Strongly paired fermions

Alexandros Gezerlis

UNIVERSITY of GUELPH

TALENT/INT Course on
Nuclear forces and their impact on structure, reactions and astrophysics
July 4, 2013

Strongly paired fermions

Neutron matter & cold atoms

Strongly paired fermions

BCS theory of superconductivity

Strongly paired fermions

**Beyond weak coupling:
Quantum Monte Carlo**

fermions

Bibliography

Michael Tinkham
"Introduction to Superconductivity, 2nd ed."
Chapter 3

(readable introduction to basics of BCS theory)

D. J. Dean & M. Hjorth-Jensen
"Pairing in nuclear systems"
Rev. Mod. Phys. 75, 607 (2003)

(neutron-star crusts and finite nuclei)

S. Giorgini, L. P. Pitaevskii, and S. Stringari
"Theory of ultracold Fermi gases"
Rev. Mod. Phys. 80, 1215 (2008)

(nice snapshot of cold-atom physics – also strong pairing)

How cold are cold atoms?

1908: Heike Kamerlingh Onnes liquefied ^4He at 4.2 K

1911: Onnes used ^4He to cool down Hg discovering superconductivity (zero resistivity) at 4.1 K

How cold are cold atoms?

1908: Heike Kamerlingh Onnes
liquefied ^{4}He at 4.2 K

1911: Onnes used ^{4}He to cool down Hg
discovering superconductivity (zero
resistivity) at 4.1 K

1938: Kapitsa / Allen-Misener find
superfluidity (frictionless flow)
in ^{4}He at 2.2 K

1972: Osheroff-Richardson-Lee encounter
superfluidity in fermionic ^{3}He at mK

How cold are cold atoms?

1908: Heike Kamerlingh Onnes liquefied ^{4}He at 4.2 K

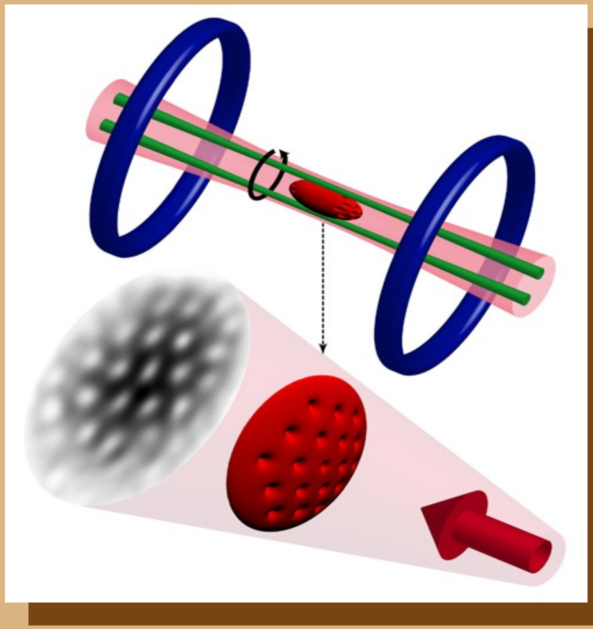
1911: Onnes used ^{4}He to cool down Hg discovering superconductivity (zero resistivity) at 4.1 K

1938: Kapitsa / Allen-Misener find superfluidity (frictionless flow) in ^{4}He at 2.2 K

1972: Osheroff-Richardson-Lee encounter superfluidity in fermionic ^{3}He at mK

1995: Cornell-Wieman / Ketterle create Bose-Einstein condensation in ^{87}Rb at nK

2003: Jin / Grimm / Ketterle managed to use fermionic atoms (^{40}K and ^{6}Li)

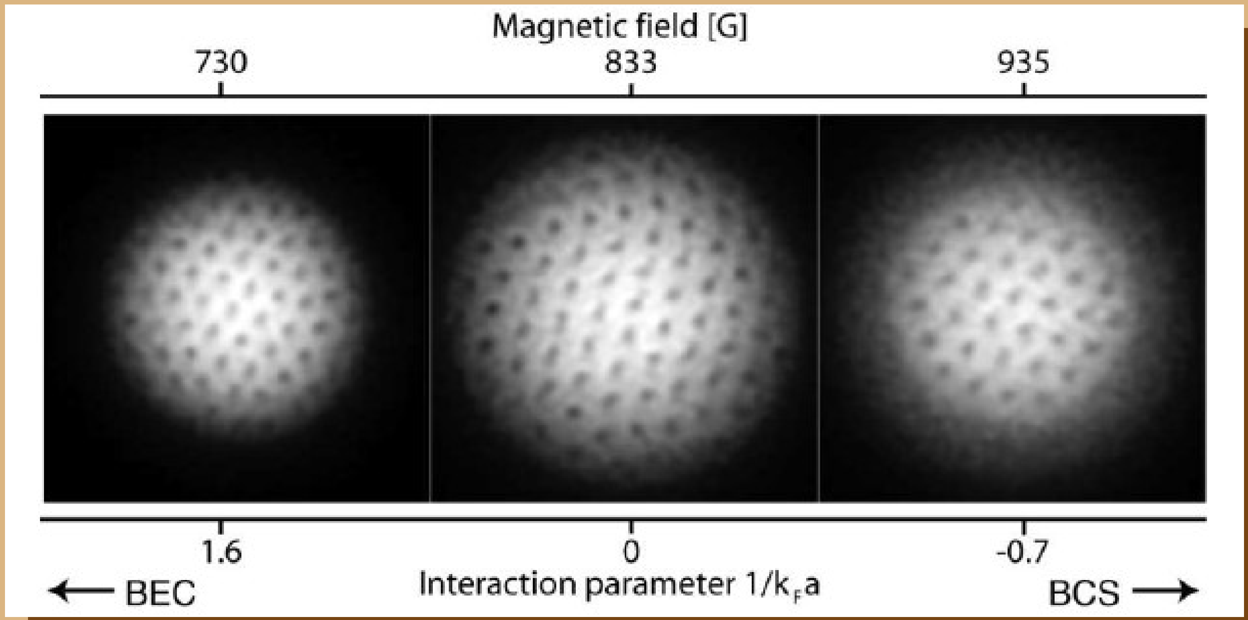


Credit: Wolfgang Ketterle group

Cold atoms overview

30K foot overview of the experiments

- Particles in a (usually anisotropic) trap
- Hyperfine states of ^{6}Li or ^{40}K (and now both!)
- 1, 2, 3 (4?) components; equal populations or polarized gases
- Cooling (laser, sympathetic, evaporative) down to nK (close to low-energy nuclear physics?)

