Recent progress on the Fermi gas from auxiliary-field QMC

Shiwei Zhang

- Auxiliary-field QMC (AFQMC)
  - Connection with lattice methods
  - Technical advances in FG (e.g. low-rank decomp - scaling N^3 -> N)
  - Conceptual difference for general interactions: controlling sign problem (any realistic materials)
- Precision computation in the 2D Fermi gas
  - Ground state: EOS, gaps, n(k), …
  - BKT Tc, contact, response

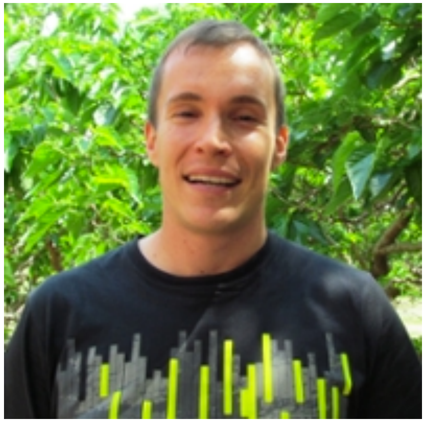
FLATIRON INSTITUTE
Center for Computational Quantum Physics

Collaborators:

Yuanyao He
(Northwest U, China)

Peter Rosenberg
(Sherbrooke, Canada)

Hao Shi
(Delaware)

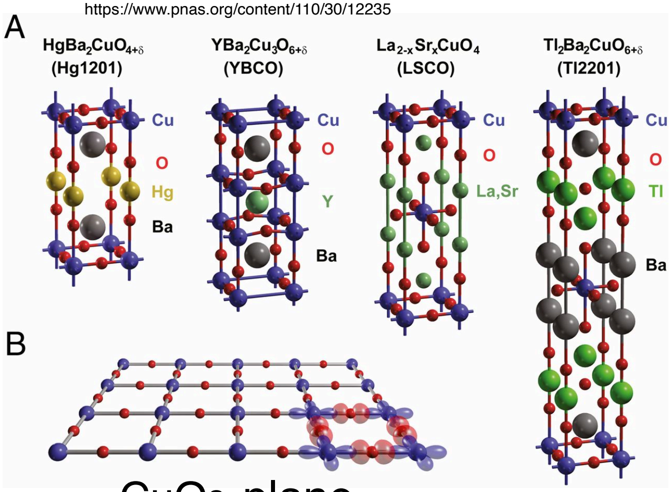


Ettore Vitali
(Cal State Fresno)

The many electron problem

- We know the electronic Hamiltonian well!

https://www.pnas.org/content/110/30/12235



CuO_2 plane
in cuprates

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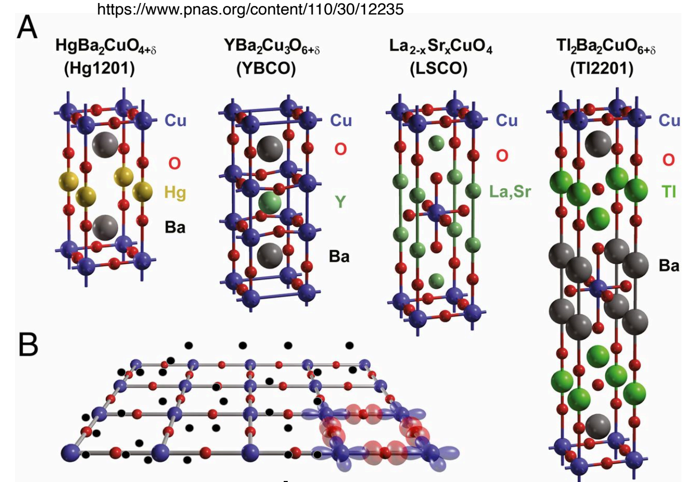

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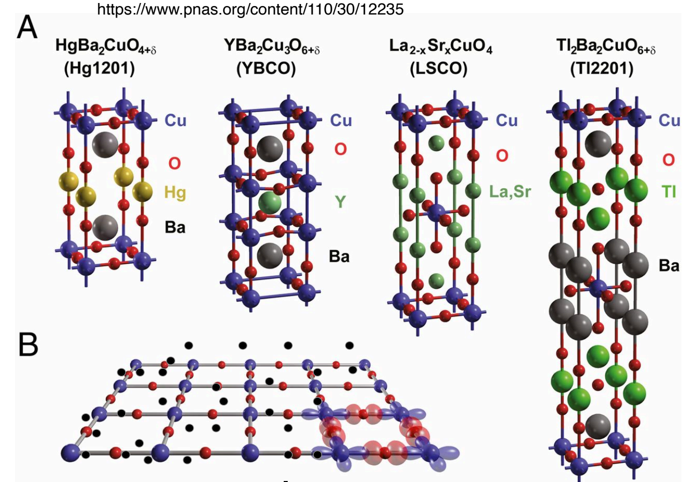

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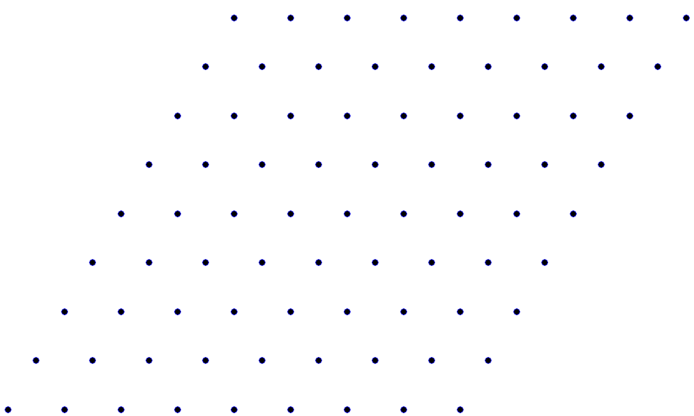

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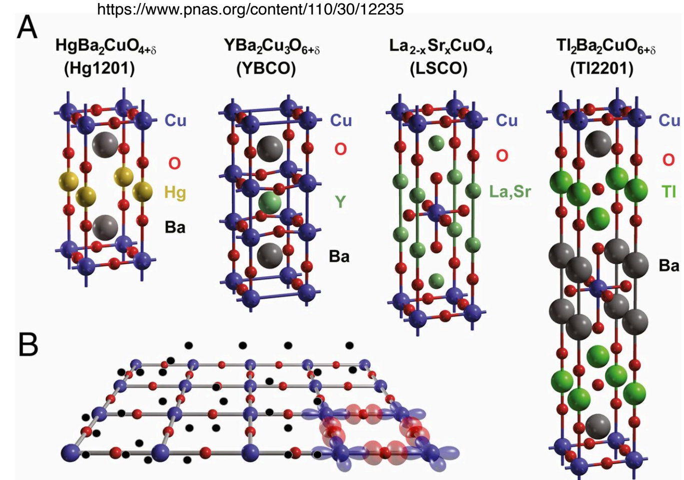

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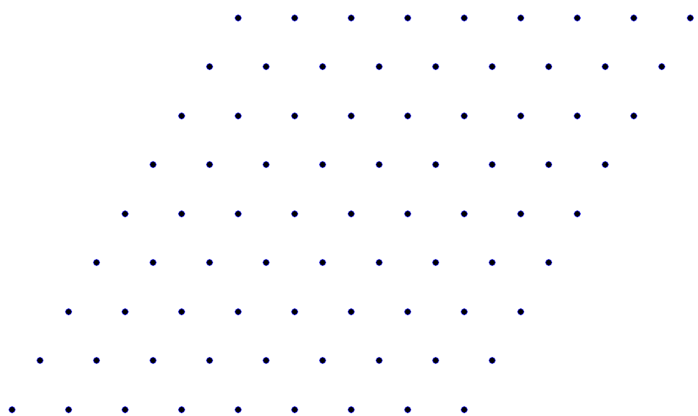

