EENEN 09
First EMMI-EFES Workshop on Neutron-Rich Nuclei

Lattice calculation of thermal properties of low-density neutron matter with pionless effective field theory

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Outline

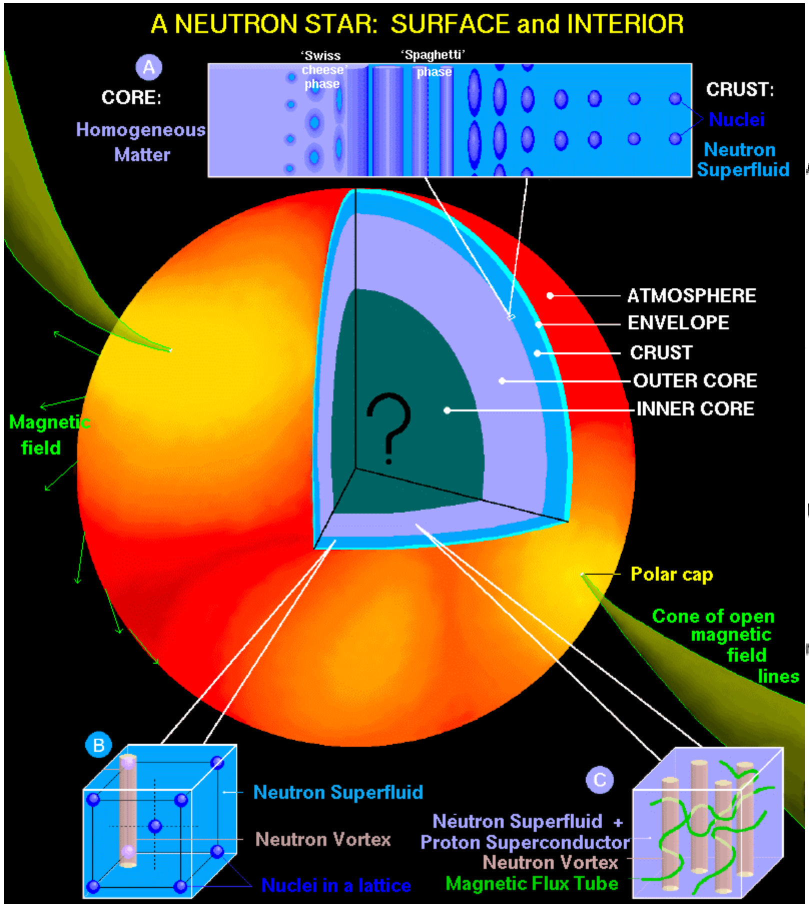
1. Motivation
2. Lattice Calculation w/ Pionless Effective Field Theory (EFT)
3. Numerical Results
    a. $^1S_0$ Pairing Gap @ T ~ 0
    b. Phase Diagram
4. Summary & Outlook

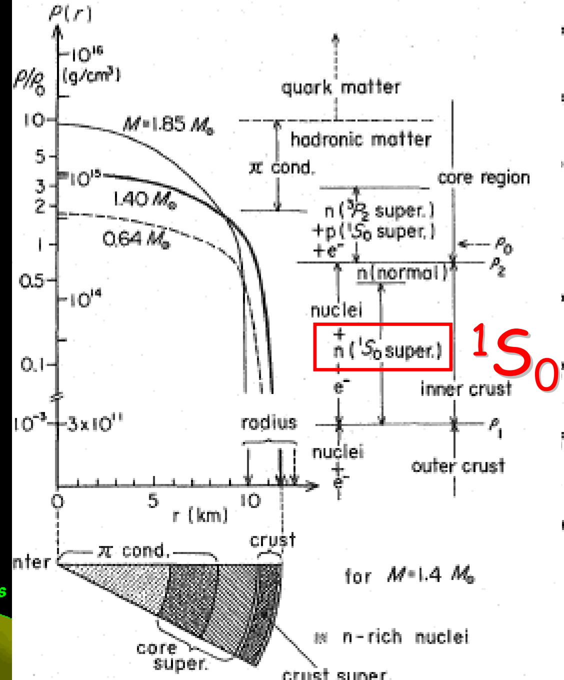
1. Motivation

- Superfluidity of Low-density Neutron Matter

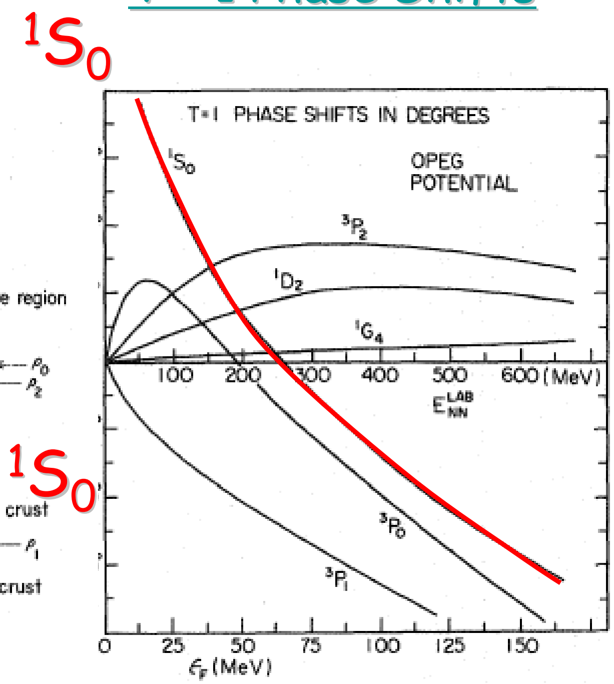
$^{2S+1}L_J$

Inner Structure of Neutron Star





T = 1 Phase Shifts



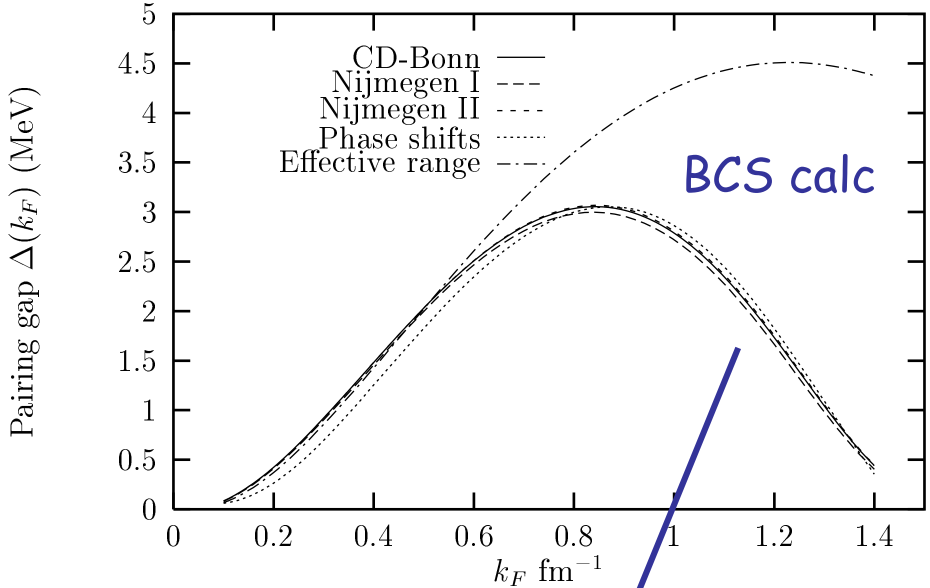
1-1. Nucleon-nucleon scattering phase shifts for the isospin $T=1$ pair as a function of the scattering energy E_{NN}^{LAB} ($=4\epsilon_F$; ϵ_F the Fermi energy) in the laboratory frame, calculated with the OPEG-1 potential.