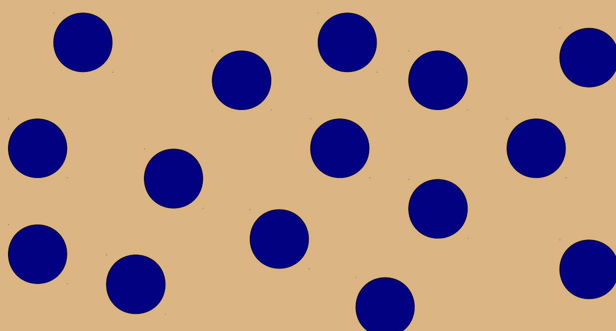


Credit: Martin Zwierlein

Connection between the two

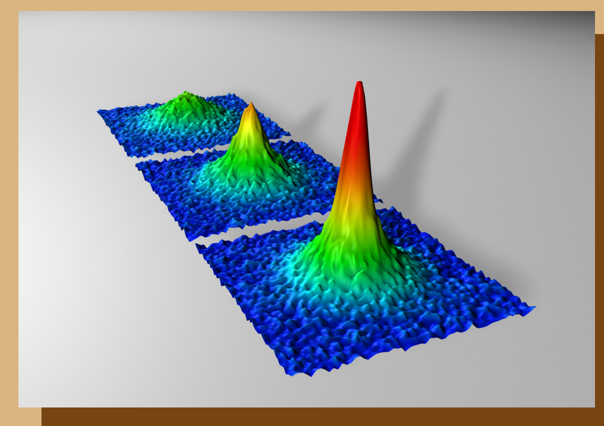
Neutron matter

- MeV scale
- $O(10^{57})$ neutrons



Cold atoms

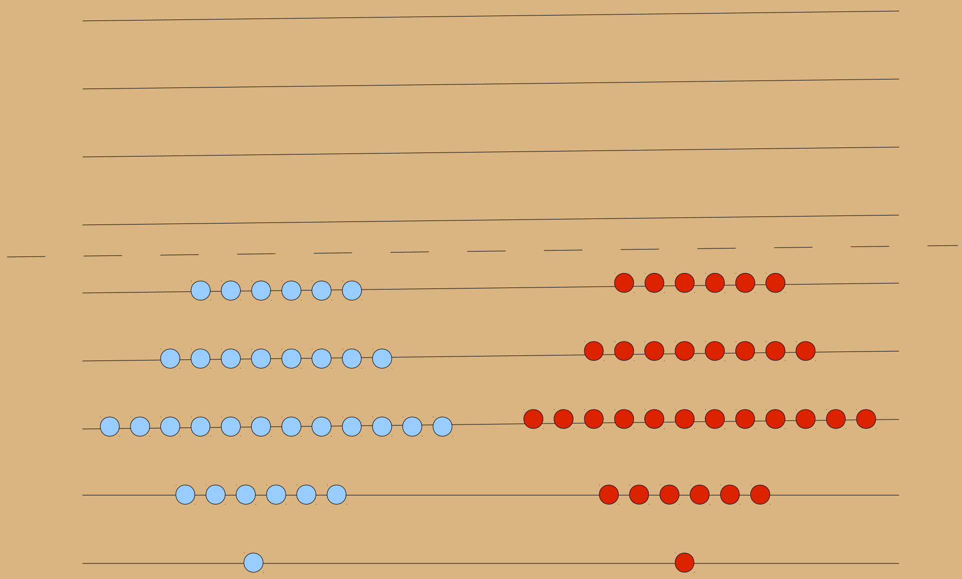
- peV scale
- O(10) or $O(10^5)$ atoms



Credit: University of Colorado

- Very similar E/E_{FG}
- Weak to intermediate to strong coupling

Fermionic dictionary



Energy of a free Fermi gas: $E_{FG} = 3/5 N E_F$

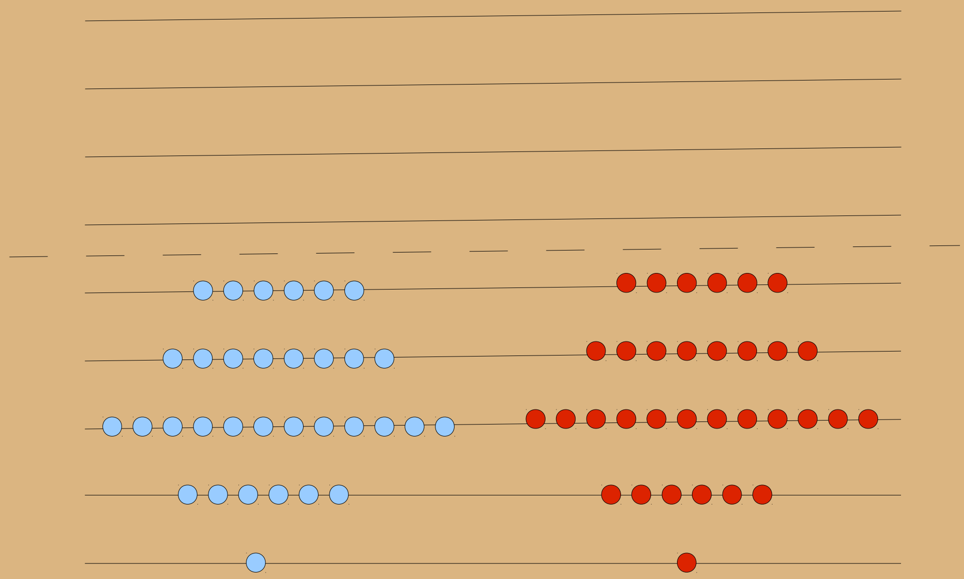
Fermi energy: $E_F = \hbar^2 k_F^2 / 2m$

Fermi wave number: k_F

Number density: $\rho = g k_F^3 / 6\pi^2$

Scattering length: a

Fermionic dictionary



Energy of a free Fermi gas: $E_{FG} = 3/5 N E_F$

Fermi energy: $E_F = \hbar^2 k_F^2 / 2m$

Fermi wave number: k_F

Number density: $\rho = g k_F^3 / 6\pi^2$

Scattering length: a

In what follows, the dimensionless quantity $k_F a$ is called the "coupling"

From weak to strong

Weak coupling

- $k_F a \to 0$
- Studied for decades
- Experimentally difficult
- Pairing exponentially small
- Perturbative expansion

$$\frac{E}{E_{FG}} = 1 + \frac{10}{9\pi} k_F a + \frac{4}{21\pi^2}(11 - 2\ln 2)(k_F a)^2$$

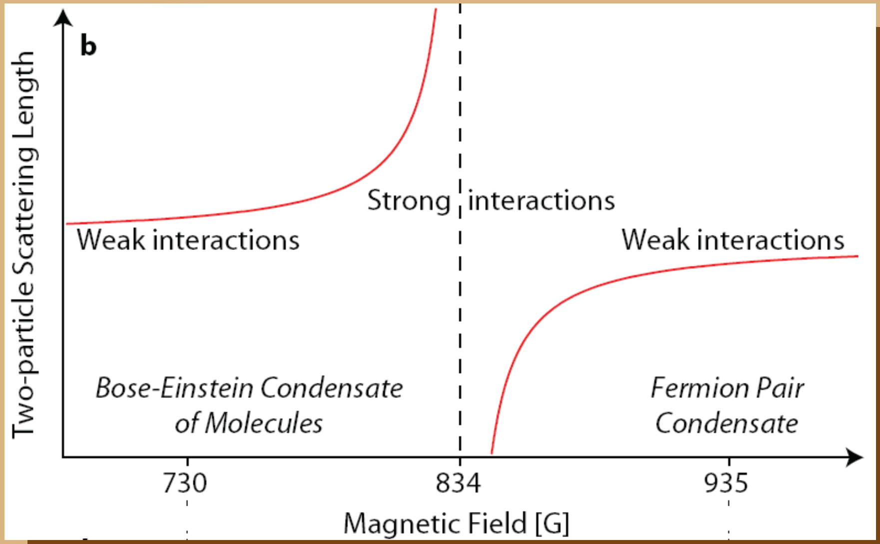
Strong coupling

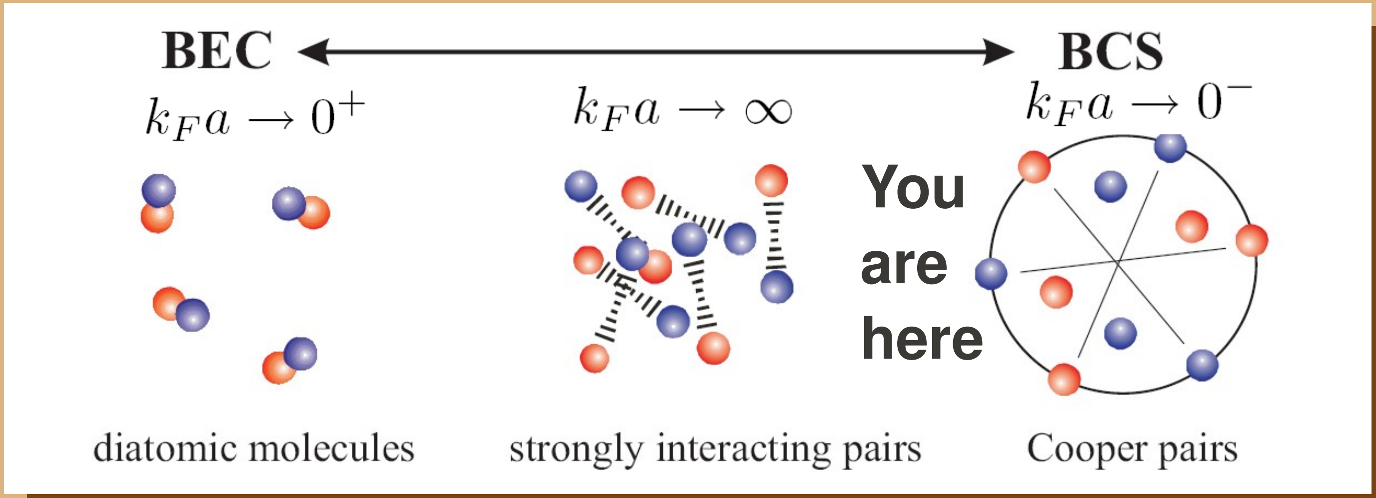
- $k_F a \to \infty$
- More recent (2000s)
- Experimentally probed
- Pairing significant
- Non-perturbative

From weak to strong experimentally

Using “Feshbach” resonances one can tune the coupling

Credit: Thesis of Martin Zwierlein





Credit: Thesis of Cindy Regal

From weak to strong experimentally

Using "Feshbach" resonances one can tune the coupling

In nuclear physics

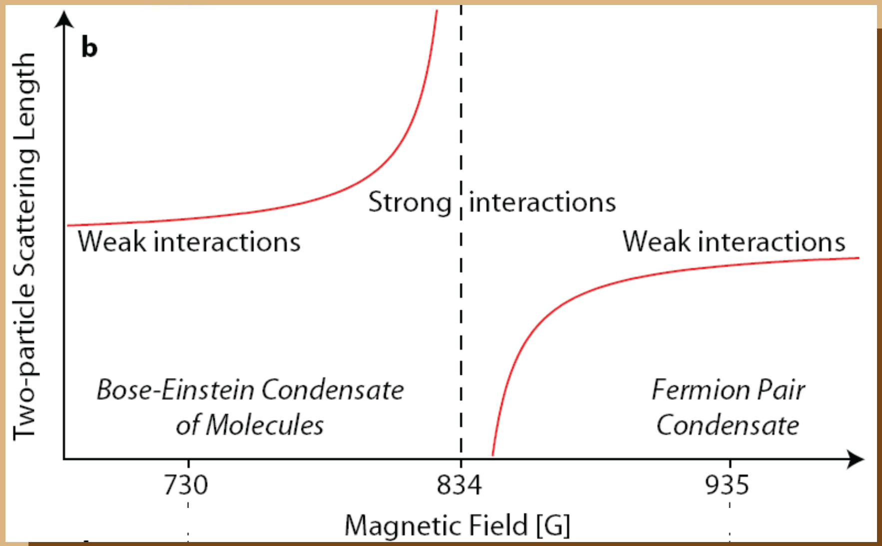
$a =$ -18.5(4) fm

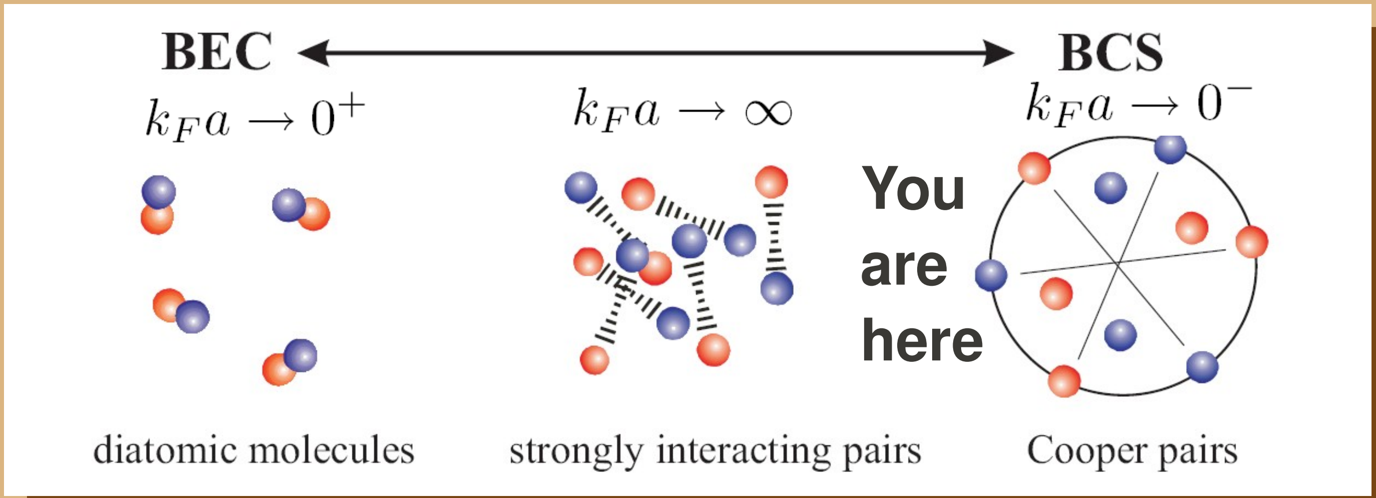
$r_e = 2.80(11)$ fm

are fixed, so all we can "tune" is the density

(N.B.: there is no stable dineutron)