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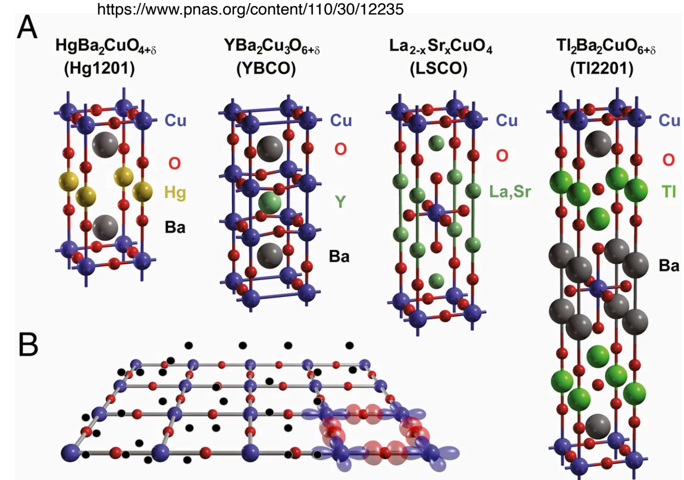

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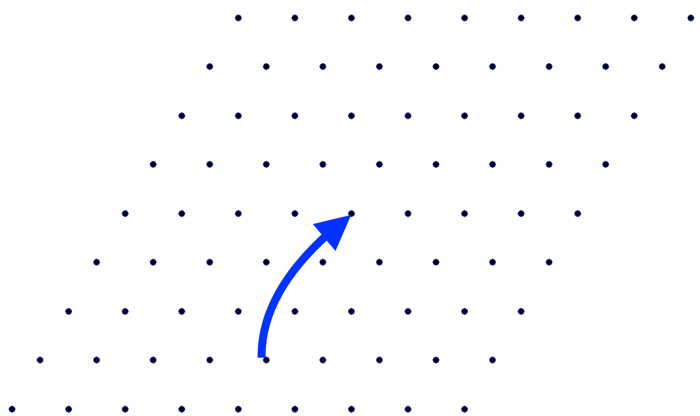

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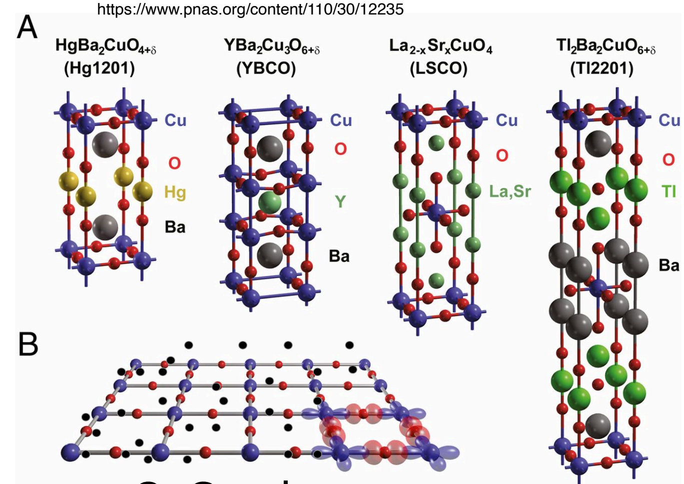

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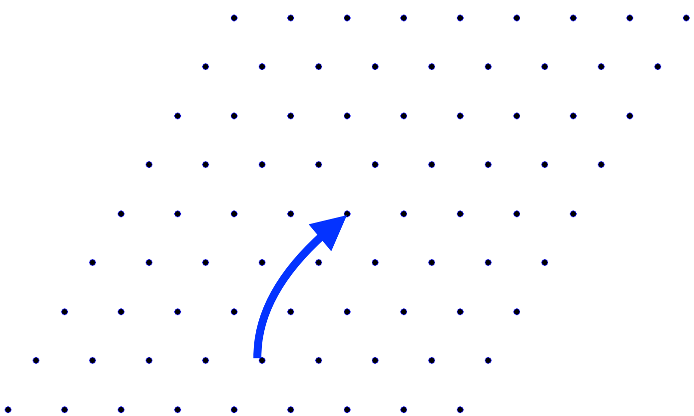

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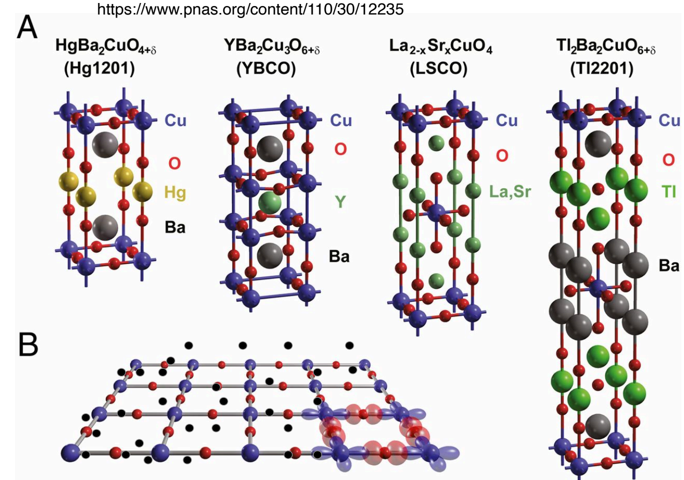

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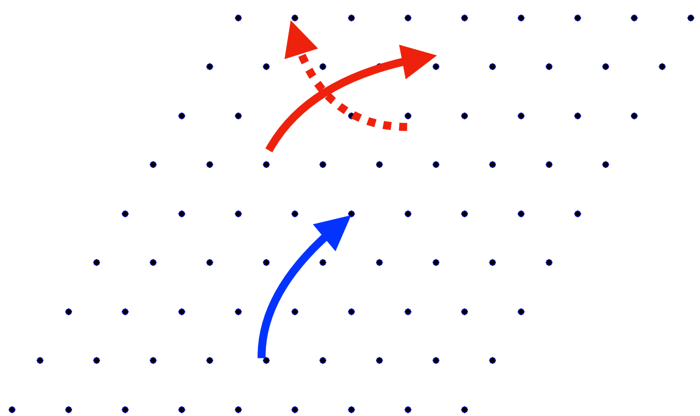

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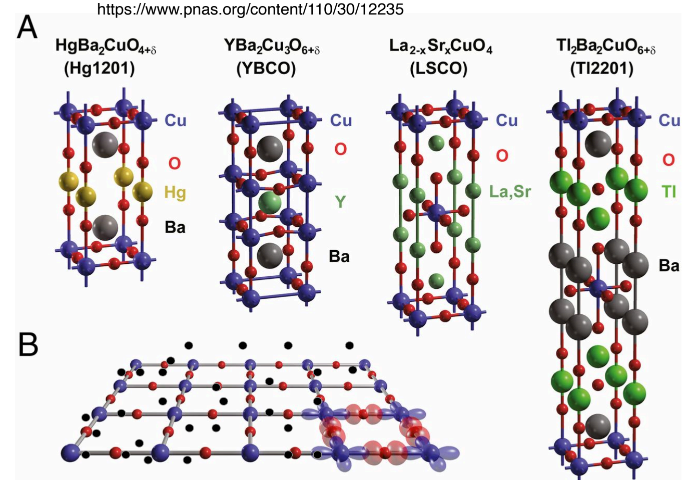

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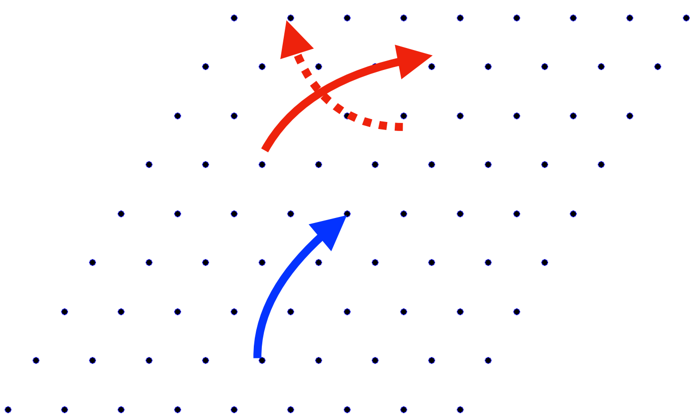