- T. Takatsuka & R. Tamagaki, PTP Suppl. 112, 27 (1993)

- http://www.astroscu.unam.mx/neutrones/NS-Picture/NS-Picture.html

1. Motivation

- ## $^1S_0$ Pairing gap Δ (Neutron Matter)



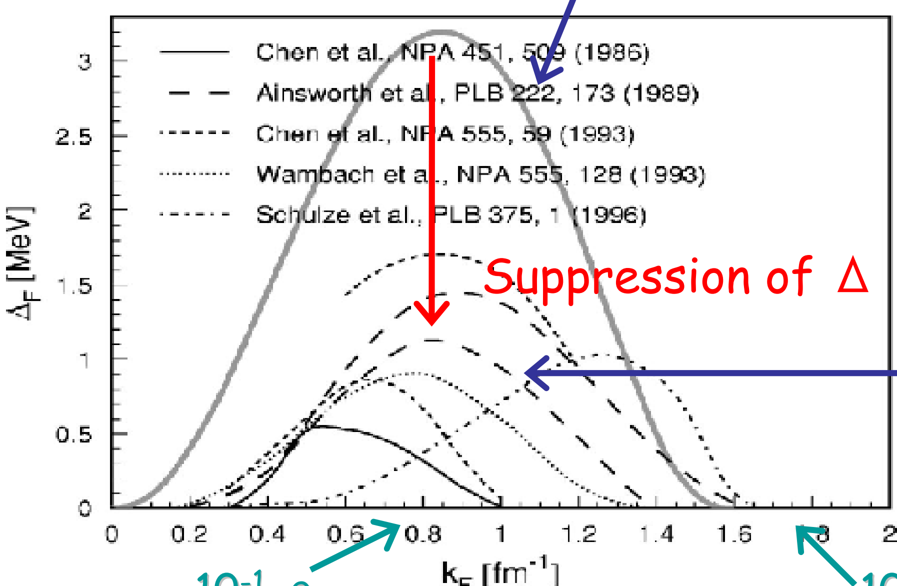
BCS equation

$$\Delta(k) = -\frac{1}{\pi}\int_0^\infty \mathrm{d}k' k'^2 V(k,k')\frac{\Delta(k')}{E(k')}$$

$$E(k') = \sqrt{(\epsilon(k) - \epsilon(k'))^2 + \Delta(k')^2}$$

$$\epsilon(k) = \frac{k^2}{2m} + \Sigma(k) - \mu$$

$k_F \sim 1.68$ fm^{-1} ($\rho \sim 0.16$ fm^{-3}) for neutron matter



Polarization effects (screening)

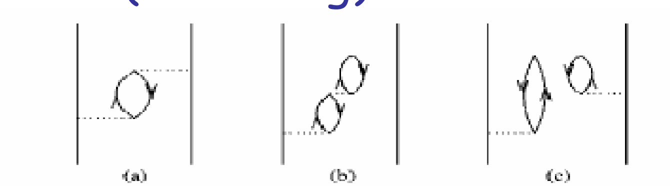


FIG. 13. (a) The second-order diagram with particle-hole intermediate states. The external legs can be particles or holes. (b) and (c) are examples of the third-order Tamm-Dancoff approximation or the random-phase approximation diagrams. The dotted lines represent the interaction vertex.

- D. J. Dean & M. Hjorth-Jensen, Rev. Mod. Phys. 75, 607 (2003)

1. Motivation

- Nuclear many-body ab-initio calculation based on the underlying theory (QCD)

↑ ↑

Monte Carlo method on a Lattice

Quantum Monte Carlo (QMC),

Hybrid Monte Carlo (HMC), …

NN Effective Field Theory (EFT)

Pionful EFT,

Pionless EFT, …

Simplest nuclear many-body system ← Low-density Neutron Matter

- References (Lattice EFT Calculations of Neutron/Nuclear Matter)

- H.-M. Mueller, S. E. Koonin, R. Seki, & U. van Kolck, PRC 61, 044320 (2000)
- D. Lee, B. Borasoy, & T. Schafer, PRC 70, 064002 (2004)
- D. Lee, & T. Schafer, PRC 72, 024006 (2005); PRC 73, 015201 (2006); PRC 73, 015202 (2006)
- T. Abe, & R. Seki, arXiv:0708.2523 (2007)
- B. Borasoy, E. Epelbaum, H Krebs, D. Lee, U.-G. Meissner, Eur. Phys. J. A35, 357 (2008)
- D. Lee, arXiv:0804.3501 (Review article)
- …

2. Lattice Calc. w/ Pionless EFT

- Introduction of χ EFT (Andreas Nogga's talk)

- EFT

  Power Counting

$$T(Q \sim M_{lo}) = \mathcal{N} \sum_{\nu=\nu_{min}}^{\infty} c_{\nu}(M_{hi}, \Lambda) \left(\frac{Q}{M_{hi}}\right)^{\nu} \mathcal{F}_{\nu}\left(\frac{Q}{M_{lo}}; \frac{\Lambda}{M_{lo}}\right)$$

$$\nu = \nu_{min}\ (LO),\ \nu_{min} + 1\ (NLO) \cdots$$

  Renormalization-Group (RG) Invariance

$$\frac{\partial T(Q \sim M_{lo})}{\partial \Lambda} = 0$$

- Observables are cutoff-independent order by order in low-energy expansion

- Pionful EFT, χ EFT

  Explicit degrees of freedom: $N,\ \pi$

$$M_{hi} \sim M_{QCD}, \quad M_{lo} \sim m_{\pi}$$

- Pionless EFT

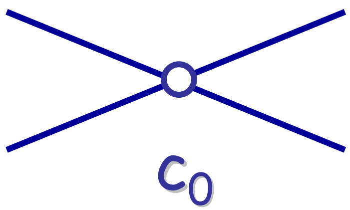
  Explicit degrees of freedom: N

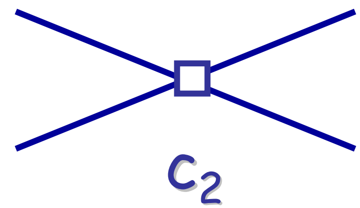
$$M_{hi} \sim m_{\pi}, \quad M_{lo} \sim Q \ll m_{\pi}$$