Credit: Thesis of Martin Zwierlein





Credit: Thesis of Cindy Regal

$$a = a_{bg}\left(1 - \frac{\Delta B}{B - B_0}\right)$$

paired

Normal vs paired

A normal gas of spin-1/2 fermions is described by two Slater determinants (one for spin-up, one for spin-down), which in second quantization can be written as :

$$|\psi_{normal}\rangle = \prod_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{\mathbf{k}\downarrow} |0\rangle$$

The Hamiltonian of the system contains a one-body and a two-body operator:

$$\mathcal{H} = \sum_{\mathbf{k}\sigma} \epsilon(\mathbf{k}) c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}\mathbf{q}'\sigma\sigma'} \langle \mathbf{k}|V|\mathbf{k}'\rangle \delta_{\mathbf{k}+\mathbf{q},\mathbf{k}'+\mathbf{q}'} c^{\dagger}_{\mathbf{k}'\sigma} c^{\dagger}_{\mathbf{q}'\sigma'} c_{\mathbf{q}\sigma'} c_{\mathbf{k}\sigma}$$

However, it's been known for many decades that there exists a lower-energy state that includes particles *paired* with each other

BCS theory of superconductivity I

Start out with the wave function:

$$|\psi_{BCS}\rangle = \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow})|0\rangle \qquad (\, u^2_{\mathbf{k}} + v^2_{\mathbf{k}} = 1 \,)$$

and you can easily evaluate the average particle number:

$$\bar{N} = \langle \hat{N} \rangle = \langle \psi_{BCS} | \sum_{\mathbf{k}} \left(c^{\dagger}_{\mathbf{k}\uparrow} c_{\mathbf{k}\uparrow} + c^{\dagger}_{\mathbf{k}\downarrow} c_{\mathbf{k}\downarrow} \right) | \psi_{BCS} \rangle = 2 \sum_{\mathbf{k}} v^2_{\mathbf{k}}$$

BCS theory of superconductivity I

Start out with the wave function:

$$|\psi_{BCS}\rangle = \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow})|0\rangle \qquad (u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1)$$

and you can easily evaluate the average particle number:

$$\bar{N} = \langle \hat{N} \rangle = \langle \psi_{BCS} | \sum_{\mathbf{k}} \left(c^{\dagger}_{\mathbf{k}\uparrow} c_{\mathbf{k}\uparrow} + c^{\dagger}_{\mathbf{k}\downarrow} c_{\mathbf{k}\downarrow} \right) |\psi_{BCS}\rangle = 2 \sum_{\mathbf{k}} v_{\mathbf{k}}^2$$

Now start (again!) with the reduced Hamiltonian:

$$\mathcal{H} = \sum_{\mathbf{k}\sigma} \epsilon(\mathbf{k}) c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\mathbf{k}'} \langle \mathbf{k} | V | \mathbf{k}' \rangle c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow}$$

where $\epsilon(\mathbf{k}) = \frac{\hbar^2 k^2}{2m}$ is the energy of a single particle with momentum $\mathbf{k}$

Now, if μ is the chemical potential, add $-\mu \hat{N}$ to get:

$$\langle \mathcal{H} - \mu \hat{N} \rangle = 2 \sum_{\mathbf{k}} \xi(\mathbf{k}) v_{\mathbf{k}}^2 + \sum_{\mathbf{k}\mathbf{k}'} \langle \mathbf{k} | V | \mathbf{k}' \rangle u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{k}'} v_{\mathbf{k}'}$$ where $\xi(\mathbf{k}) = \epsilon(\mathbf{k}) - \mu$

BCS theory of superconductivity II

A straightforward minimization leads us to define:

$$\Delta(\mathbf{k}) = -\sum_{\mathbf{k}'} \langle \mathbf{k}|V|\mathbf{k}'\rangle \frac{\Delta(\mathbf{k}')}{2E(\mathbf{k}')}$$ BCS gap equation

Where $\Delta(\mathbf{k})$ is the excitation energy gap, while:

$$E(\mathbf{k}) = \sqrt{\xi(\mathbf{k})^2 + \Delta(\mathbf{k})^2}$$

is the quasiparticle excitation energy. Solve self-consistently with the particle-number equation, which also helps define the momentum distribution:

$$\langle N\rangle = \sum_{\mathbf{k}} \left[1 - \frac{\xi(\mathbf{k})}{E(\mathbf{k})}\right] = 2\sum_{\mathbf{k}} n(\mathbf{k})$$

BCS theory of superconductivity II

A straightforward minimization leads us to define:

$$\Delta(\mathbf{k}) = -\sum_{\mathbf{k}'} \langle \mathbf{k}|V|\mathbf{k}'\rangle \frac{\Delta(\mathbf{k}')}{2E(\mathbf{k}')}$$ BCS gap equation

Where $\Delta(\mathbf{k})$ is the excitation energy gap, while:

$$E(\mathbf{k}) = \sqrt{\xi(\mathbf{k})^2 + \Delta(\mathbf{k})^2}$$

is the quasiparticle excitation energy. Solve self-consistently with the particle-number equation, which also helps define the momentum distribution:

$$\langle N \rangle = \sum_{\mathbf{k}} \left[1 - \frac{\xi(\mathbf{k})}{E(\mathbf{k})}\right] = 2\sum_{\mathbf{k}} n(\mathbf{k})$$

$$2u_{\mathbf{k}}v_{\mathbf{k}} = \frac{\Delta(\mathbf{k})}{E(\mathbf{k})}$$

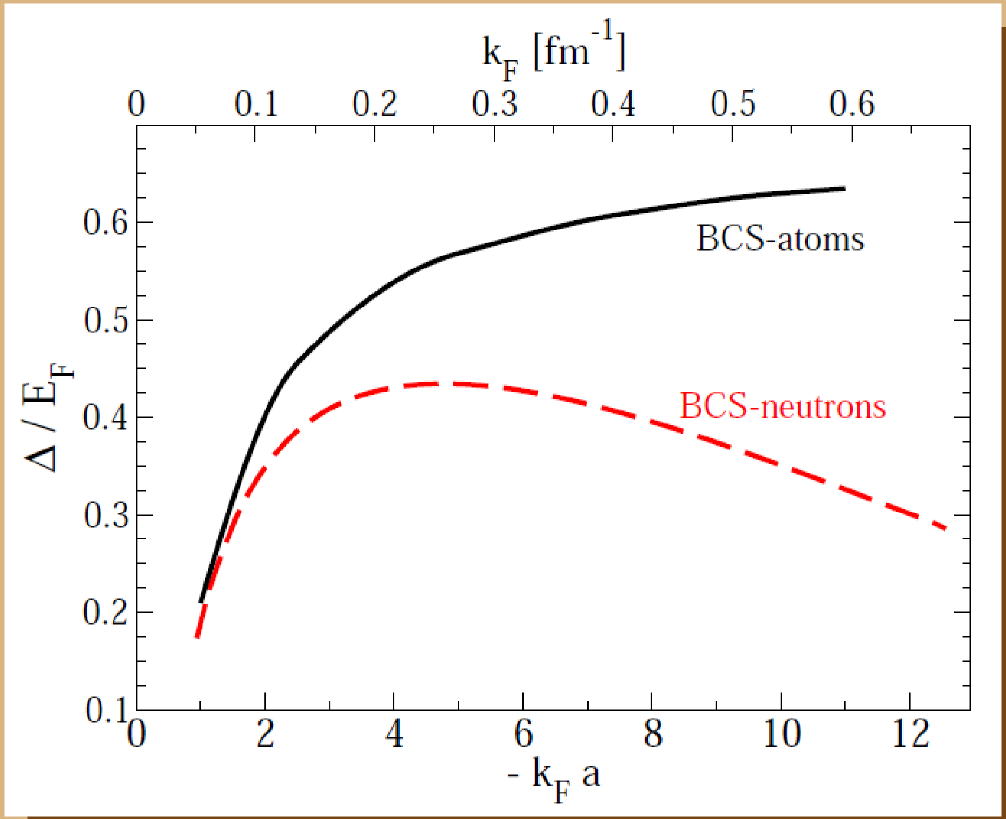
$$v_{\mathbf{k}}^2 - u_{\mathbf{k}}^2 = \frac{\xi(\mathbf{k})}{E(\mathbf{k})}$$

BCS theory of superconductivity III

Solving the two equations in the continuum:

$$\Delta(\mathbf{k}) = -\sum_{\mathbf{k}'} \langle \mathbf{k}|V|\mathbf{k}'\rangle \frac{\Delta(\mathbf{k}')}{2E(\mathbf{k}')} \qquad \langle N\rangle = \sum_{\mathbf{k}} \left[1 - \frac{\xi(\mathbf{k})}{E(\mathbf{k})}\right]$$

with and without an effective range gives:



Note that both of these are large (see below). One saturates asymptotically while the other closes.

