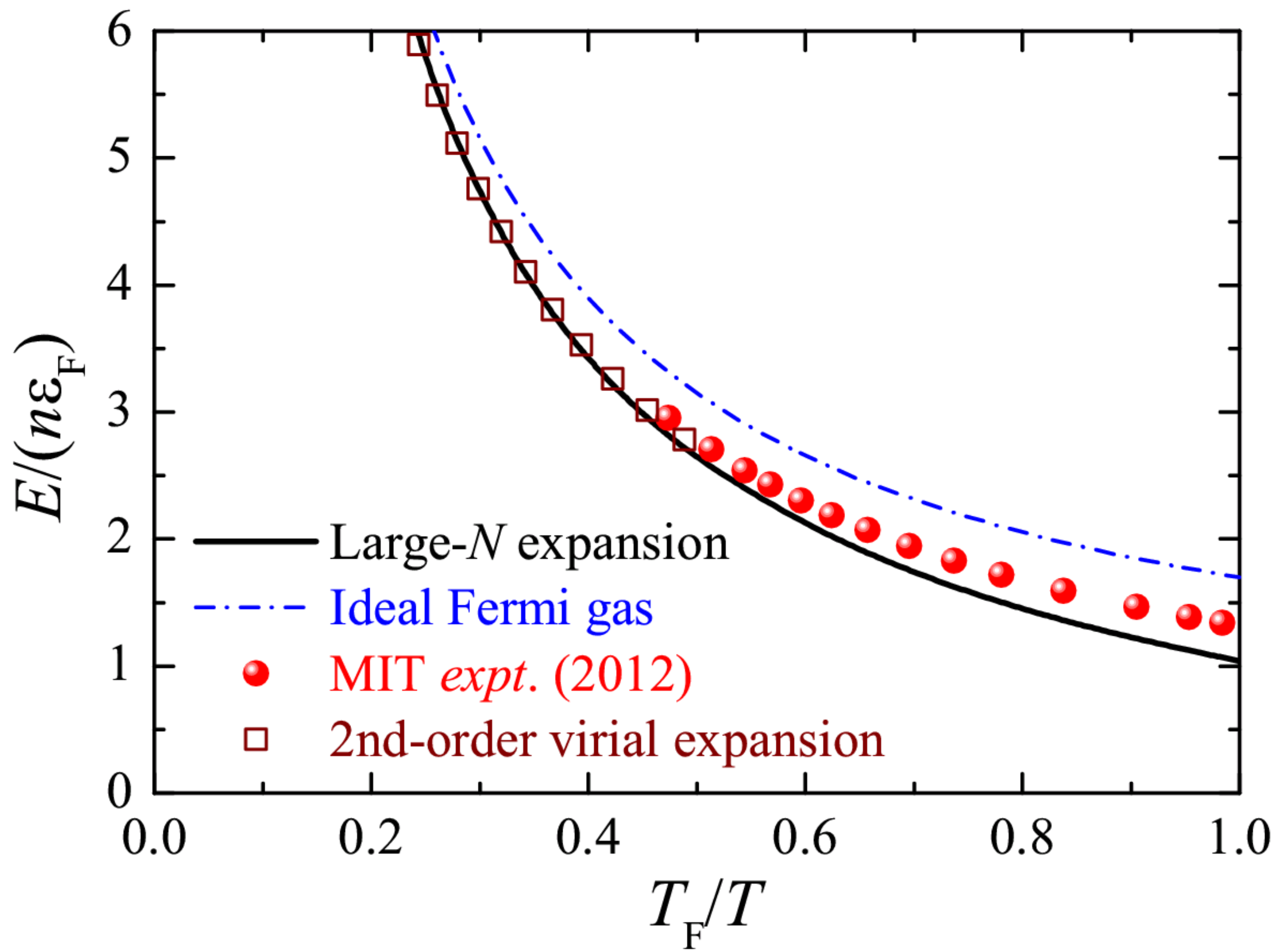
$$\mu(N) = \mu_0 + \mu_1/N + O(1/N^2)$$

$$E(N) = E_0 + E_1/N + O(1/N^2)$$



Compute corrections in the small parameter $1/N$ and obtain a systematic expansion of the linear dependence