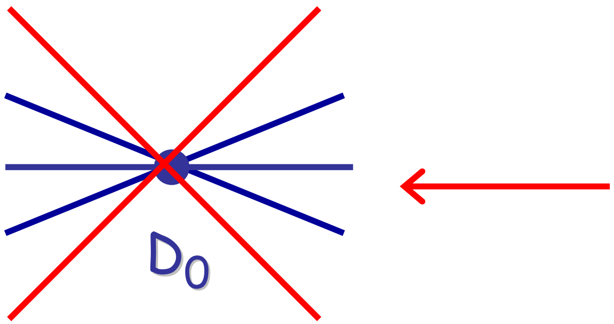
2. Lattice Calc. w/ Pionless EFT

- Power counting in Pionless EFT up to NLO

- LO (NN & 3N contact terms)
- NLO (NN p^2-dep. contact term)







Pauli principle (neutron matter)

3N contact term already appears @ LO in pionless EFT
P. F. Bedaque, H. W. Hammer, U. van Kolck, Nucl. Phys. A676, 357 (2000)
c.f.) 3N contact term appears @ N2LO in pionful EFT

- T. Abe, R. Seki, & A. N. Kocharian, PRC 70, 014315 (2004)

2. Lattice Calc. w/ Pionless EFT

Lattice Hamiltonian

- Non-relativistic Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2M}\sum_\sigma \int \mathrm{d}\mathbf{r}\, \hat{\psi}^\dagger_\sigma(\mathbf{r})\vec{\nabla}^2\hat{\psi}_\sigma(\mathbf{r}) + \frac{1}{2}\sum_{\sigma\sigma'}\int \mathrm{d}\mathbf{r}\int \mathrm{d}\mathbf{r}'\, \hat{\psi}^\dagger_\sigma(\mathbf{r})\hat{\psi}^\dagger_{\sigma'}(\mathbf{r}')V(\mathbf{r}-\mathbf{r}')\hat{\psi}_{\sigma'}(\mathbf{r}')\hat{\psi}_\sigma(\mathbf{r})$$

w/ $V(\mathbf{r}-\mathbf{r}') = c_0\,\delta\left(\mathbf{r}-\mathbf{r}'\right) - c_2\left(\vec{\nabla}^2_{\mathbf{r}}\delta\left(\mathbf{r}-\mathbf{r}'\right) + \vec{\nabla}^2_{\mathbf{r}'}\delta\left(\mathbf{r}-\mathbf{r}'\right)\right)$

$$V(\mathbf{p}',\mathbf{p}) = c_0 + c_2\left(\mathbf{p}^2 + \mathbf{p}'^2\right) \qquad \vec{r}\to a\vec{n} \quad \left(-\frac{Na}{2}\le an\le \frac{Na}{2}\right)$$

- Non-relativistic Lattice Hamiltonian

$$\hat{c}_{i\sigma} = a^{3/2}\hat{\psi}_\sigma(\mathbf{r}) \quad \hat{c}^\dagger_{i\sigma} = a^{3/2}\hat{\psi}^\dagger_\sigma(\mathbf{r})$$

$$\hat{H}_{LO} = -t\sum_{\langle i,j\rangle\sigma}\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + 6t\sum_{i\sigma}\hat{n}_{i\sigma} - \mu\sum_{i\sigma}\hat{n}_{i\sigma} + \frac{c_0}{a^3}\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$$

c_0 (LO) $\qquad t = (2Ma^2)^{-1}$

$$\hat{H}_{NLO} = -t\sum_{\langle i,j\rangle\sigma}\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + 6t\sum_{i\sigma}\hat{n}_{i\sigma} - \mu\sum_{i\sigma}\hat{n}_{i\sigma} + \left(\frac{c_0}{a^3} + 12\frac{c_2}{a^5}\right)\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} + \frac{c_2}{a^5}\sum_{\langle i,j\rangle\sigma\sigma'}\hat{n}_{i\sigma}\hat{n}_{j\sigma'}$$

c_0 & c_2 (NLO)

c.f.) Attractive Hubbard Model

$$\hat{H}_{AHM} = -t\sum_{\langle i,j\rangle\sigma}\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} - \mu\sum_{i\sigma}\hat{n}_{i\sigma} + U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$$

Extended Attractive Hubbard Model

$$\hat{H}_{EAHM} = -t\sum_{\langle i,j\rangle\sigma}\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} - \mu\sum_{i\sigma}\hat{n}_{i\sigma} + U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} + V\sum_{\langle i,j\rangle\sigma\sigma'}\hat{n}_{i\sigma}\hat{n}_{j\sigma'}$$

2. Lattice Calc. w/ Pionless EFT

Effective Range Expansion on the Lattice

- **Potential Terms**

$$V(\mathbf{r}) = c_0(\Lambda)\delta^3(\mathbf{r}) - c_2(\Lambda)[\overleftarrow{\nabla}^2\delta^3(\mathbf{r}) + \delta^3(\mathbf{r})\overrightarrow{\nabla}^2] + \cdots$$

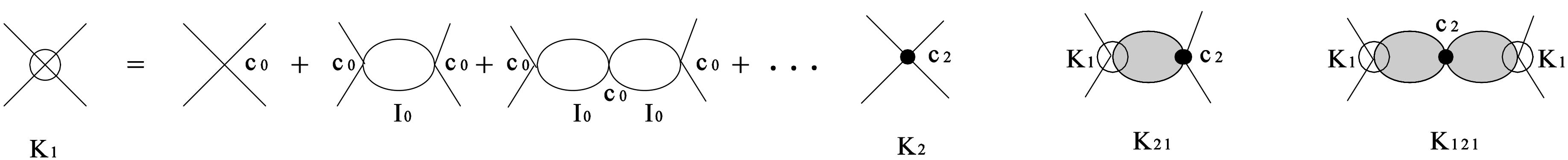
$$V(\mathbf{p}', \mathbf{p}) = c_0(\Lambda) + c_2(\Lambda)(p^2 + p'^2) + \cdots$$

- **K (reaction) Matrix**

Luscher's method ~ K matrix with asymptotically standing-wave boundary condition

$$K_0^{-1}(p) \;=\; p\cot\delta_0(p) = -\frac{1}{a_0} + \frac{1}{2}r_0 p^2 + \mathcal{O}(p^4)$$

$$-\frac{4\pi}{M}K_0(p) = K_1 + K_2 + 2\cdot K_{21} + K_{121} + \mathcal{O}(c_2^2, p^4)$$



$$K_1 \;\equiv\; c_0(\Lambda) + c_0(\Lambda)I_0(p,\Lambda)c_0(\Lambda) + c_0(\Lambda)I_0(p,\Lambda)c_0(\Lambda)I_0(p,\Lambda)c_0(\Lambda) + \cdots$$

$$K_2 \equiv 2p^2 c_2$$

$$K_{121} \equiv 2K_1^2 c_2 I_0 I_2$$

$$K_{21} \equiv K_1 c_2 (I_2 + p^2 I_0)$$

- R. Seki, & U. van Kolck, PRC 73, 044006 (2006)