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DFT

- "standard model"

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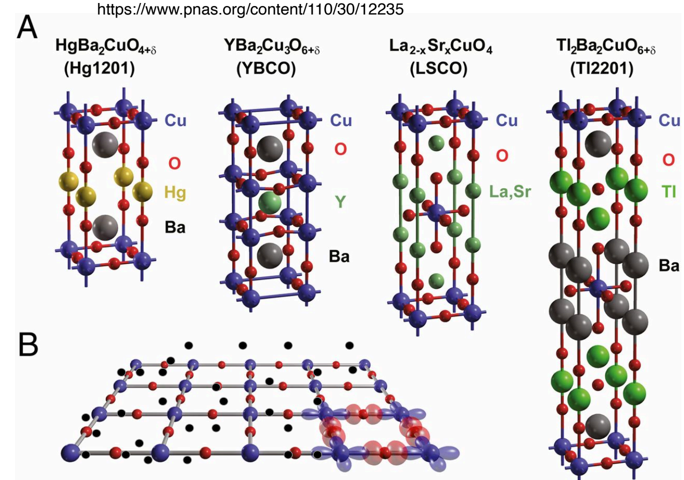

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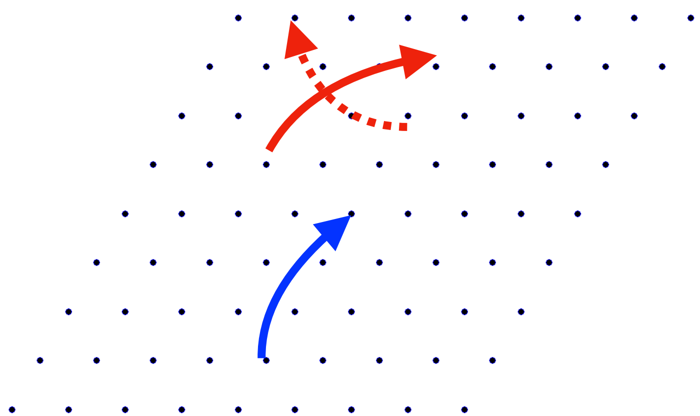

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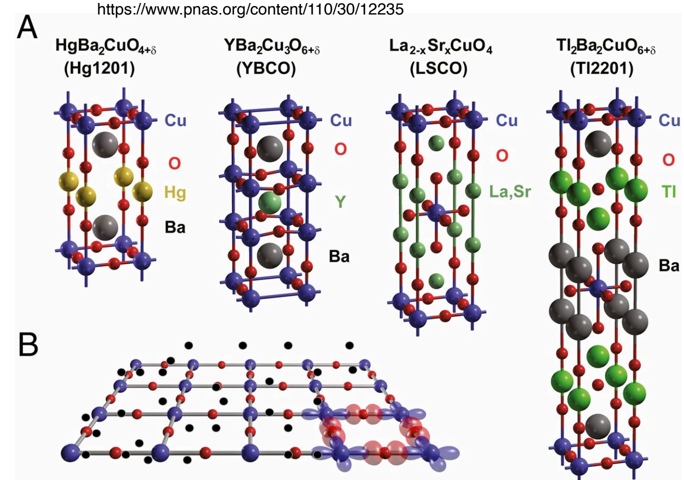

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DFT

- "standard model"
- mean-field-like

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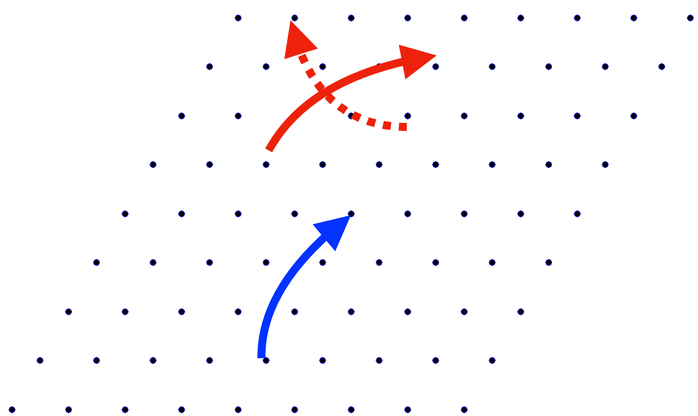

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$$\sum_i f_c(n_i)\hat{n}_i$$

DFT

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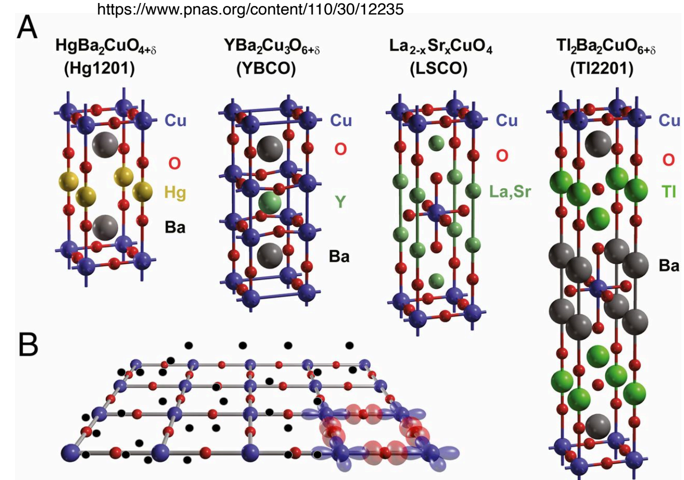

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Benchmark and multi-messenger

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Towards the solution of the many-electron problem in real materials: equation of state of the hydrogen chain with state-of-the-art many-body methods

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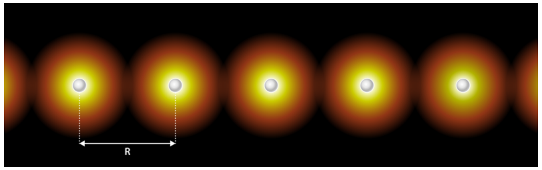
PRX (2017)



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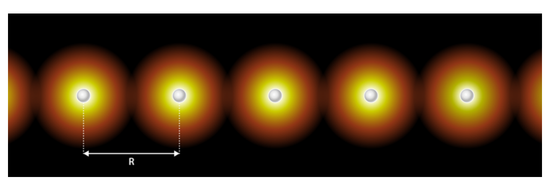

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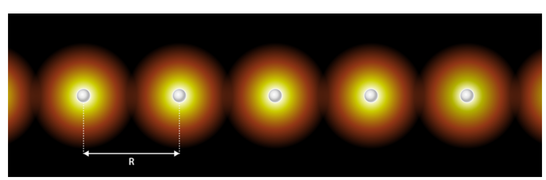

VIEWPOINT

The Rich Inner Life of the Hydrogen Chain

Dieter Vollhardt
Center for Electronic Correlations and Magnetism, University of Augsburg, Augsburg, Germany

September 14, 2020 • *Physics* 13, 142

A one-dimensional chain of hydrogen atoms displays a wide variety of many-body effects—suggesting that the chain can be a useful model system for condensed-matter physics.