BCS at weak coupling

The BCS gap at weak coupling, $|k_F a| << 1$, is exponentially small:

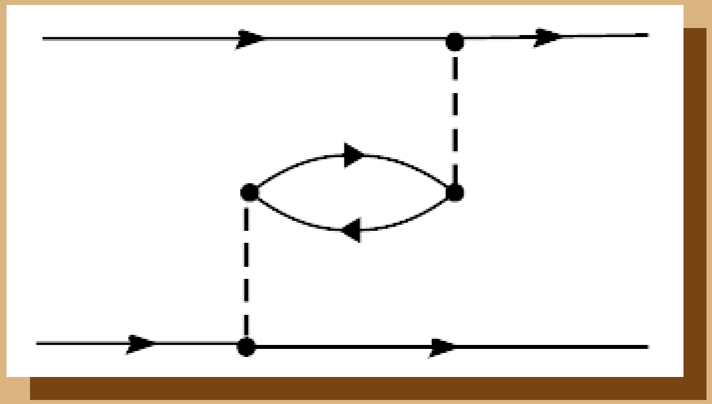
$$\Delta^0_{BCS}(k_F) = \frac{8}{e^2}\frac{\hbar^2 k_F^2}{2m}\exp\left(\frac{\pi}{2ak_F}\right)$$

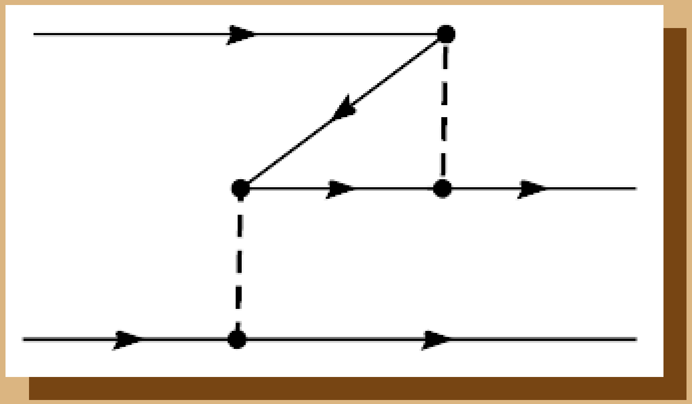
BCS at weak coupling

The BCS gap at weak coupling, $|k_F a| << 1$, is exponentially small:

$$\Delta^0_{BCS}(k_F) = \frac{8}{e^2}\frac{\hbar^2 k_F^2}{2m}\exp\left(\frac{\pi}{2ak_F}\right)$$

Note that even at vanishing coupling this is not the true answer.
A famous result by Gorkov and Melik-Barkhudarov states that
due to screening:





the answer is smaller by a factor of $1/(4e)^{1/3} \approx 0.45$:

$$\Delta^0_{GMB}(k_F) = \frac{1}{(4e)^{1/3}}\frac{8}{e^2}\frac{\hbar^2 k_F^2}{2m}\exp\left(\frac{\pi}{2ak_F}\right)$$

Strongly

Fermionic superfluidity

Transition temperature below which we have superfluidity, T_c, is directly related to the size of the pairing gap at zero temperature.

	T_c	T_c/T_F
Conventional superconductors	5 K	$5 \cdot 10^{-5}$
^{3}He	2.7 mK	$5 \cdot 10^{-4}$
High-T_c superconductors	100 K	10^{-2}
Neutron matter	10^{10} K	0.1
Atomic Fermi gases	200 nK	0.2

Fermionic superfluidity

Transition temperature below which we have superfluidity, T_c,
is directly related to the size of the pairing gap at zero temperature.

	T_c	T_c/T_F
Conventional superconductors	5 K	$5 \cdot 10^{-5}$
^{3}He	2.7 mK	$5 \cdot 10^{-4}$
High-T_c superconductors	100 K	10^{-2}
Neutron matter	10^{10} K	0.1
Atomic Fermi gases	200 nK	0.2

Fermionic superfluidity

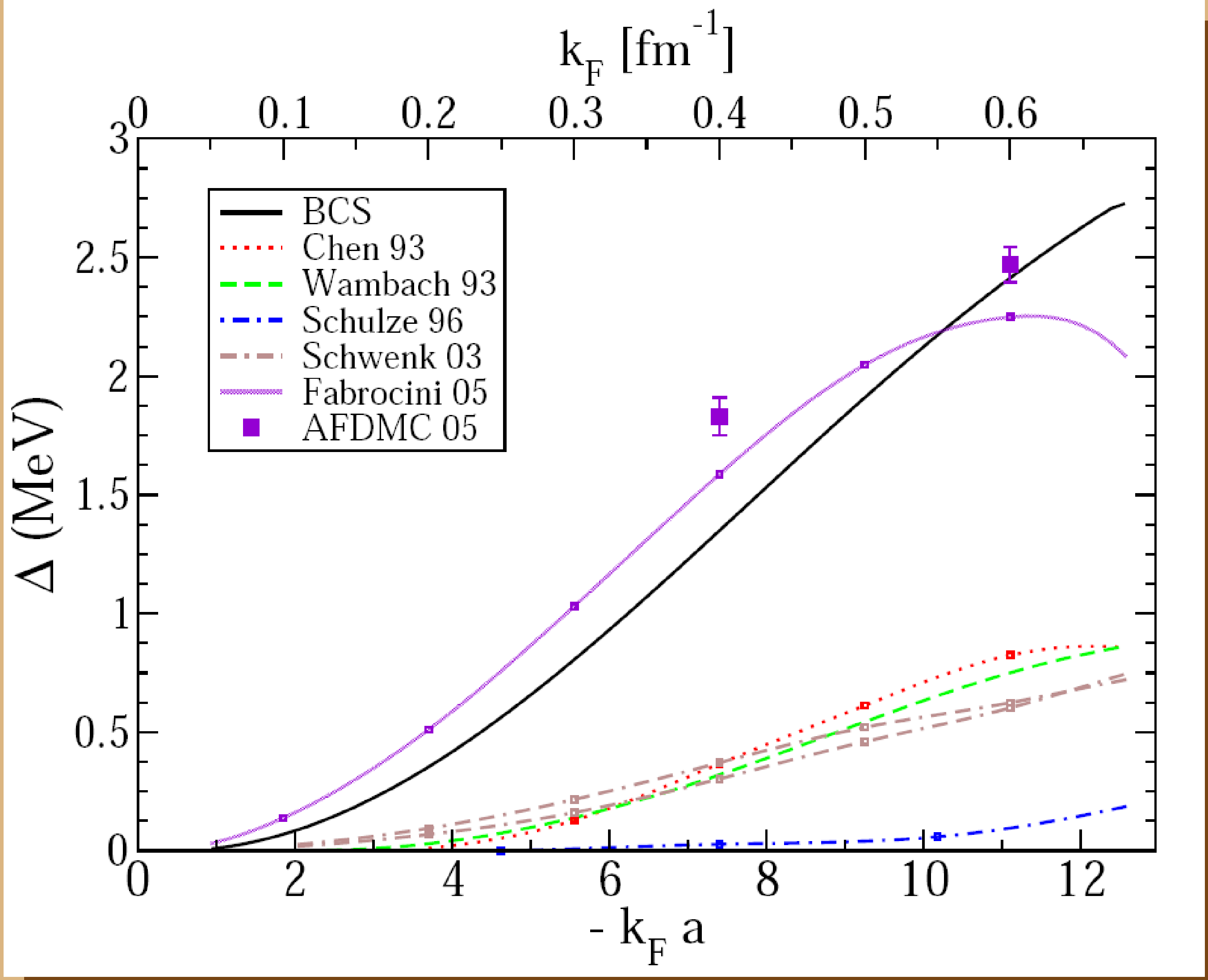
Transition temperature below which we have superfluidity, T_c,
is directly related to the size of the pairing gap at zero temperature.

	T_c	T_c/T_F
Conventional superconductors	5 K	$5 \cdot 10^{-5}$
^{3}He	2.7 mK	$5 \cdot 10^{-4}$
High-T_c superconductors	100 K	10^{-2}
Neutron matter	10^{10} K	0.1
Atomic Fermi gases	200 nK	0.2

Note: inverse of pairing gap gives coherence length/Cooper pair size.
Small gap means huge Cooper pair. Large gap, smaller pair size.

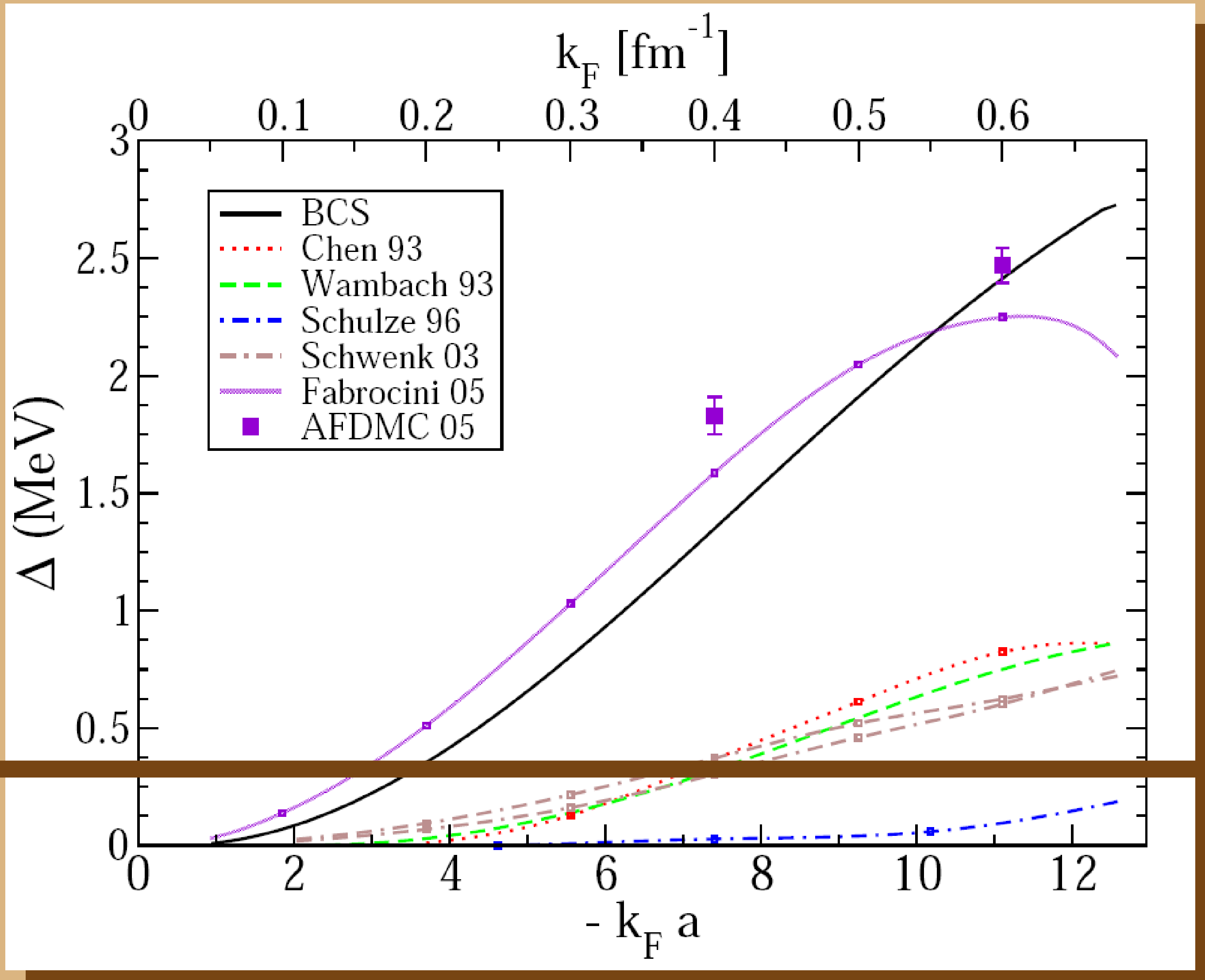
$^1S_0$ neutron matter pairing gap

No experiment → no consensus



$^1S_0$ neutron matter pairing gap

No experiment → no consensus



Strong pairing

How to handle beyond-BCS pairing?