Observables (a_0, r_0) — Coupling Constants & Regularization Scale $(c_0, c_2, \ldots, \Lambda(\sim\pi/a))$

$$\frac{M}{4\pi}\frac{1}{a_0} = \frac{1}{c_0(a)} + \frac{M}{2\pi^2}\left(L_1(a) + 2\frac{c_2(a)}{c_0(a)}L_3(a)\right) + \cdots$$

$$\frac{M}{16\pi}r_0 = \frac{c_2(a)}{c_0^2(a)} - \frac{Ma}{4\pi^3}R(0) + \cdots$$

$$V(\mathbf{p}',\mathbf{p}) = c_0 + c_2\left(\mathbf{p}^2 + \mathbf{p}'^2\right)$$

where

$$L_1\left(\frac{\pi}{a}\right) = \frac{1}{8\pi a}\wp\int_{-\pi}^{\pi}\frac{dxdydz}{3-(\cos x+\cos y+\cos z)} \equiv \frac{\pi}{a}\theta_1 = \frac{\pi}{a}\cdot 1.58796\cdots$$

$$L_3\left(\frac{\pi}{a}\right) = \frac{1}{4\pi a^3}\int_{-\pi}^{\pi}dxdydz \equiv \theta_3\left(\frac{\pi}{a}\right)^3 = \left(\frac{\pi}{a}\right)^3\cdot\frac{2}{\pi}$$

$$R\left(\left(\frac{pa}{\pi}\right)^2\right) = \frac{1}{16}\wp\int_{-\pi}^{\pi}\frac{dxdydz}{[3-(\cos x+\cos y+\cos z)][3-a^2p^2/2-(\cos x+\cos y+\cos z)]}$$

$$= 0.754330\cdots + \mathcal{O}\left(\left(\frac{pa}{\pi}\right)^2\right)$$

- Potential parameters, c_0 & c_2, are determined from the above coupled equations by reproducing the $^1S_0$ scattering length, a_0, & effective range, r_0, on the lattice.

- R. Seki, & U. van Kolck, PRC 73, 044006 (2006)

- Set up

- <u>Calculation Method</u>

  - Detarminantal Quantum Monte Carlo (DQMC)
  - LO (c_0) & NLO (c_0 & c_2) calc.
    (NLO calc.: All orders in c_0 included, c_2 treated perturbatively)

$$\begin{aligned} e^{-\Delta\beta\hat{H}} &= e^{-\Delta\beta(\hat{H}_0+\hat{H}')} \\ &\approx (1-\Delta\beta\hat{H}')e^{-\Delta\beta\hat{H}_0} \end{aligned}$$

- R. Seki, & U. van Kolck, Phys. Rev. *C* **73**, 044006 (2006); and references therein.

- <u>Parameter set up</u>

  - k_F = 15, 30, 60, 90, 120 MeV
  - Temporal lattice: N_t = 4 – 128
  - Spatial lattice: $N_s = 4^3 - 10^3$
  - Lattice filling: n = 1/16, 1/8, 3/16, 1/4, 3/8, 1/2

Sample # ~ 2,000 – 10,000 with 25 - 100 thermalization steps
Performed @ NERSC Seaborg, Bassi, Franklin, Titech Grid & TSUBAME

3. Numerical Results

a. $^1S_0$ Pairing Gap @ T ~ 0

k_F = 0.15 fm^{-1}(30 MeV)
a = 12.82 fm
t = 0.1261 MeV
Ns = 8^3

- S-wave Pair Correlation Function

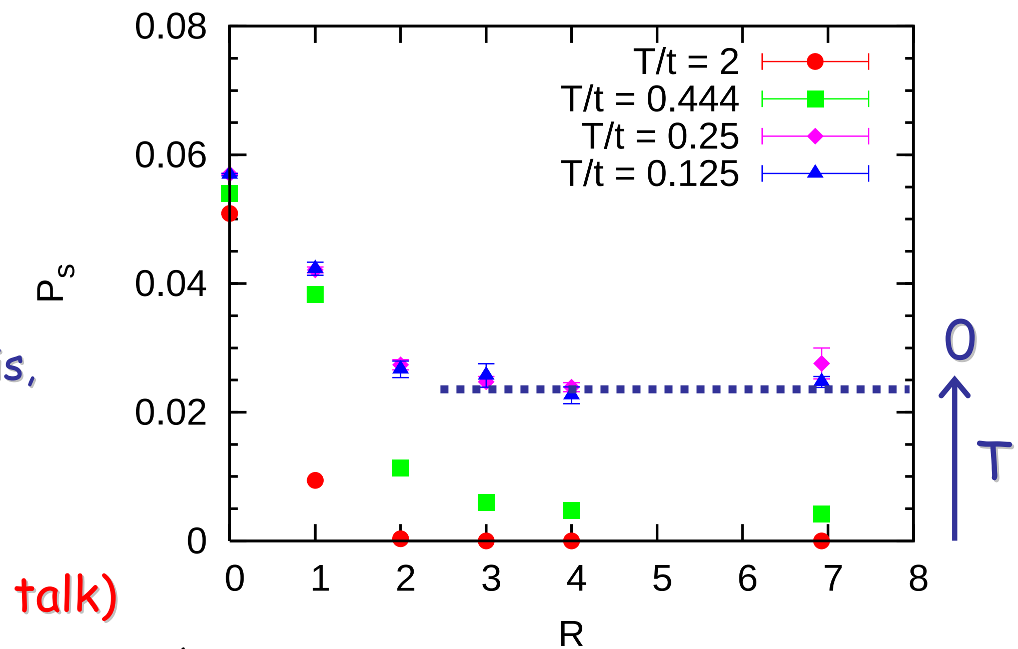
$$P_s(R) \equiv \frac{1}{N_s}\sum_i \langle \hat{\Delta}^\dagger_{i+R}\hat{\Delta}_i \rangle$$

w/ S-wave pair field $\hat{\Delta}_i \equiv \hat{c}_{i\uparrow}\hat{c}_{i\downarrow}$ & # of spatial lattice sites N_s

- Estimation of Δ

$$\Delta \sim \frac{c_0}{a^3} \times \sqrt{P_s}$$

- M. Guerrero, G. Ortiz, & E. Gubernatis, Phys. Rev. B **62**, 600 (2000)



- Definition of Δ (Heiko Hergert's talk)