Benchmark and multi-messenger

- Mobilized most methods from physics and chemistry - unusual in CM

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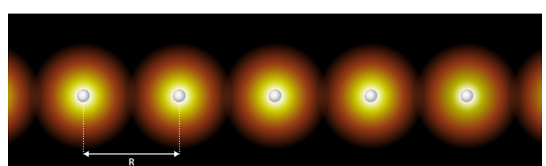

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- The 10-atom chain (molecule)
  - minimal basis
  - -> complete basis set (CBS) limit

- Infinite chain (TDL)
  - minimal basis (extended Hubbard)
  - results at joint CBS+TDL: THE curve

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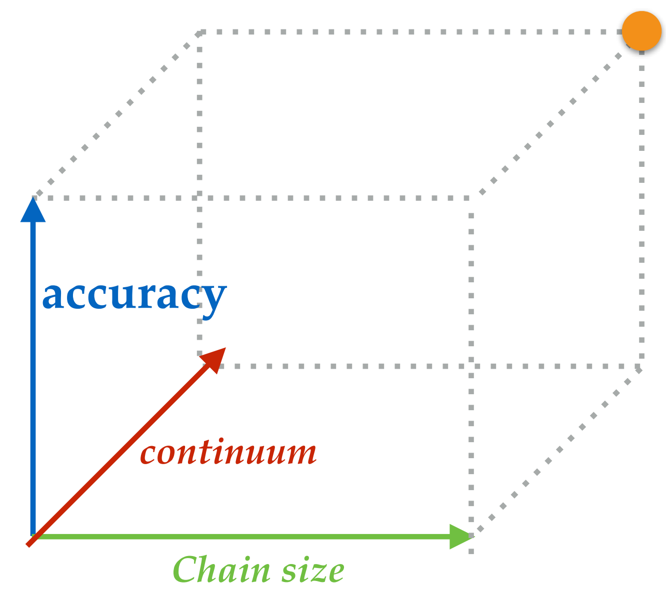
3-fold challenge



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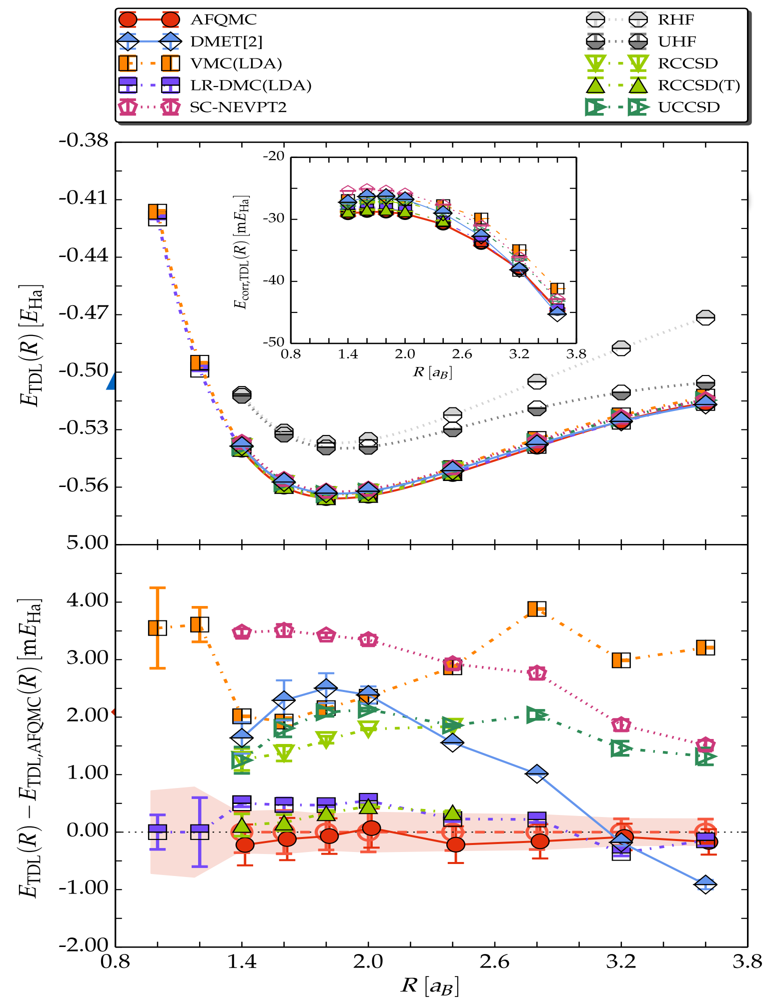
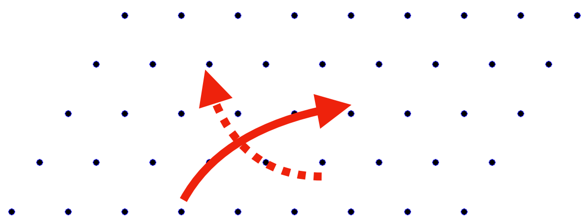
- Highlights
  - Create handshake points: meticulous comparisons and cross-checks
  - large reference data - chem accuracy
  - insights about technical needs; spurred many developments

EOS



What does AFQMC do?

Interaction can be decoupled:



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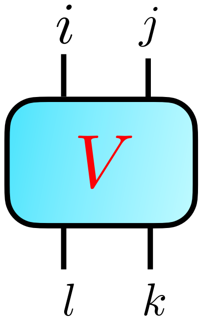

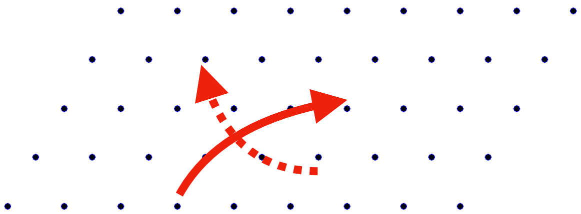

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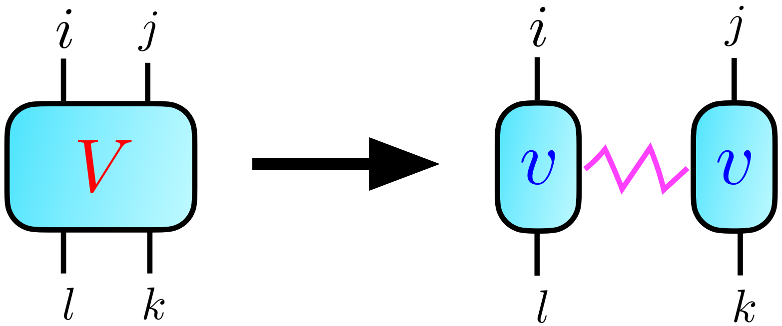

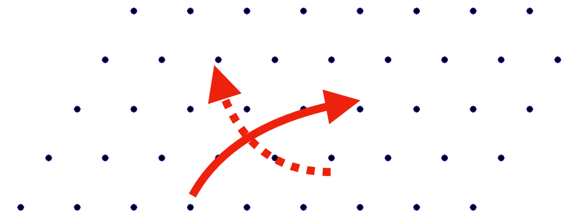

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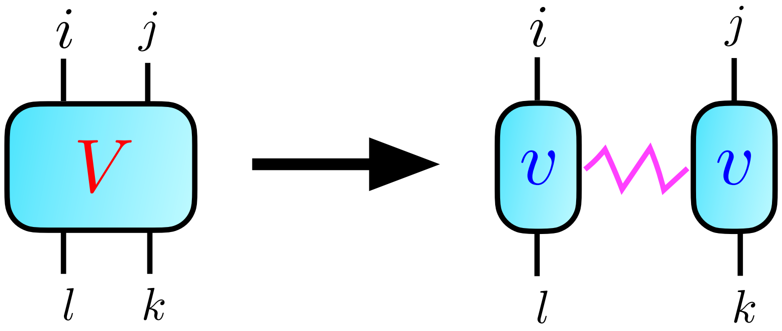

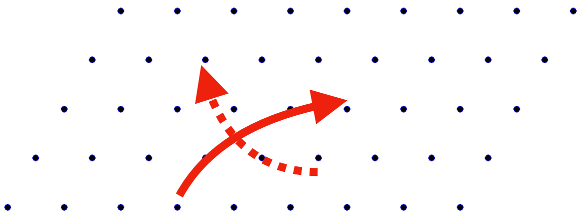

$$e^{-\tau V}$$

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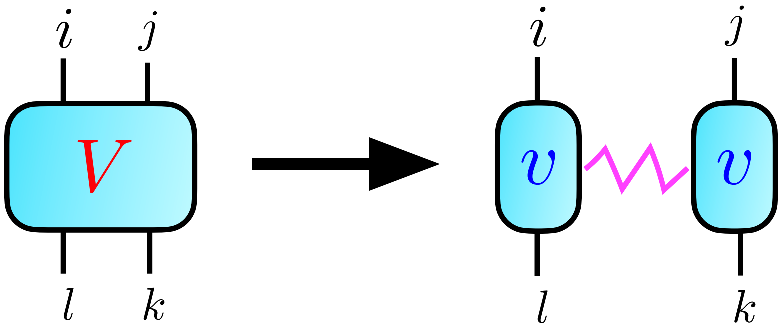