Quantum Monte Carlo is a dependable, *ab initio* approach to the many-body problem, unused for pairing in the past, since the gap is given as a difference:

$$\Delta = E(N+1) - \frac{1}{2}\left[E(N) + E(N+2)\right]$$

and in traditional systems this energy difference was very small. However, for strongly paired fermions this is different.

Continuum Quantum Monte Carlo

Rudiments of Diffusion Monte Carlo:

$$\Psi(\tau \to \infty) = \lim_{\tau \to \infty} e^{-(\mathcal{H} - E_T)\tau} \Psi_V$$

$$\to \alpha_0 e^{-(E_0 - E_T)\tau} \Psi_0$$

Continuum Quantum Monte Carlo

Rudiments of Diffusion Monte Carlo:

$$\Psi(\tau \to \infty) = \lim_{\tau \to \infty} e^{-(\mathcal{H} - E_T)\tau} \Psi_V$$
$$\to \alpha_0 e^{-(E_0 - E_T)\tau} \Psi_0$$

How to do? Start somewhere and evolve

$$\psi(\mathbf{R}, \tau) = \int G(\mathbf{R}, \mathbf{R}', \tau) \psi(\mathbf{R}', 0) d\mathbf{R}'$$

With a standard propagator

$$G(\mathbf{R}, \mathbf{R}', \tau) = \langle \mathbf{R} | e^{-(H - E_0)\tau} | \mathbf{R}' \rangle$$

Cut up into many time slices

$$G(\mathbf{R}, \mathbf{R}', \Delta\tau) \approx e^{-\frac{V(\mathbf{R}) + V(\mathbf{R}')}{2} \Delta\tau} \left(\frac{m}{2\pi\hbar^2\tau} \right)^{\frac{3A}{2}} e^{-\frac{m|\mathbf{R} - \mathbf{R}'|^2}{2\hbar^2\tau}}$$

Continuum Quantum Monte Carlo

Rudiments of wave functions in Diffusion Monte Carlo

Normal gas

Two Slater determinants, written either using the antisymmetrizer:

$$\Phi_S(\mathbf{R}) = \mathcal{A}[\phi_n(r_1)\phi_n(r_2)\ldots\phi_n(r_{\frac{N}{2}})]\ \ \mathcal{A}[\phi_n(r_{1'})\phi_n(r_{2'})\ldots\phi_n(r_{\frac{N}{2}'})]$$

Continuum Quantum Monte Carlo

Rudiments of wave functions in Diffusion Monte Carlo

Normal gas

Two Slater determinants, written either using the antisymmetrizer:

$$\Phi_S(\mathbf{R}) = \mathcal{A}[\phi_n(r_1)\phi_n(r_2)\ldots\phi_n(r_{\frac{N}{2}})]\ \mathcal{A}[\phi_n(r_{1'})\phi_n(r_{2'})\ldots\phi_n(r_{\frac{N}{2}'})]$$

or actual determinants (e.g. 7 + 7 particles):

$$\Phi_S(\mathbf{R}) = \begin{vmatrix} \phi_1(r_1) & \phi_1(r_2) & \ldots & \phi_1(r_7) \\ \phi_2(r_1) & \phi_2(r_2) & \ldots & \phi_2(r_7) \\ \phi_3(r_1) & \phi_3(r_2) & \ldots & \phi_3(r_7) \\ \phi_4(r_1) & \phi_4(r_2) & \ldots & \phi_4(r_7) \\ \phi_5(r_1) & \phi_5(r_2) & \ldots & \phi_5(r_7) \\ \phi_6(r_1) & \phi_6(r_2) & \ldots & \phi_6(r_7) \\ \phi_7(r_1) & \phi_7(r_2) & \ldots & \phi_7(r_7) \end{vmatrix} \begin{vmatrix} \phi_1(r_1') & \phi_1(r_2') & \ldots & \phi_1(r_7') \\ \phi_2(r_1') & \phi_2(r_2') & \ldots & \phi_2(r_7') \\ \phi_3(r_1') & \phi_3(r_2') & \ldots & \phi_3(r_7') \\ \phi_4(r_1') & \phi_4(r_2') & \ldots & \phi_4(r_7') \\ \phi_5(r_1') & \phi_5(r_2') & \ldots & \phi_5(r_7') \\ \phi_6(r_1') & \phi_6(r_2') & \ldots & \phi_6(r_7') \\ \phi_7(r_1') & \phi_7(r_2') & \ldots & \phi_7(r_7') \end{vmatrix}$$

Continuum Quantum Monte Carlo

Rudiments of wave functions in Diffusion Monte Carlo

Superfluid gas

BCS determinant for fixed particle number, using the antisymmetrizer:

$$\Phi_{BCS}(\mathbf{R}) = \mathcal{A}[\phi(r_{11'})\phi(r_{22'})\ldots\phi(r_{\frac{N}{2}\frac{N}{2}'})]$$

Continuum Quantum Monte Carlo

Rudiments of wave functions in Diffusion Monte Carlo

Superfluid gas

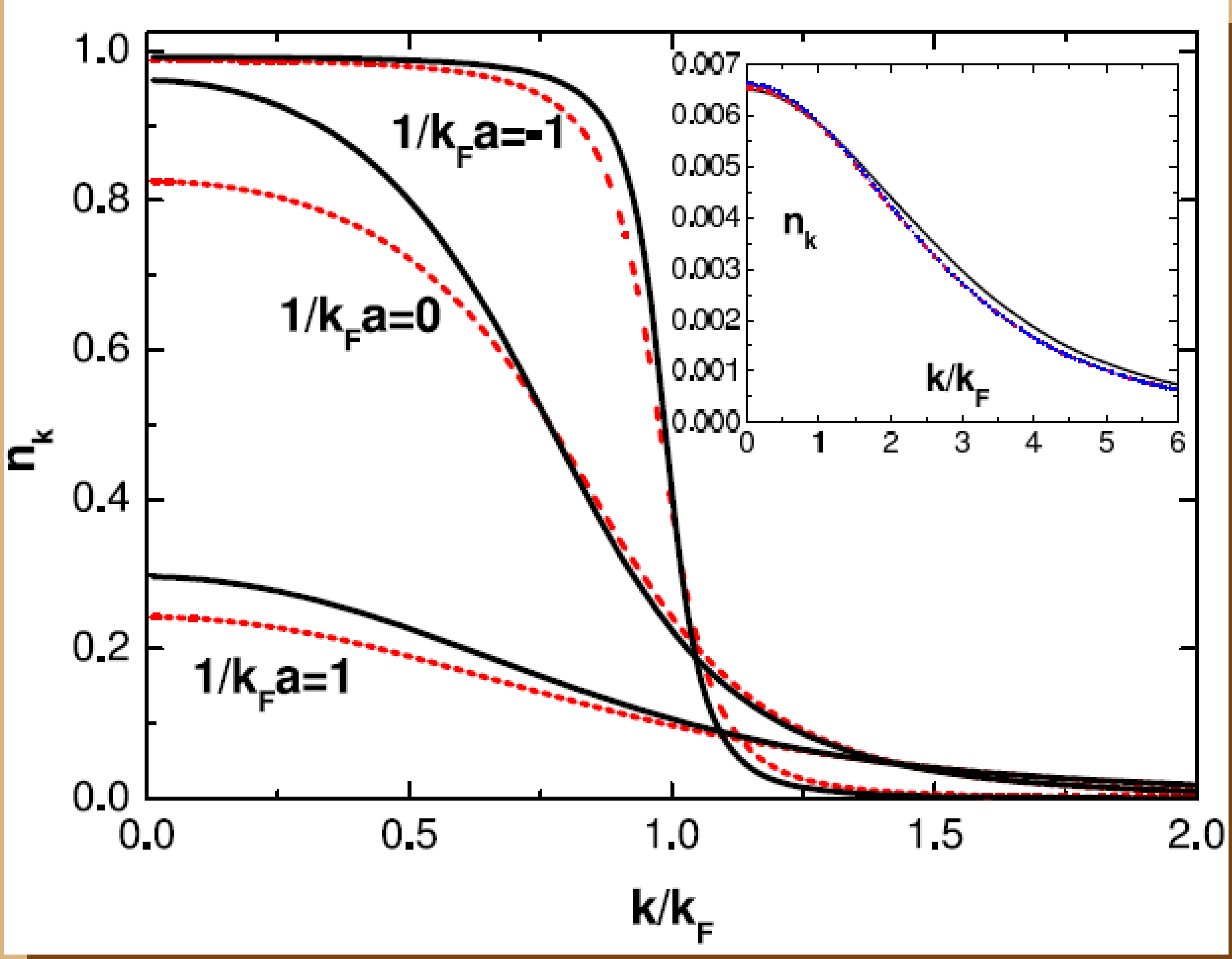
BCS determinant for fixed particle number, using the antisymmetrizer:

$$\Phi_{BCS}(\mathbf{R}) = \mathcal{A}[\phi(r_{11'})\phi(r_{22'})\ldots\phi(r_{\frac{N}{2}\frac{N}{2}'})]$$

or, again, a determinant, but this time of pairing functions:

$$\begin{vmatrix} \phi(r_{11'}) & \phi(r_{12'}) & \ldots & \phi(r_{1\frac{N}{2}'}) \\ \phi(r_{21'}) & \phi(r_{22'}) & \ldots & \phi(r_{2\frac{N}{2}'}) \\ \vdots & \vdots & \vdots\vdots\vdots & \vdots \\ \phi(r_{\frac{N}{2}1'}) & \phi(r_{\frac{N}{2}2'}) & \ldots & \phi(r_{\frac{N}{2}\frac{N}{2}'}) \end{vmatrix}$$