Large-N Expansion Theory: **Benchmark**



Benchmark of $1/N$ expansion for attractive unitary Fermi gas:

Comparison with MIT measurement and the 2nd virial expansion

ϵ Expansion Theory

ϵ Expansion Theory: a expansion around four or two spatial dimensions

developed by Nishida and Son Phys. Rev. Lett. 97, 050403 $\epsilon = 4 - \mathrm{d}$ or $\bar{\epsilon} = d - 2$

Two dimensions: a system of non-interacting composite bosons in 2D.

Four dimensions: mean field approximation is good

NSR

$$\Omega = -k_B T \sum_{\mathbf{k}\sigma} \ln\left(1 + e^{-\beta \xi_{\mathbf{k}\sigma}}\right) + k_B T \sum_{\mathbf{q}, i\nu_n} \ln\left[-\Gamma^{-1}\left(\mathbf{q}, i\nu_n\right)\right]$$

$$\sum_{\mathbf{k}} \equiv \int \frac{d\mathbf{k}}{(2\pi)^d} = \frac{2}{(4\pi)^{d/2}\Gamma\left(\frac{d-1}{2}\right)\pi^{1/2}} \int_0^\infty k^{d-1} dk \int_0^\pi (\sin\theta)^{d-2} d\theta = \frac{2}{(4\pi)^{d/2}\Gamma\left(\frac{d}{2}\right)} \int_0^\infty k^{d-1} dk.$$