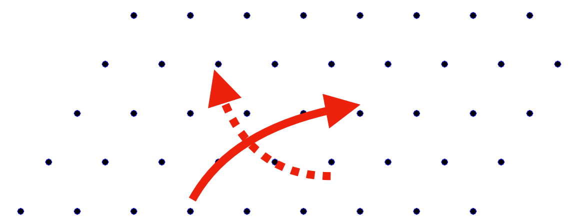

$$e^{-\tau V} \longrightarrow e^{v^2} = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-\sigma^2} e^{2\sigma v} d\sigma$$

Hubbard-Strotonovich

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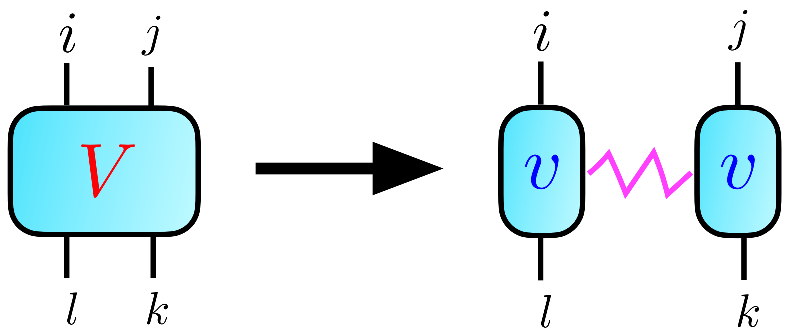
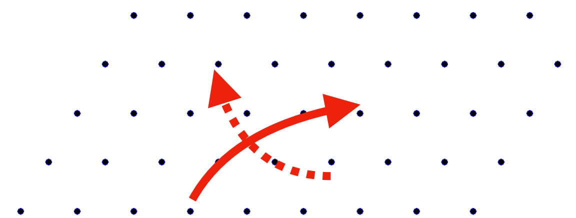
Interaction can be decoupled:

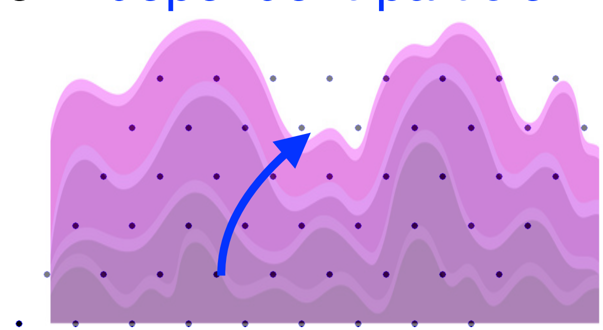




$$e^{-\tau V} \longrightarrow e^{v^2} = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-\sigma^2} e^{2\sigma v} d\sigma$$

Hubbard-Strotonovich

Many-body propagator —> linear combination of independent-particle propagators in auxiliary-fields



Connection to lattice QCD methods

Auxiliary-field methods

	models (attractive, sym, +U 1/2-filling, ...)	models (Doped, multi-orbital, SOC, spin-imbalance, ...)	Molecules/solids (Quantum chemistry, ab initio materials, ...)
ground -state	Projector MC		
finite-T	DQMC/BSS AFMC LMC		

Auxiliary-field methods

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finite-T	DQMC/BSS AFMC LMC	FT CP-AFQMC	FT AFQMC

Sign/phase problem

Auxiliary-field methods

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Sign/phase problem

Sugiyama & Kooning, Ann Phys '86

Blankenbecler, Scalapino, Sugar, PRD '81

SZ, Carlson, Gubernatis, PRL '95; PRB '97

SZ, PRL '99; He et al, PRB '19

SZ & Krakauer, PRL '03; Shi & SZ, JCP '21

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AFDMC

Sign/phase problem

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ground -state	Projector MC		MC
finite-T	DQMC/BSS AFMC LMC		MC

AFDMC

Fermi gas:

- No sign problem -> exact
- But be careful w/ infinite variance

  Shi & SZ, PRE '16
- Algorithmic advances to reach/ exceed expt precision

Sign/phase problem

Sugiyama & Kooning, Ann Phys '86

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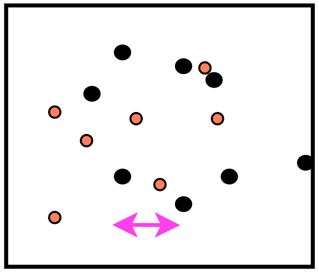
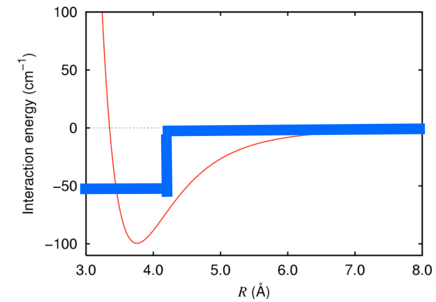
Ultracold atomic Fermi gas



$$H = -\frac{\hbar^2}{2m}\left(\sum_{i}^{N/2}\nabla_i^2 + \sum_{j}^{N/2}\nabla_j^2\right) + \sum_{i,j} V(r_{ij})$$

inter-particle spacing d >> range of V



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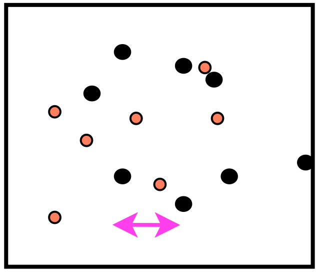

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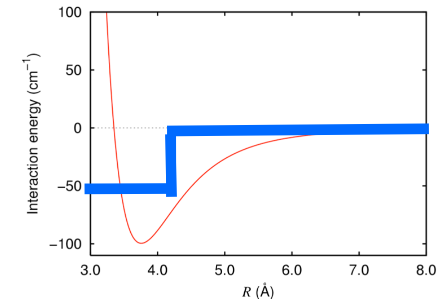
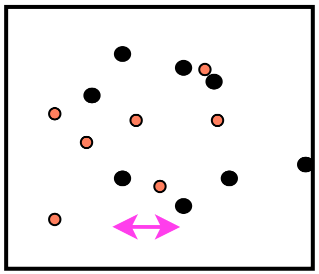


In 3D, can tune V to modify 2-body s-wave scattering length:

Ultracold atomic Fermi gas



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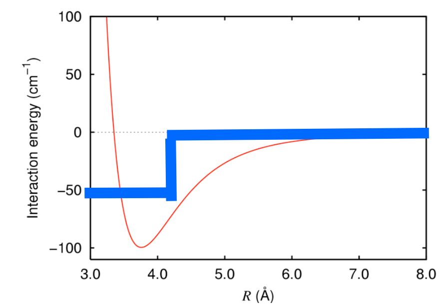


In 3D, can tune V to modify 2-body s-wave scattering length:

V depth	large	unitarity	small
2-body scattering length	>0	infinity	<0
physics	molecule		unbound