Odd-even mass staggering: $\Delta(N) \equiv E(N) - \frac{1}{2}[E(N+1) - E(N-1)]$

- Finite-size Scaling of Δ

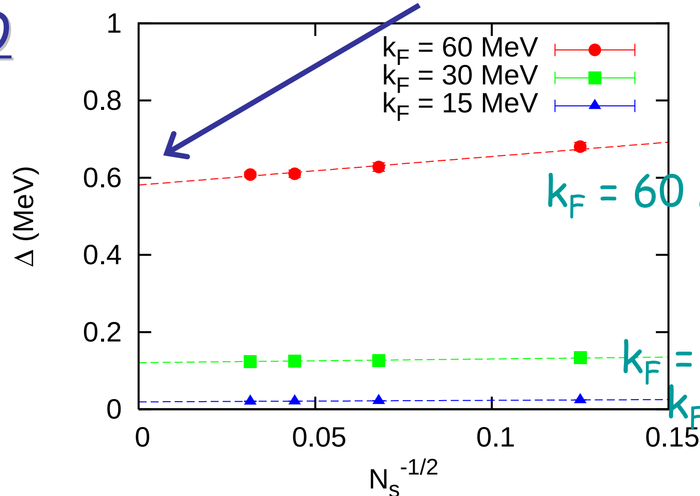
thermodynamic limit

(w/ Ns = 4^3, 6^3, 8^3, 10^3)

$$\Delta(k_F, T \sim 0, N_s \to \infty, a)$$

Ns -> ∞

LO

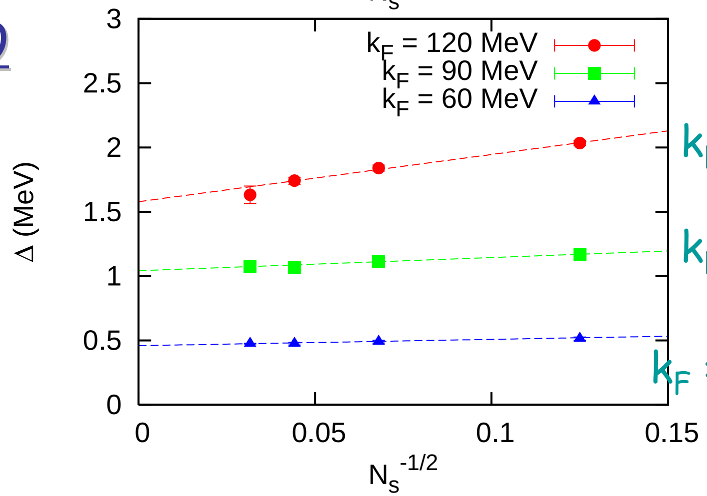


k_F = 60 MeV

k_F = 30 MeV

k_F = 15 MeV

NLO



k_F = 120 MeV

k_F = 90 MeV

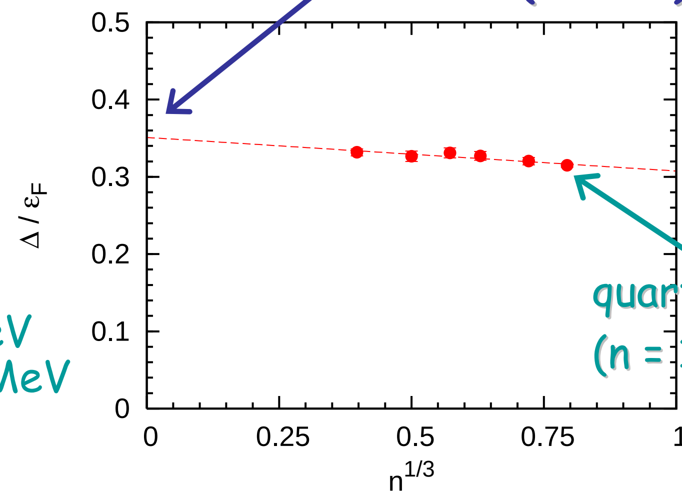
k_F = 60 MeV

continuum limit

(w/ n = 1/16, 1/8, 3/16, 1/4, 3/8, 1/2)

$$\Delta(k_F, T \sim 0, N_s \to \infty, a \to 0)$$

n -> 0 (a -> 0)

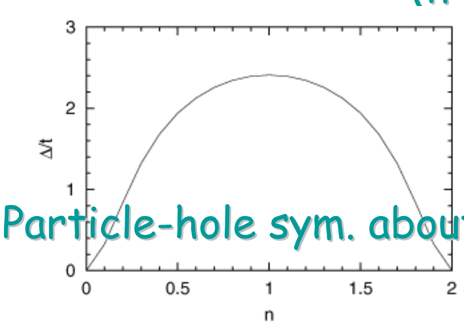


quarter-filling (n = 1/2)

half-filling (n = 1)

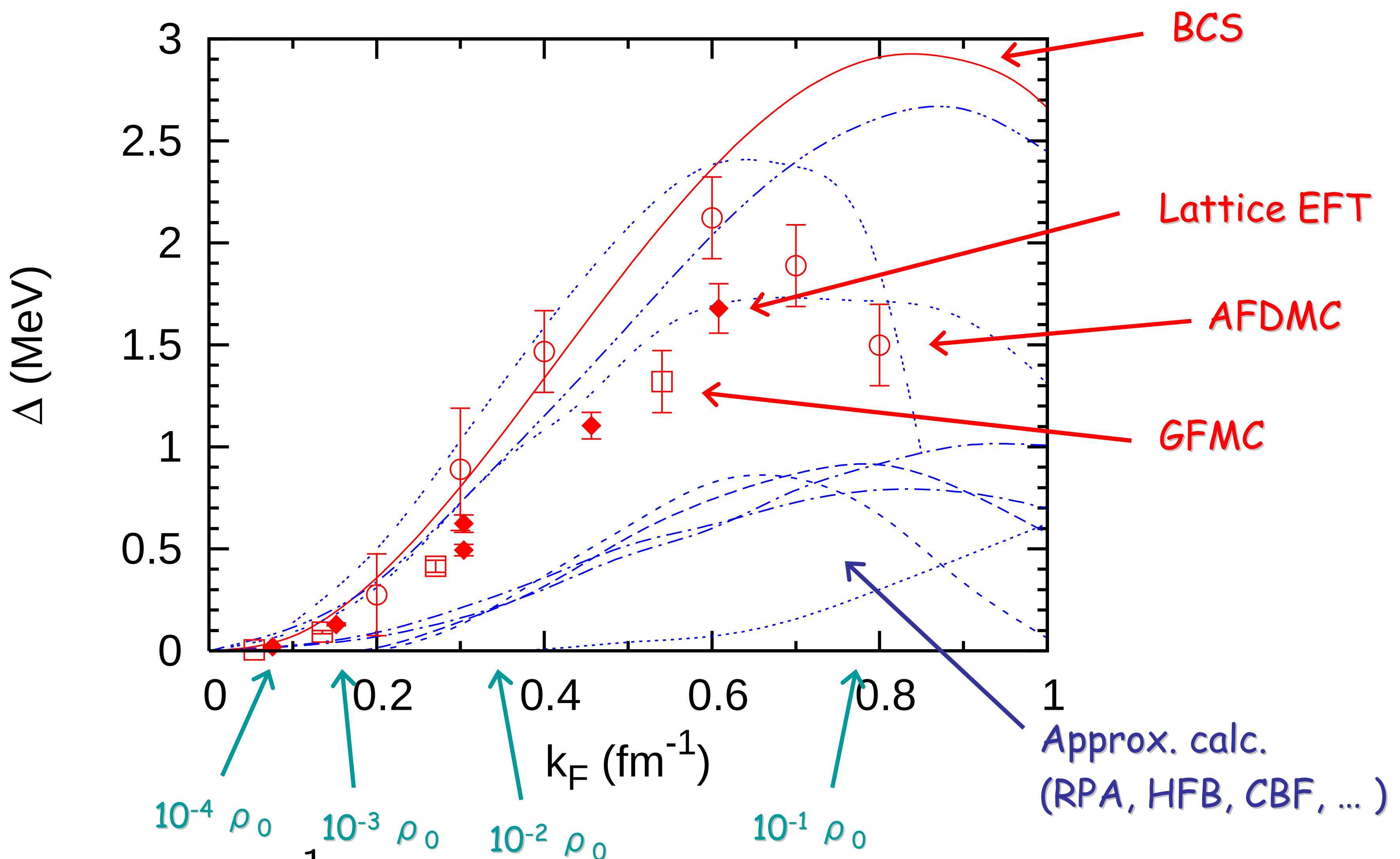
k_F = 0.3 fm^{-1}(60 MeV)