Momentum distribution: results

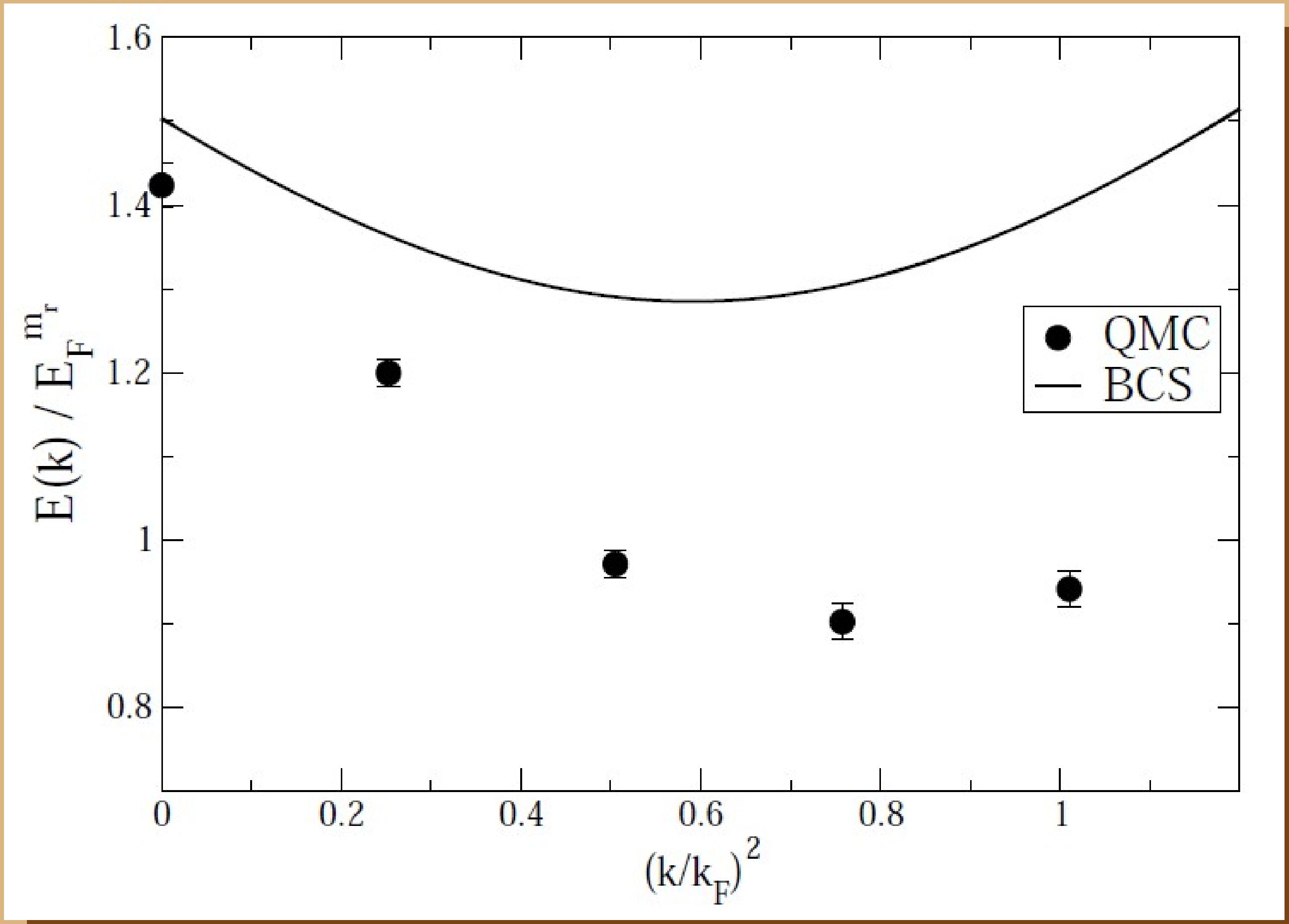


G. E. Astrakharchik, J. Boronat, J. Casulleras, and S. Giorgini, Phys. Rev. Lett. **95**, 230405 (2005)

- BCS line is simply
$$n(\mathbf{k}) = \frac{1}{2}\left(1 - \frac{\xi(\mathbf{k})}{E(\mathbf{k})}\right)$$
- Quantitatively changes at strong coupling. Qualitatively things are very similar.

ATOMS

Quasiparticle dispersion: results

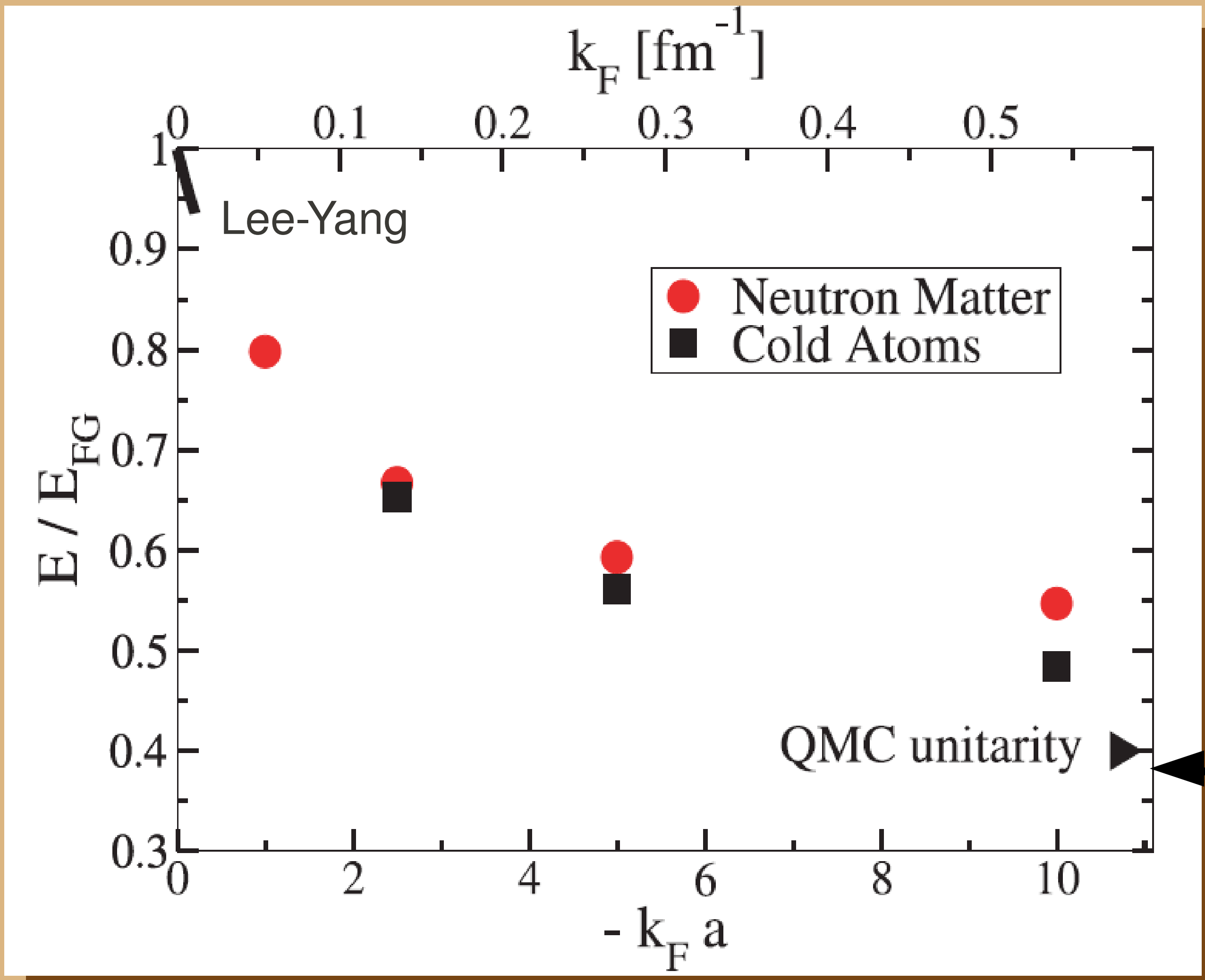


QMC results from:
J. Carlson and S. Reddy, Phys. Rev. Lett. **95**, 060401 (2005)

- BCS line is simply
$$E(\mathbf{k}) = \sqrt{\xi(\mathbf{k})^2 + \Delta(\mathbf{k})^2}$$
- Both position and size of minimum change when going from mean-field to full ab initio