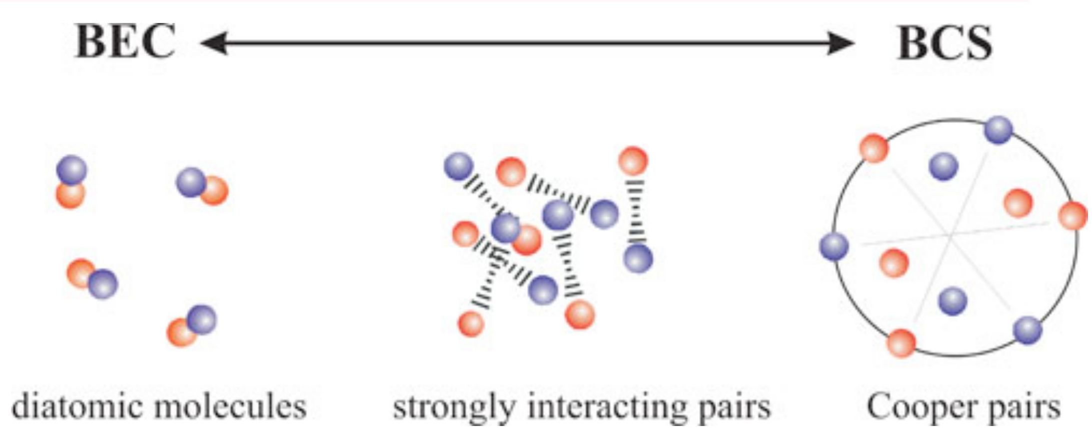
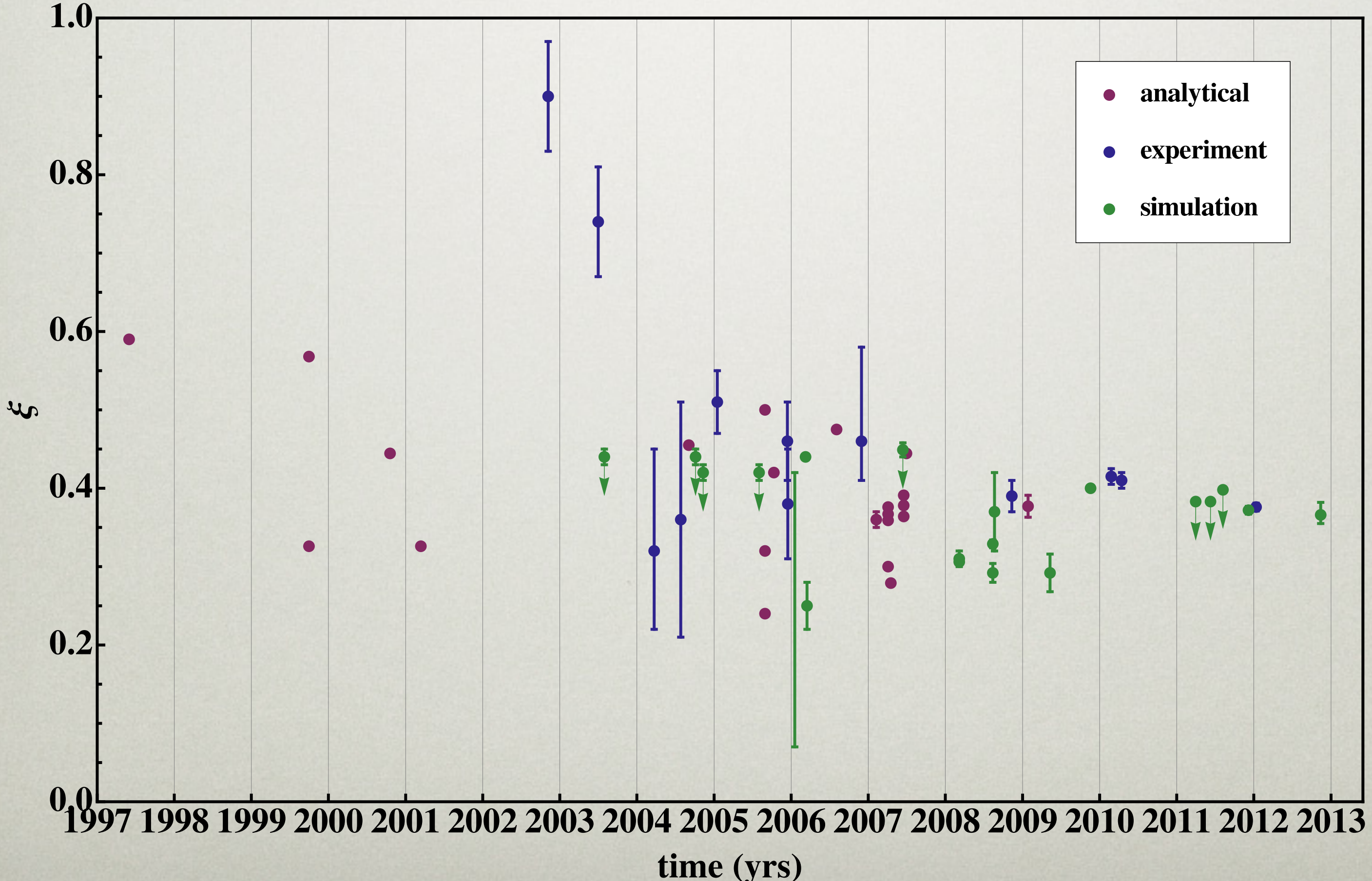


Image from D. Jin group

Precision many body physics in 3D

- Bertsch parameter M. Endres *et al* PRA 87 (2012) 023615



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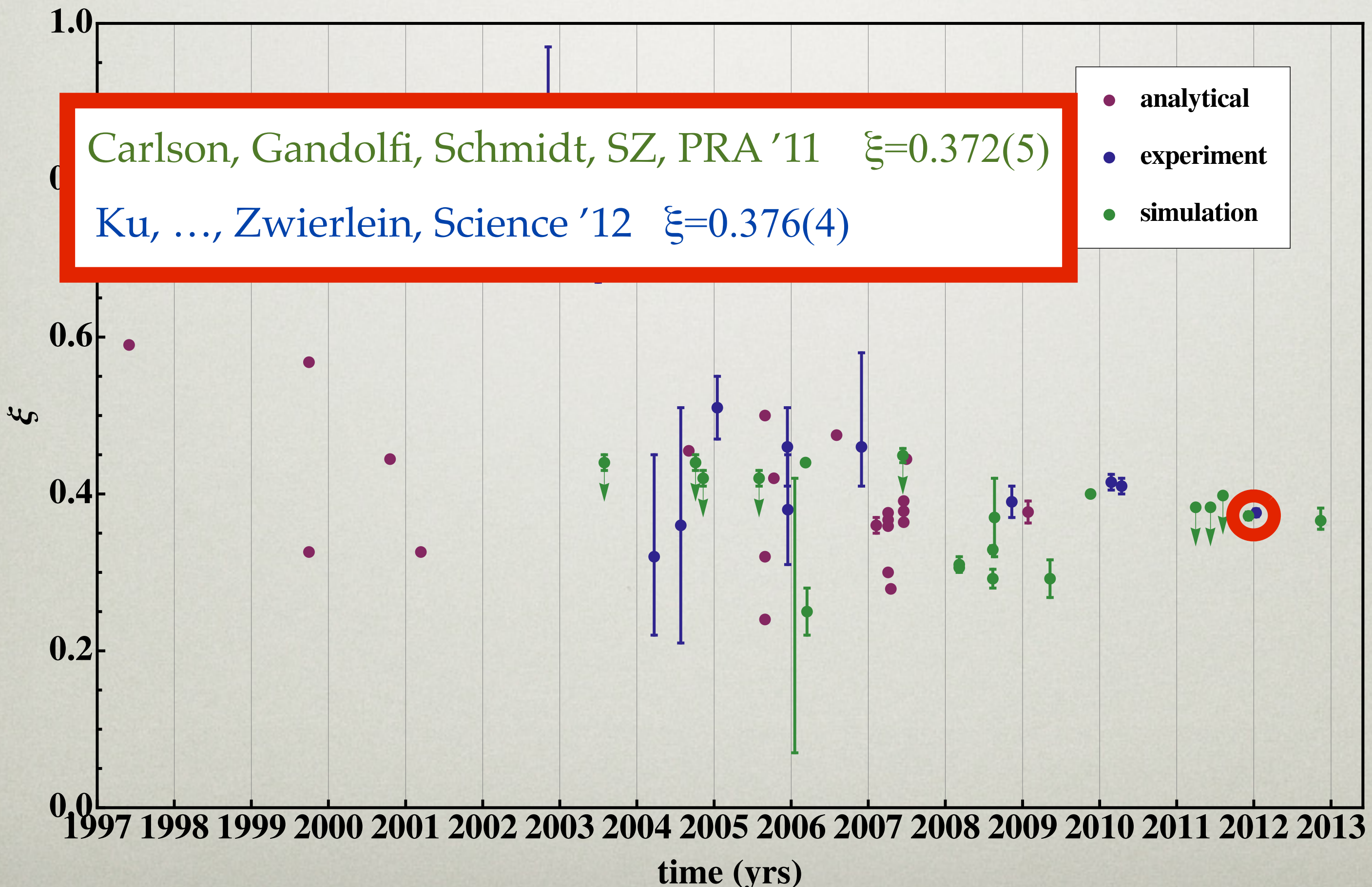
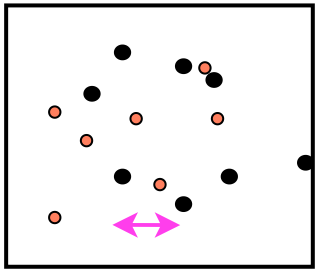