Є expansion

$$\xi_{NLO} = 0.377 \pm 0.014$$

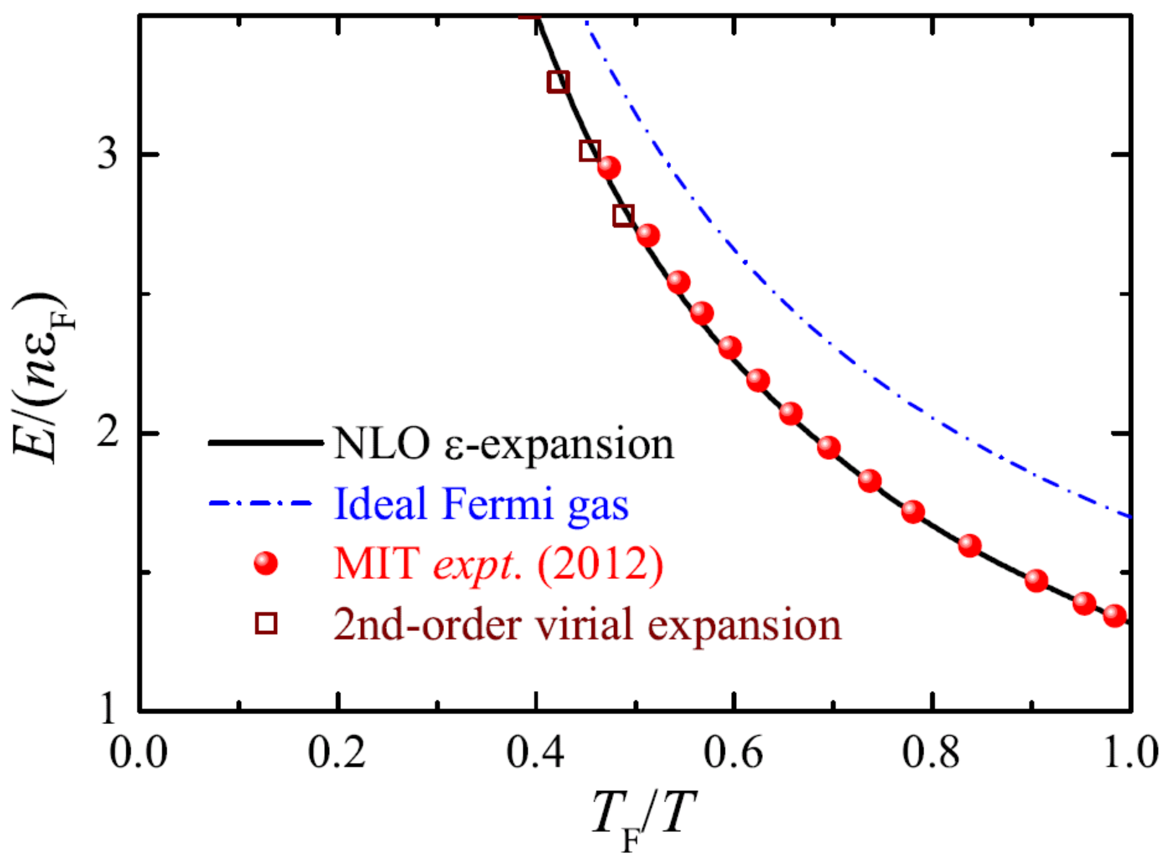
$$(T_c/T_F)_{NLO} = 0.183 \pm 0.014$$

MIT *expt.*

$$\xi = 0.376 \pm 0.005$$

$$T_c/T_F = 0.167 \pm 0.013$$

ϵ Expansion Theory: **Benchmark**

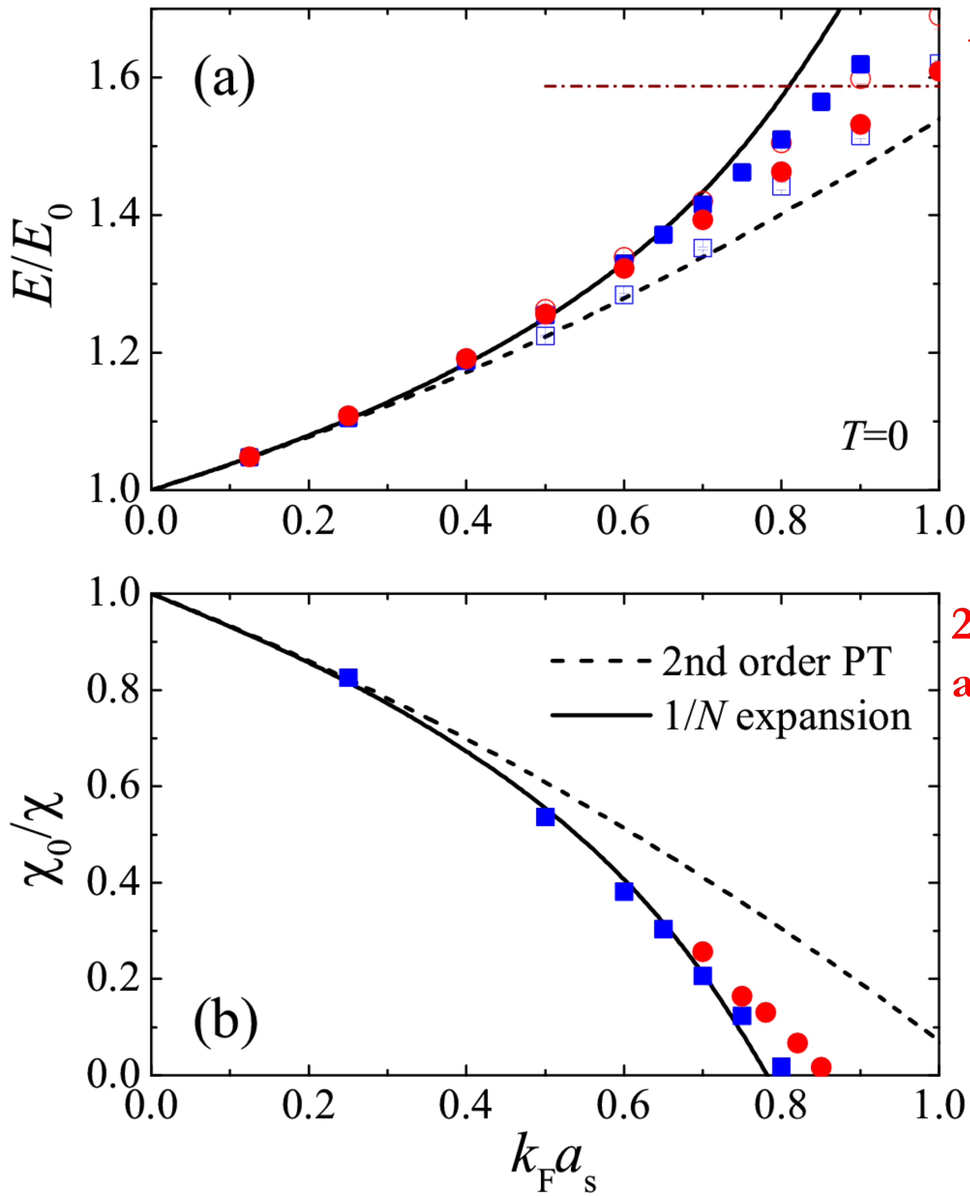


Benchmark of ϵ expansion for attractive unitary Fermi gas:

Comparison with MIT measurement and the 2nd virial expansion

Liu Physics Reports 524, 37 (2013).

Stoner Ferromagnetism at T=0



1)Stoner ferromagnetic transition

$$(k_F a_s)_c \simeq 0.78$$ (spin susceptibility diverges)

close to the QMC prediction

QMC data for hard-sphere potential (blue) and square-wall potential (red)

S. Pilati et al PRL 105, 030405(2010)

S. Y. Chang et al PNAS 108, 51 (2011)

2) agrees with the second-order perturbation at the weak coupling

$$\frac{E}{E_0} = 1 + \frac{10}{9\pi} k_F a_s + \frac{4(11 - 2\ln 2)}{21\pi^2} (k_F a_s)^2 ,$$

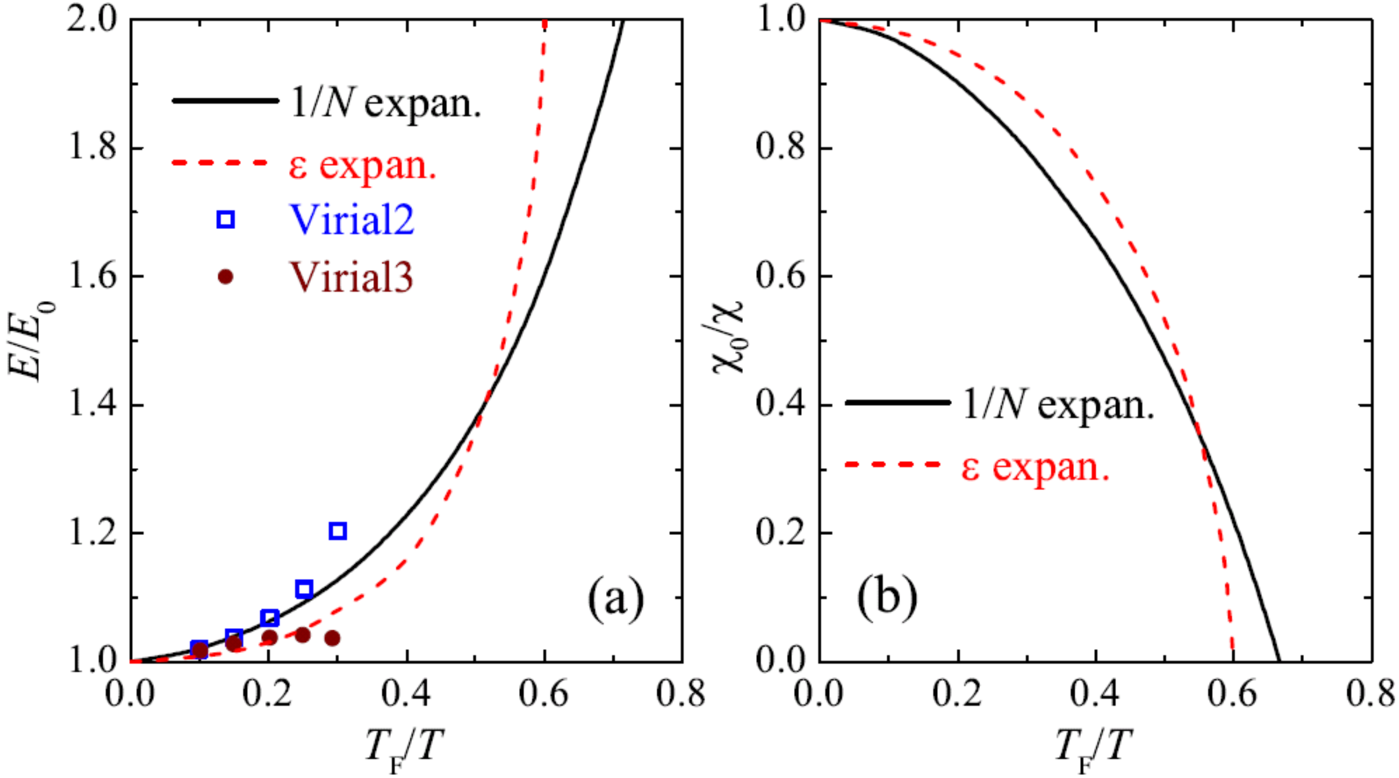
$$\frac{\chi_0}{\chi} = 1 - \frac{2}{\pi} k_F a_s - \frac{16(2 + \ln 2)}{15\pi^2} (k_F a_s)^2 .$$