Ns = 6^3



Particle-hole sym. about n = 1

- Comparison of various calculations of $^1S_0$ pairing gap of neutron matter



$$\Delta(N) \equiv E(N) - \frac{1}{2}[E(N+1) - E(N-1)] \quad \text{(AFDMC, GFMC)}$$

- T. Abe & R. Seki, arXiv:0708.2523v2 Data taken from S. Gandolfi et al., PRL 101, 132501 (2008)

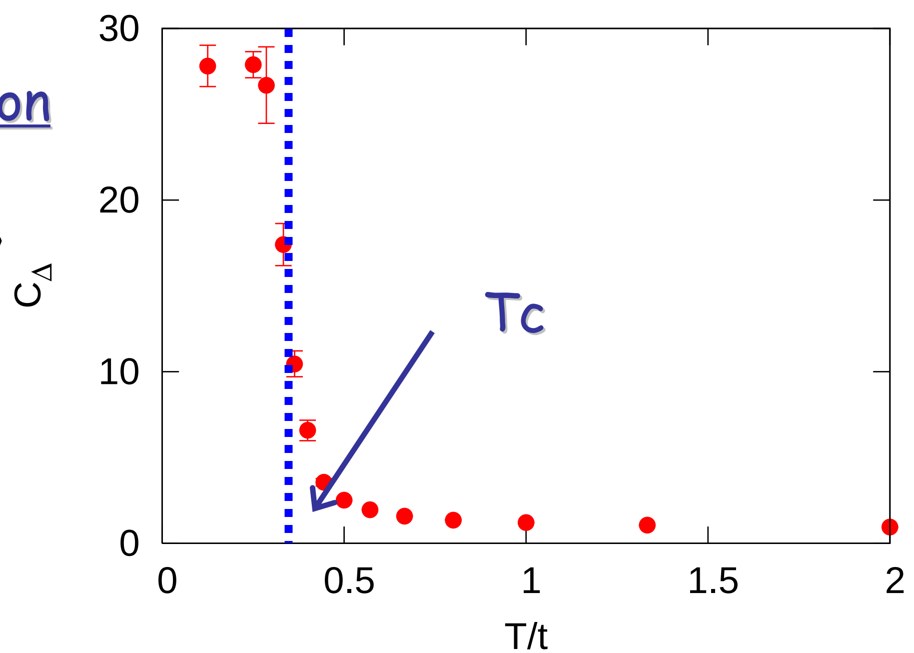
3. Numerical Results

b. Phase Diagram: $^1S_0$ Superfluid Phase Transition

- S-wave Pair Correlation Function

$$C_\Delta(T,N) \equiv \frac{1}{N_s}\sum_{i,j}\langle \hat{\Delta}_i \hat{\Delta}_j^\dagger + \hat{\Delta}_i^\dagger \hat{\Delta}_j \rangle$$

w/ $\hat{\Delta}_i \equiv \hat{c}_{i\uparrow}\hat{c}_{i\downarrow}$



- Determination of Tc

Tc is given by the inflexion point of $C_\Delta(T)$

k_F = 0.15 fm^{-1}(30 MeV)
a = 12.82 fm
t = 0.1261 MeV
N = 8^3

3. Numerical Results

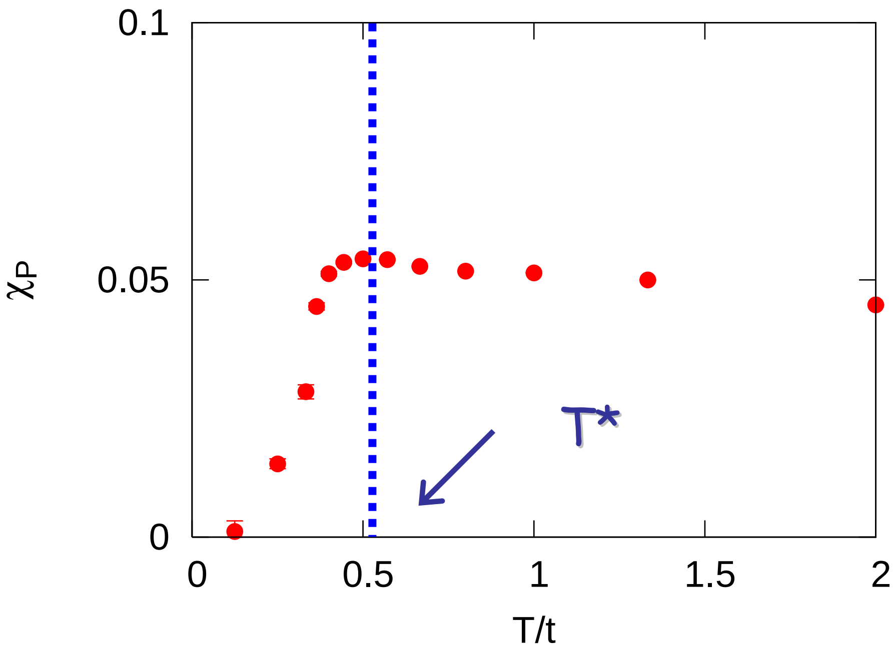
b. Phase Diagram: Pseudo Gap

k_F = 0.15 fm^{-1}(30 MeV)
a = 12.82 fm
t = 0.1261 MeV
N = 8^3

- Pauli Spin Susceptibility

$$\chi_P(T,N) \equiv \frac{1}{T}\frac{1}{N}\sum_{i,j}\langle S_i \cdot S_j \rangle$$

$$S_i = \sum_{\mu,\nu=\uparrow,\downarrow} c^\dagger_{i\mu}\boldsymbol{\sigma}_{\mu\nu}c_{i\nu},$$