Ultracold atomic Fermi gas - 2D



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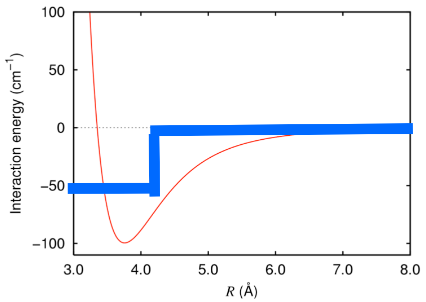

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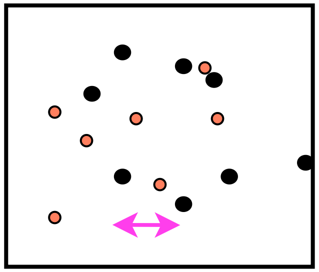

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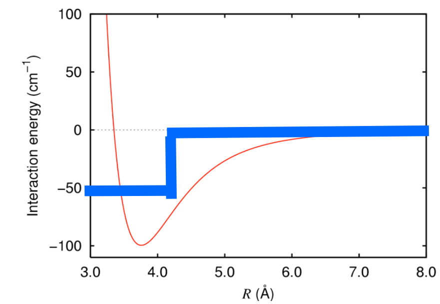


In **2D**, always bound state -- no unitarity

Pair size vs. d:

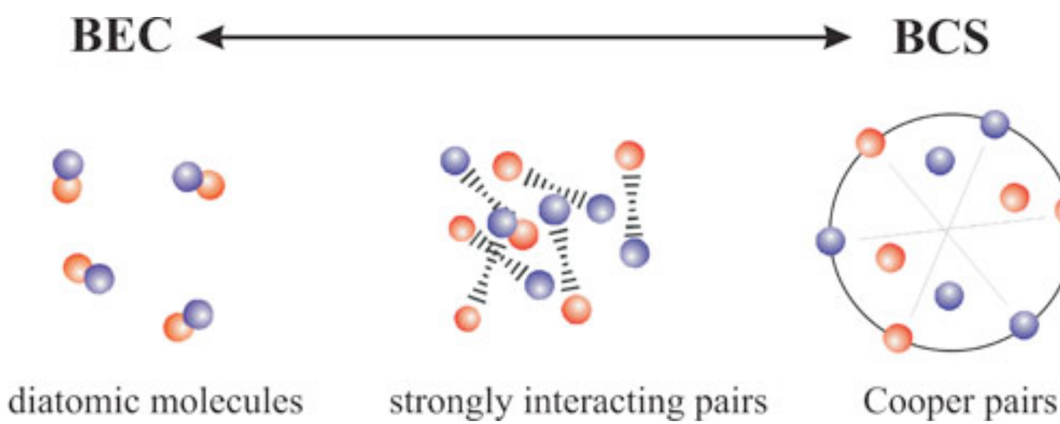
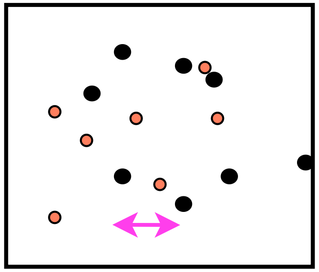


Image from D. Jin group

Ultracold atomic Fermi gas - 2D



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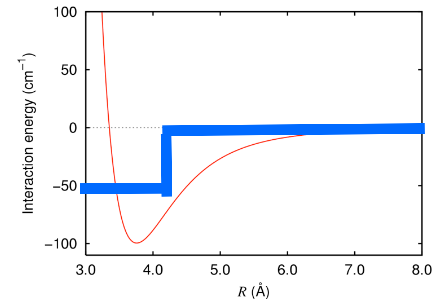

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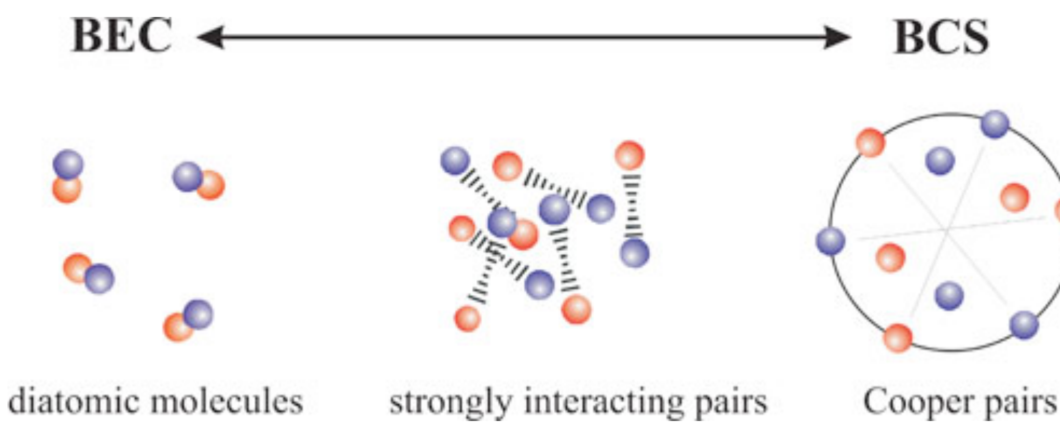
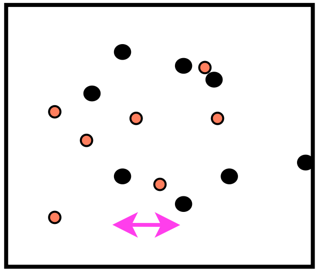


Image from D. Jin group

Expt realized (recall tremendous precision in 3D)
-- 2D important in condensed matter: cuprates, ...

Ultracold atomic Fermi gas - 2D



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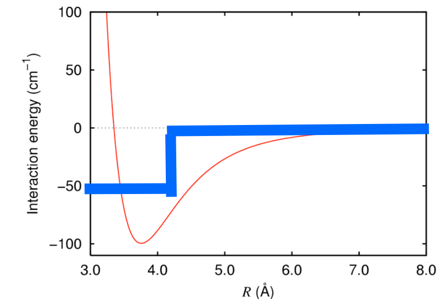

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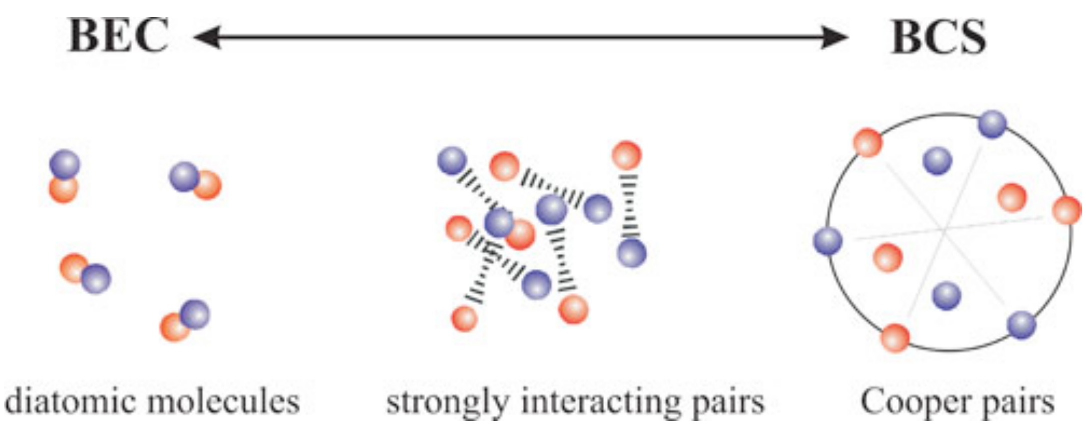