ATOMS

Equations of state: results



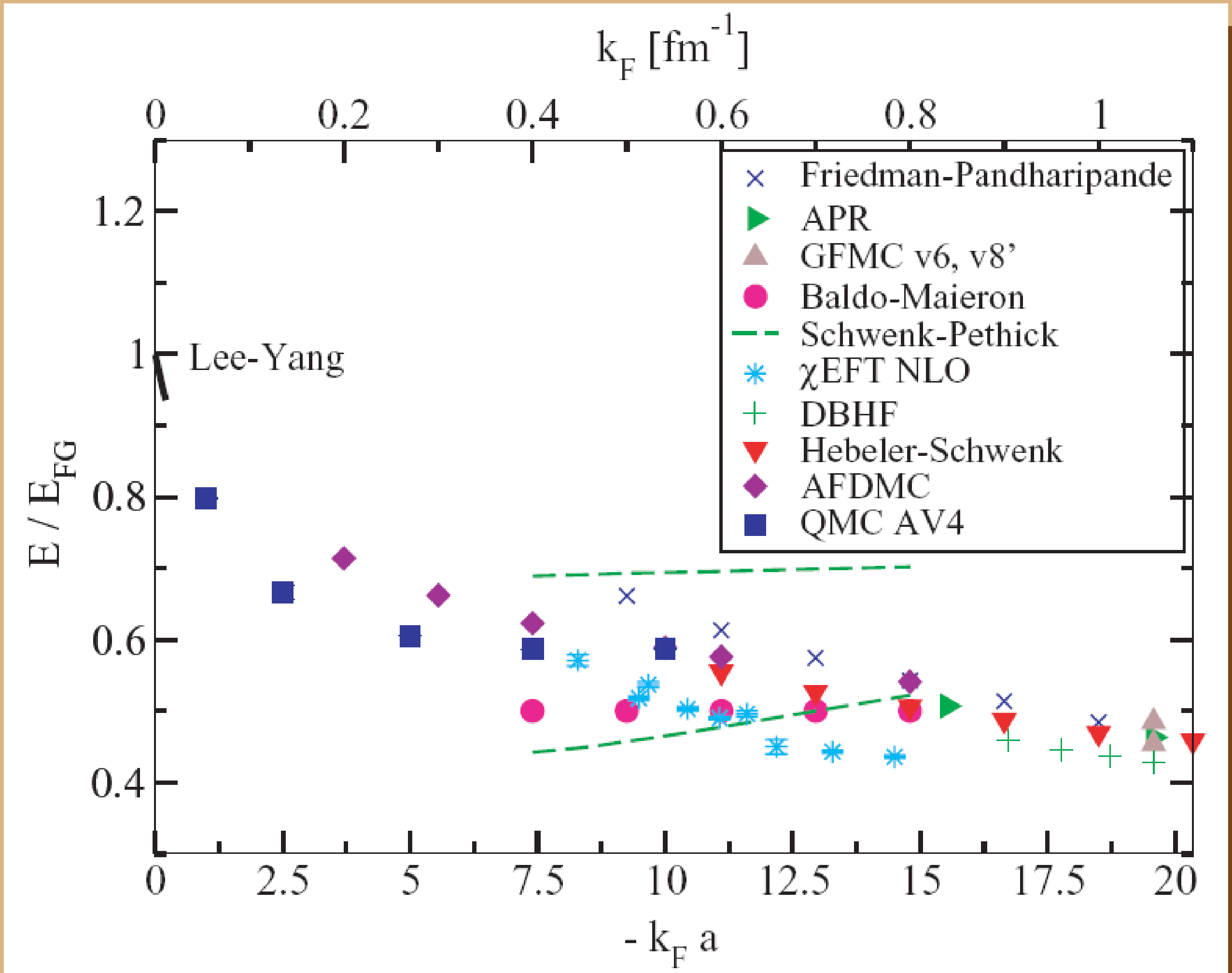
- Results identical at low density
- Range important at high density
- MIT experiment at unitarity

A. Gezerlis and J. Carlson, Phys. Rev. C **77**, 032801 (2008)

NEUTRONS

ATOMS

Equations of state: comparison

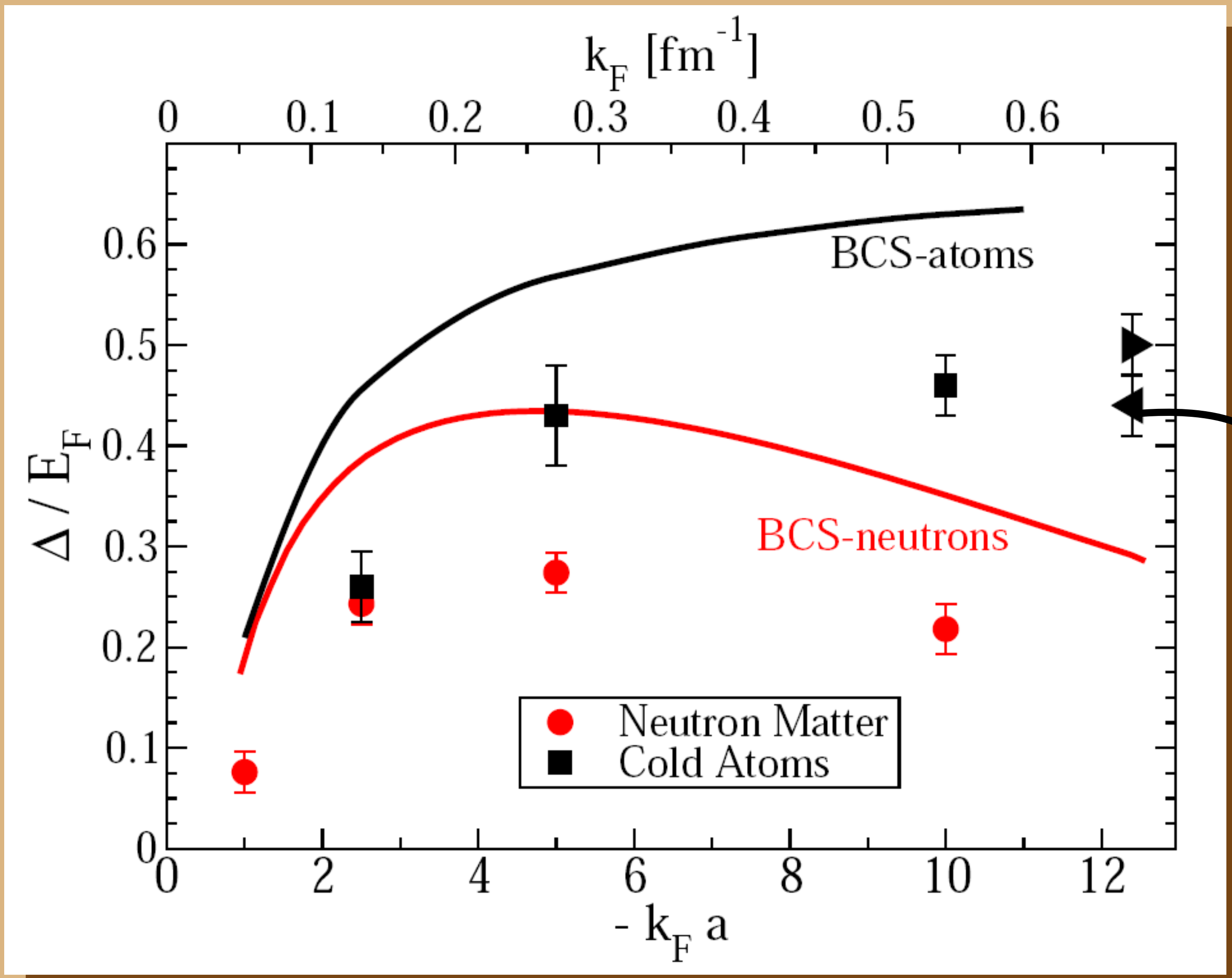


- QMC can go down to low densities; agreement with Lee-Yang trend
- At higher densities all calculations are in qualitative agreement

NEUTRONS

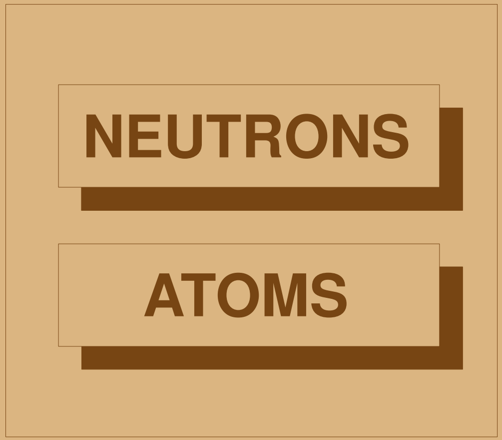
A. Gezerlis and J. Carlson, Phys. Rev. C **81**, 025803 (2010)

Pairing gaps: results

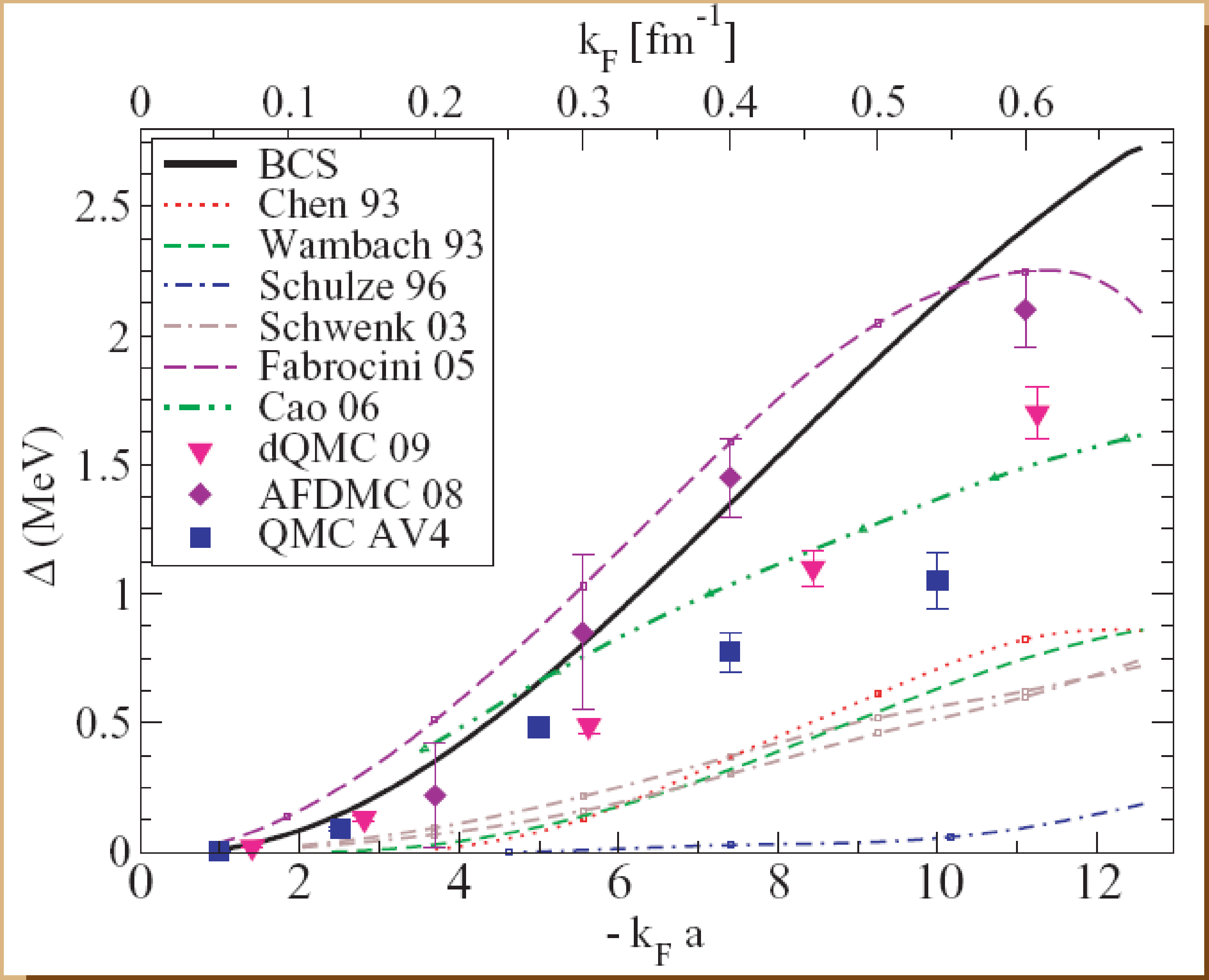


A. Gezerlis and J. Carlson, Phys. Rev. C **77**, 032801 (2008)

- Results identical at low density
- Range important at high density
- Two independent MIT experiments at unitarity