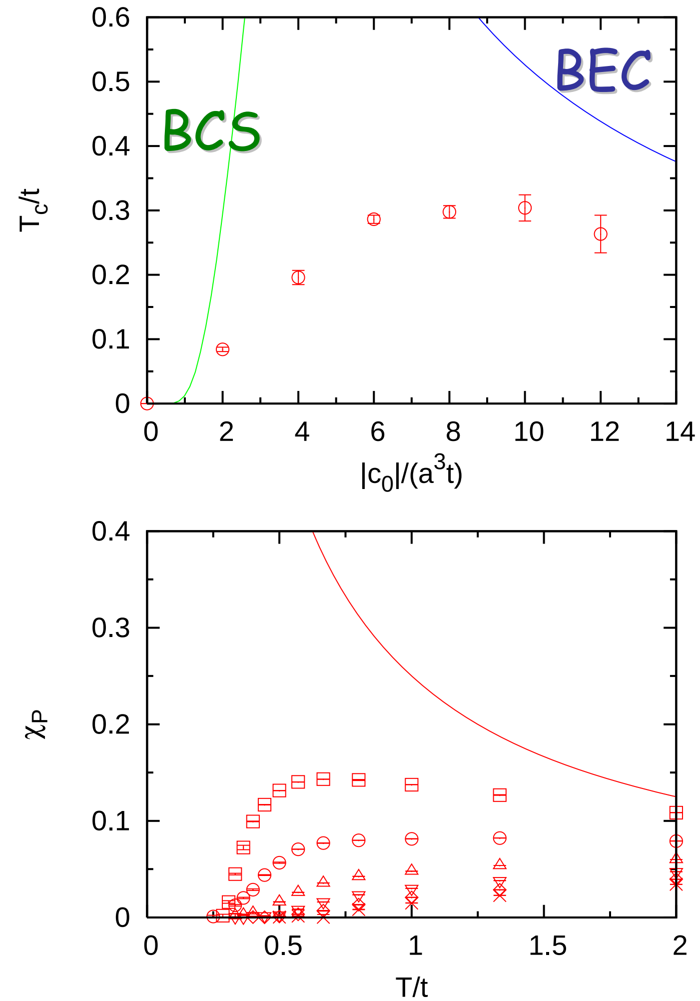
- Determination of T*

T* is identified with the maximum position of $\chi_P(T)$

$T^* \to T_c$ (BCS limit) $T^* \propto U/\ln(U/\epsilon_F)^{3/2}$ (BEC limit)

- A. Sewer, X. Zotos & H. Beck, Phys. Rev. B66, 145004 (2002)

- # BCS-BEC Crossover



$$T_c(C_0,n) = \frac{2e^\gamma}{\pi}\sqrt{\left(\frac{W}{2}+\mu\right)\left(\frac{W}{2}-\mu\right)}\exp\left(-\frac{1}{D_0(\mu)|C_0|}\right)$$

(BCS limit)

$$T_c(C_0,n) = 2\left(\frac{2\pi^2 n}{\Gamma(3/2)\zeta(3/2)}\right)^{2/3}\frac{t^2}{|C_0|}$$

(BEC limit)

$|c_0|/(a^3 t)$ = 0, 2, 4, 6, 8, 10, 12

(from top to bottom)