V. M. Galitskii, Sov. Phys. JETP 7, 104 (1958)

$$E_0 = (3/5) n \varepsilon_F \qquad \chi_0 = 3/(2n\varepsilon_F)$$

The energy and spin susceptibility of a repulsive Fermi gas as a function of interaction parameter

Stoner Instability of a Unitary Fermi Gas in the Upper Branch



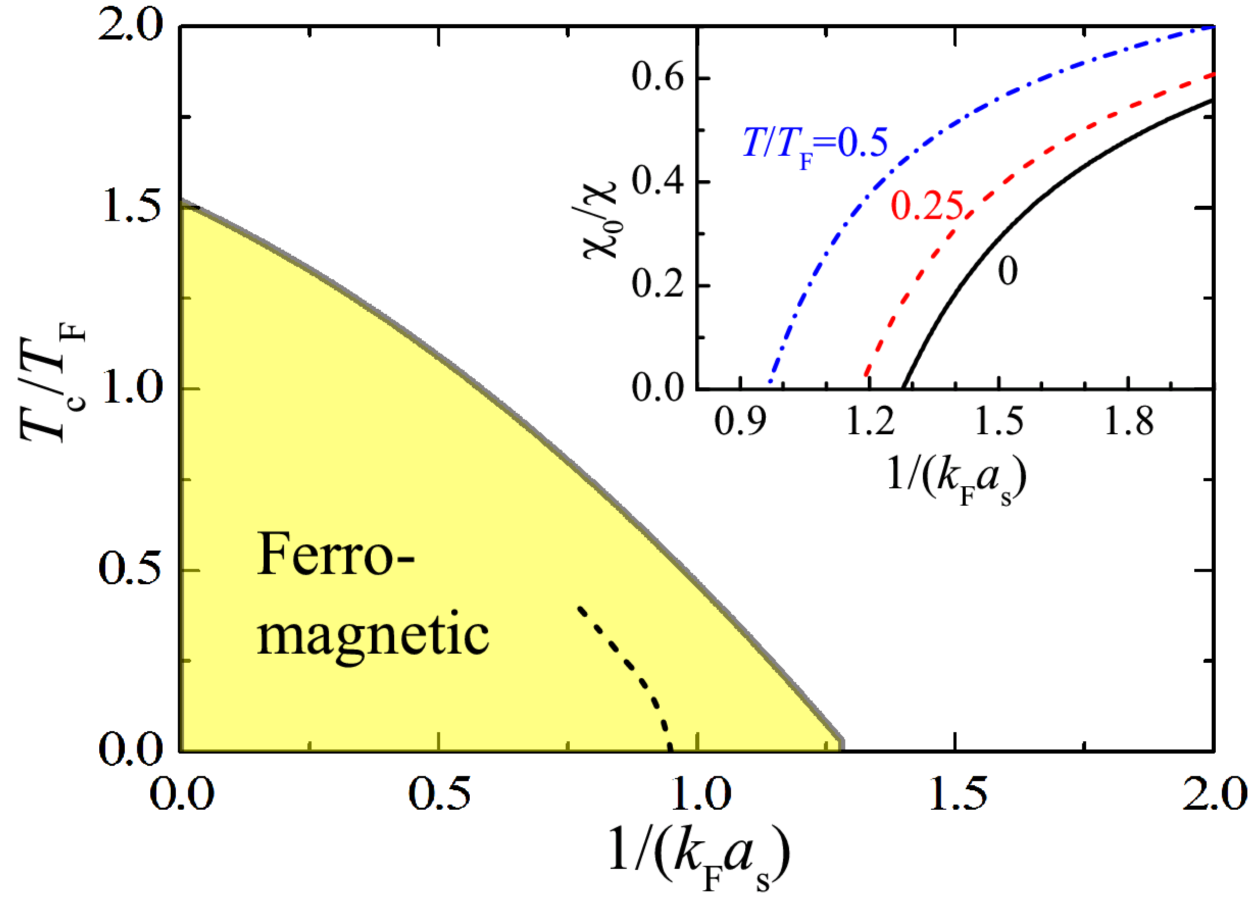
The energy and spin susceptibility of a unitary Fermi gas as a function of T_F/T

(1) at high temperature reproduce the virial expansion predictions Liu, et al., PRA 82, 023619(2010)

(2) Ferromagnetic transition (spin susceptibility diverges) at Tc~ 1.5 T_F large-N expansion