Pairing gaps: comparison



- Consistent suppression with respect to BCS; similar to Gorkov
- Disagreement with AFDMC studied extensively
- Emerging consensus

NEUTRONS

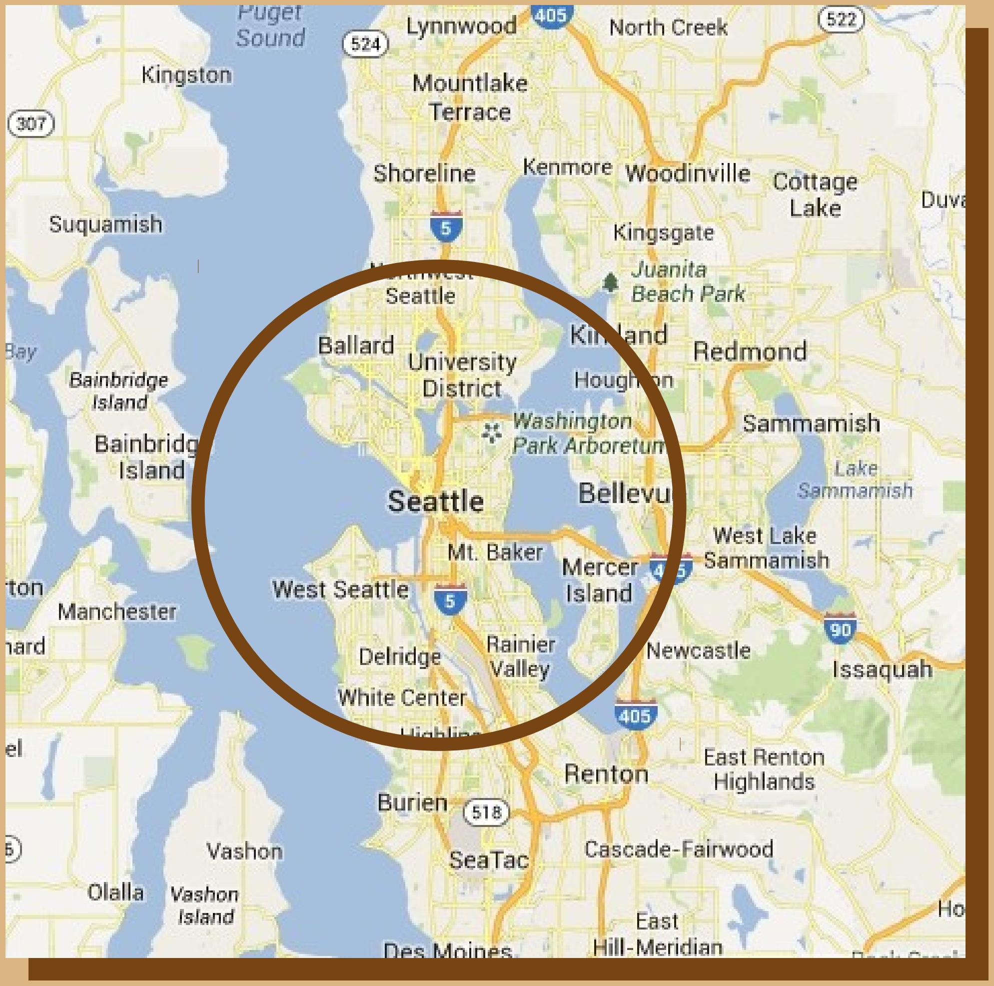
A. Gezerlis and J. Carlson, Phys. Rev. C **81**, 025803 (2010)

Physical significance: neutron stars

Ultra-dense objects

- Mass ~ 1.4 – 2.0 solar masses
- Radius ~ 10 km
- Temperature ~ 10^6 – 10^9 K
  (which you now know is cold)
- Magnetic fields ~ 10^8 T
- Rotation periods ~ ms to s

Credit: Google Maps

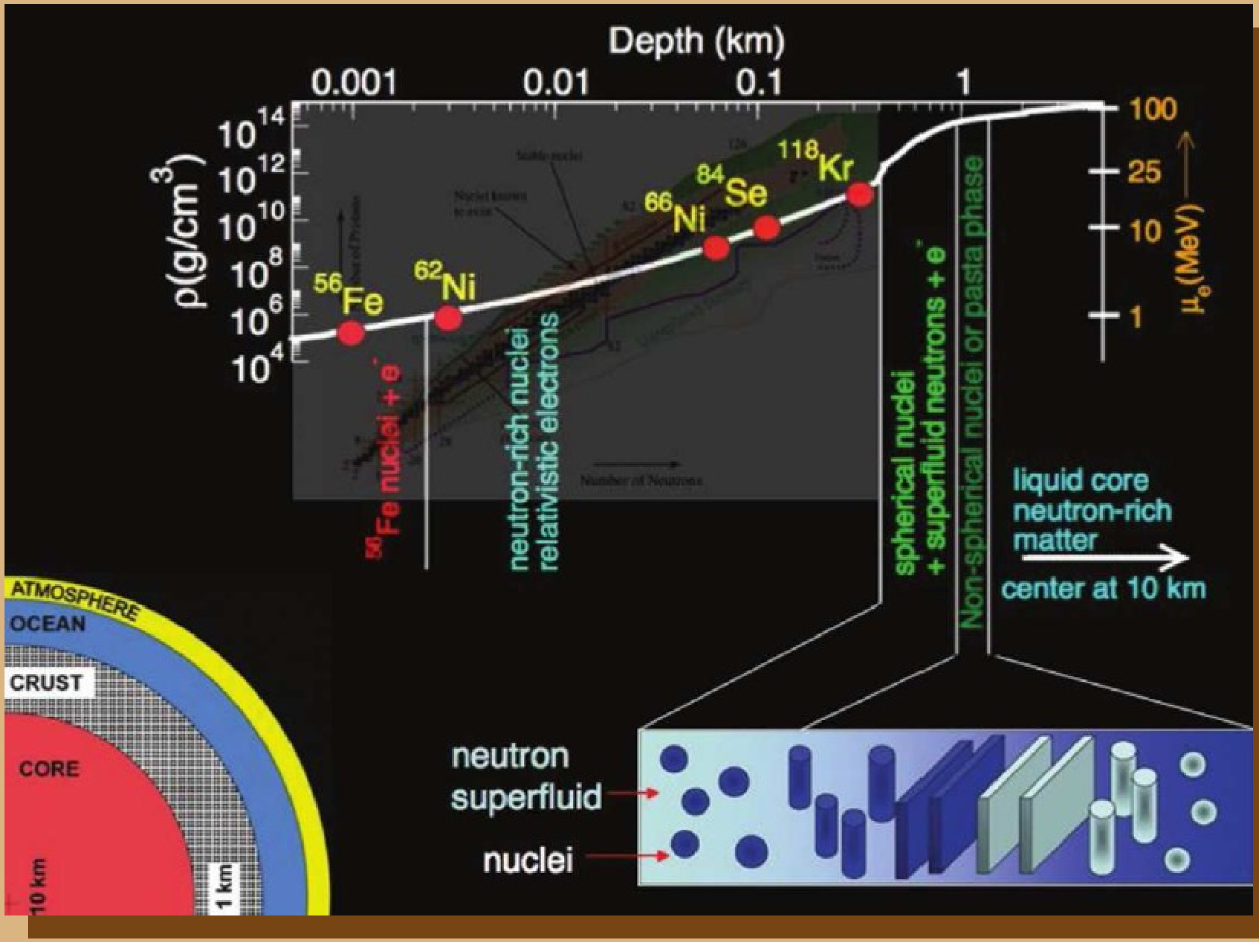


What about neutron matter?

Neutron-star crust physics

Credit: NSAC Long Range Plan 2007

- Neutrons drip
- From low to (very) high density
- Interplay of many areas of physics
- Microscopic constraints important



The meaning of it all

Neutron-star crust consequences

- Negligible contribution to specific heat consistent with cooling of transients:

  E. F. Brown and A. Cumming. Astrophys. J. **698**, 1020 (2009).

- Young neutron star cooling curves depend on the magnitude of the gap:

  D. Page, J. M. Lattimer, M. Prakash, A. W. Steiner, Astrophys. J. **707**, 1131 (2009).

- Superfluid-phonon heat conduction mechanism viable:

  D. Aguilera, V. Cirigliano, J. Pons, S. Reddy, R. Sharma, Phys. Rev. Lett. 102, 091101 (2009).

- Constraints for Skyrme-HFB calculations of neutron-rich nuclei:

  N. Chamel, S. Goriely, and J. M. Pearson, Nucl. Phys. A **812**, 27 (2008).

Conclusions

- Cold-atom experiments can help constrain nuclear theory

- Pionless theory is smoothly connected to the pionful one in the framework of neutron-star crusts

- Non-perturbative methods can be used to extract pairing gaps in addition to energies