A. Sewer, X. Zotos & H. Beck, Phys. Rev. **B66**, 140504 (2002)

- ## Finite-size Scaling for Tc & T*

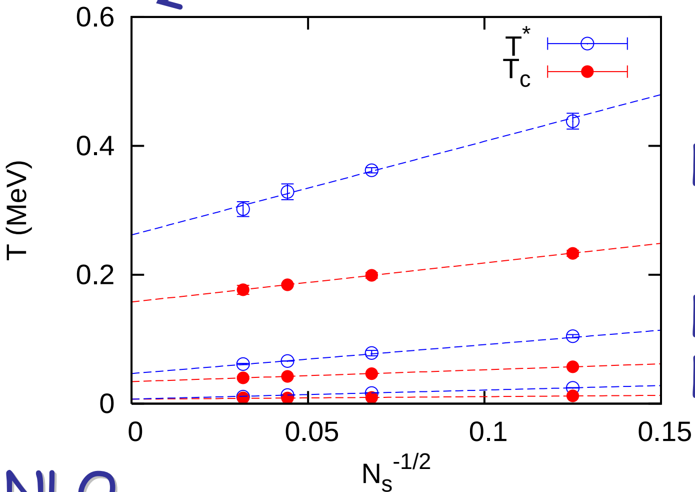
LO

thermodynamic limit

$N_s \to \infty$

continuum limit

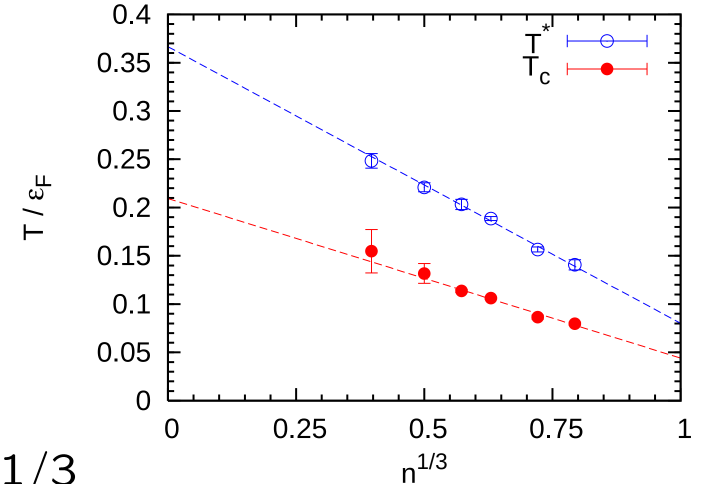
$n \to 0 \ (a \to 0)$



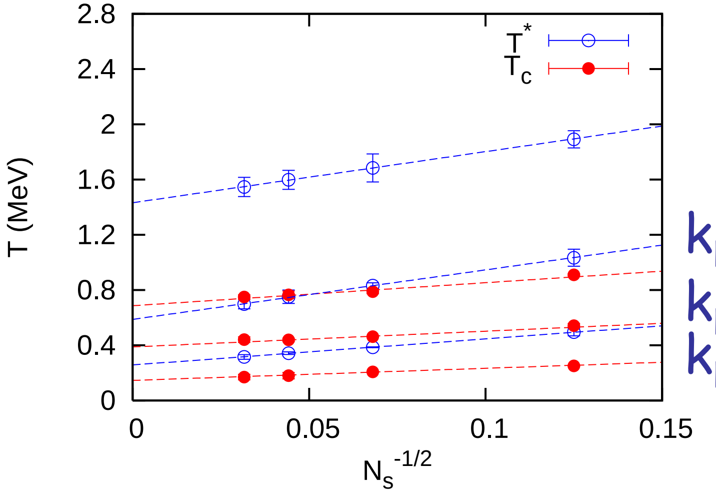
k_F = 60 MeV

k_F = 30 MeV

k_F = 15 MeV



NLO



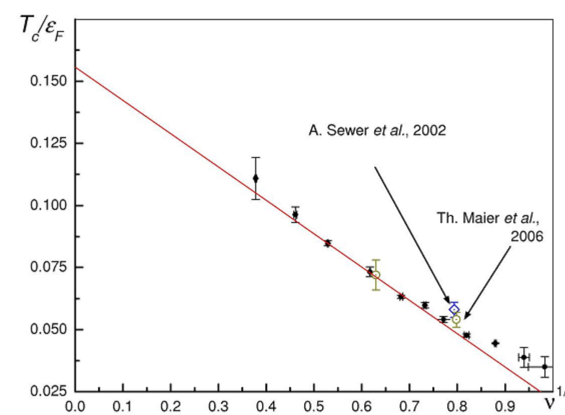
$$k_F = (3\pi^2\rho)^{1/3}$$

$$\rho = n/(2a^3)$$

k_F = 120 MeV

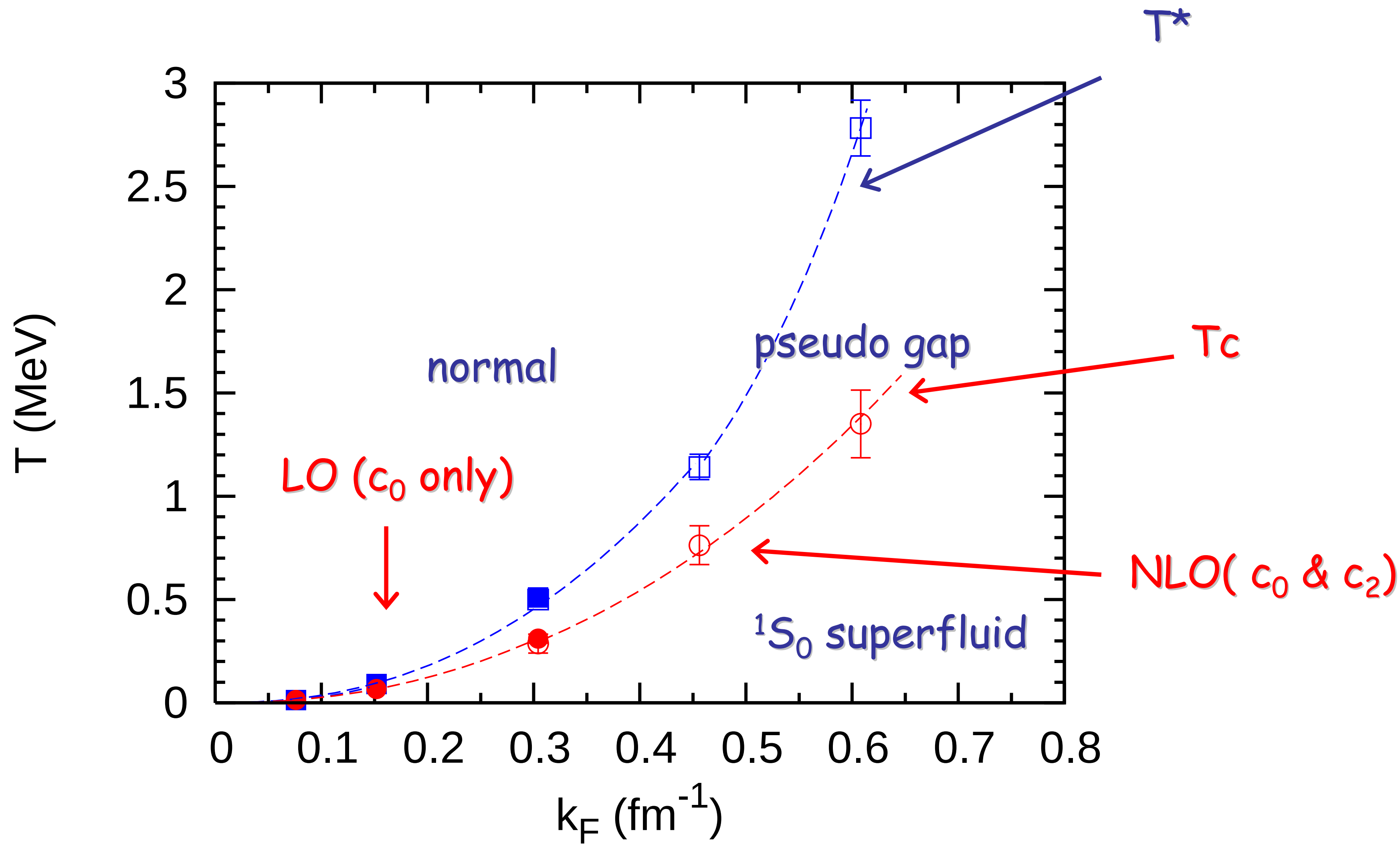
k_F = 90 MeV

k_F = 60 MeV



- E. Burovski, N. Prokofev, B. Svistunov, & M. Troyer, Phys. Rev. Lett. **96**, 160402 (2006)

Phase Diagram @ Thermodynamic & Continuum Limits



- T. Abe & R. Seki, arXiv:0708.2523v2

4. Summary & Outlook

- Lattice calculations w/ LO & NLO NN EFT @ $T \neq 0$ (DQMC) have been performed in 4^3 - 10^3 spatial & 4 – 128 temporal lattices.
- Observables are obtained by taking the thermodynamic & continuum limits.

Summary

- $^1S_0$ pairing gap @ T ~ 0 & phase diagram
  - Between BCS & calculations w/ polarization effects (reduction of Δ by ~30 - 40 % from BCS weak-coupling approx.)

- Phase diagram
  - Normal-to-superfluid phase transition, Pseudo gap above the superfluid phase
    Low-density neutron matter is the state in the BCS-BEC crossover.

✓ Importance of the pairing correlation eve at low density

Outlook

- Calculation @ higher density (w/ Pions, …)
- Other partial waves (^3P-F_2,…)
- Nuclear Matter
- Application to the finite nuclei

ρ	k_F [MeV]	Potential term
~ $0.006\rho_0$	0 - 30	1 term (a_0)
~ $0.07\rho_0$	0 - 140	2 terms (a_0, r_0)
~ $0.5\rho_0$	0 - 260	2 terms + π

$\rho_0 = 0.16$ fm^{-3}

END