Tc~ 1.6 T_F ϵ expansion

Finite-Temperature Phase Diagram

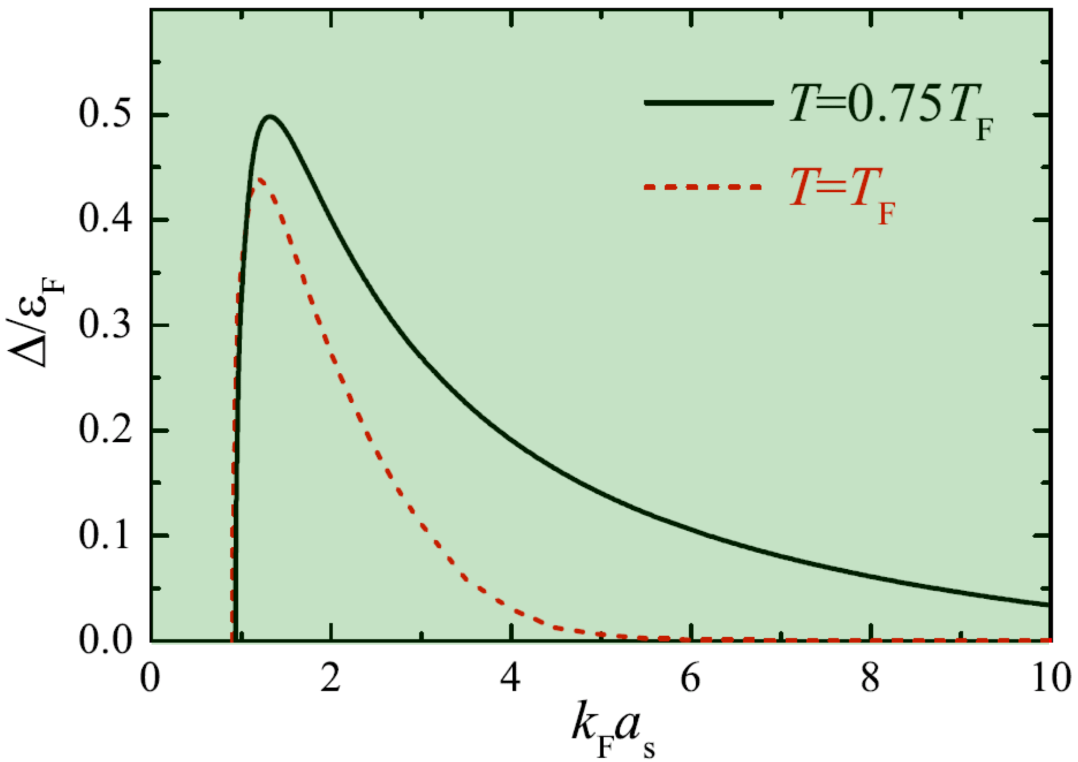


Finite-temperature phase diagram: in the shadow area the system favors spin-domain formation and exhibits Stoner ferromagnetism.

The pair formation rate

Decay rate by studying the pair formation rate

by using same method as D. Pekker, et.al., PRL 106, 050402(2011)



$k_F a_s = 2 \qquad T < 0.3 T_F \qquad \Delta \sim \varepsilon_F$

$$\omega(\mathbf{q}) = \Omega_{\mathbf{q}} + i\Delta_{\mathbf{q}}$$

$$\Gamma^{-1}(\mathbf{q}, \omega(\mathbf{q})) = 0$$

The pair formation rate is determined by

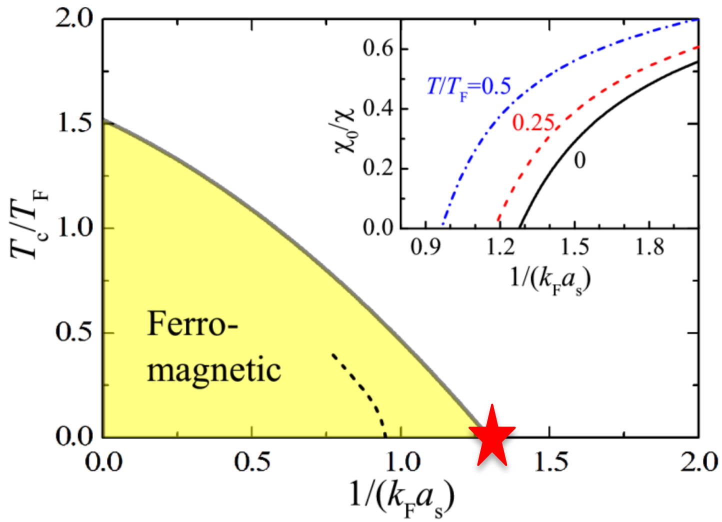
$$\frac{1}{a_s} - \sqrt{-mE} - \frac{8\pi}{m}\sum_{\mathbf{k}} \frac{f(\xi_{\mathbf{k}})}{E - 2\varepsilon_{\mathbf{k}}} = 0$$

Taking home messages:

- **New prescription for the upper branch**

$$\delta_{\mathrm{rep}}(\mathbf{q},\omega) = [\delta_{\mathrm{att}}(\mathbf{q},\omega) - \pi]\,\Theta\,[\omega - \omega_s(\mathbf{q})]$$

- **Strong-coupling theory for the repulsive branch (2nd PT and VE)**
- **Qualitative Phase diagram for Stoner transition**



- **New tools for strongly interacting Bose gases and BF mixtures**

LENS arXiv: 1605.07850

PRA, **93, 063629** (2016)