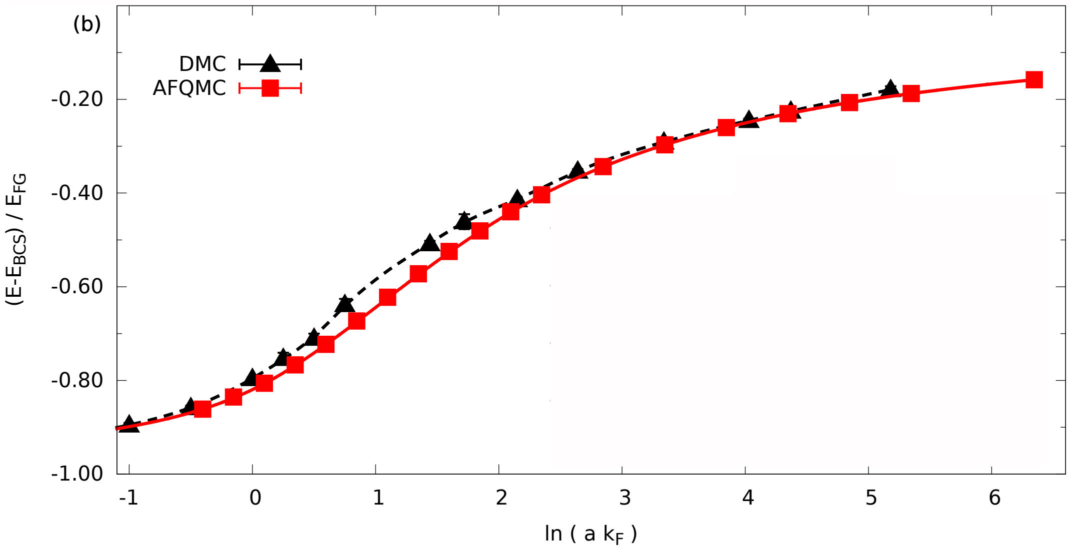
Image from D. Jin group

"Metric": $x \equiv \ln(k_F a)$, scattering length/d

Ultracold atomic Fermi gas -- 2D

Exact EOS obtained

- BCS trial wf;
  Variance control;
  sampling tricks;



DMC: prev. best (var)

Bertaina & Giorgini, PRL '11

Shi, Chiesa, SZ, PRA '15

Ultracold atomic Fermi gas -- 2D

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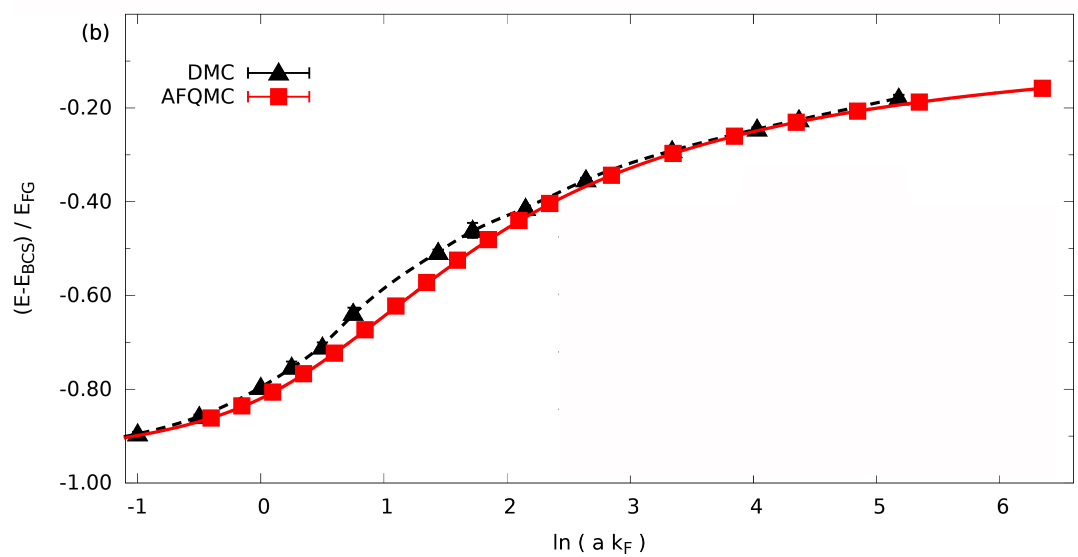
- careful extrap to TDL



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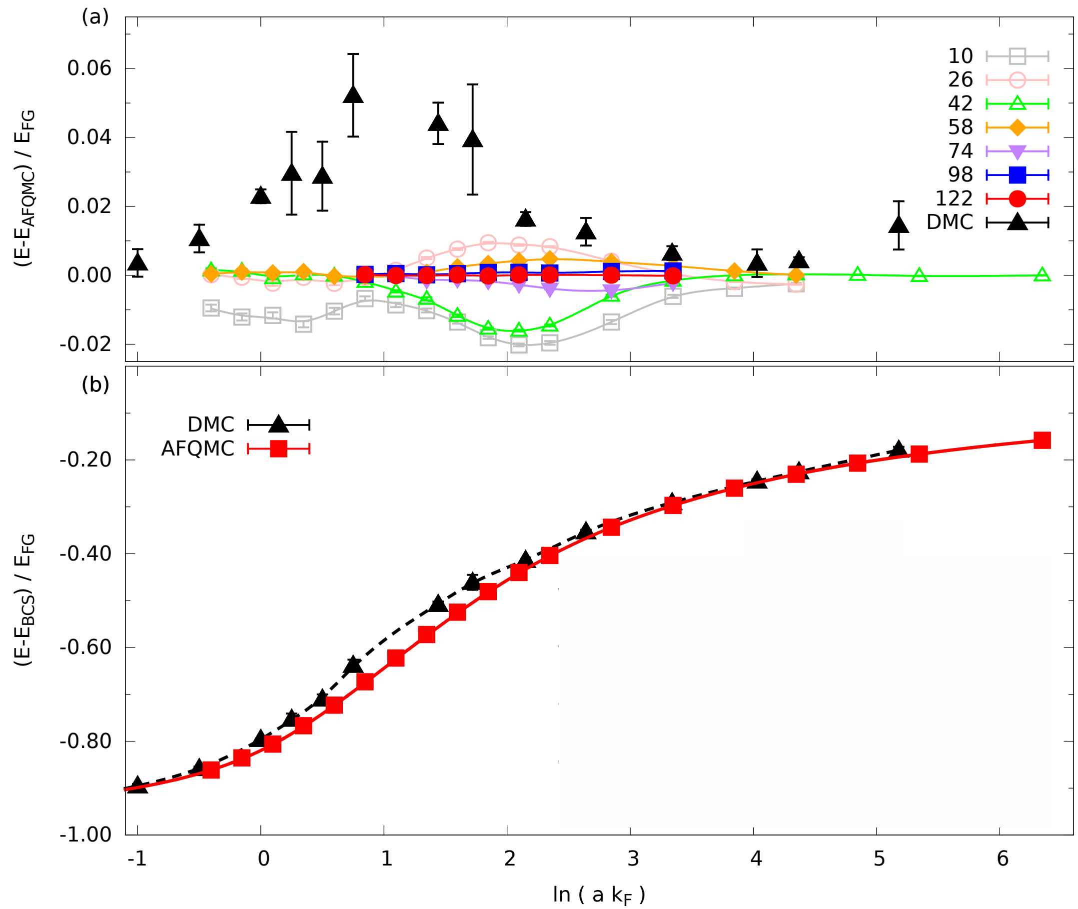

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Ultracold atomic Fermi gas -- 2D

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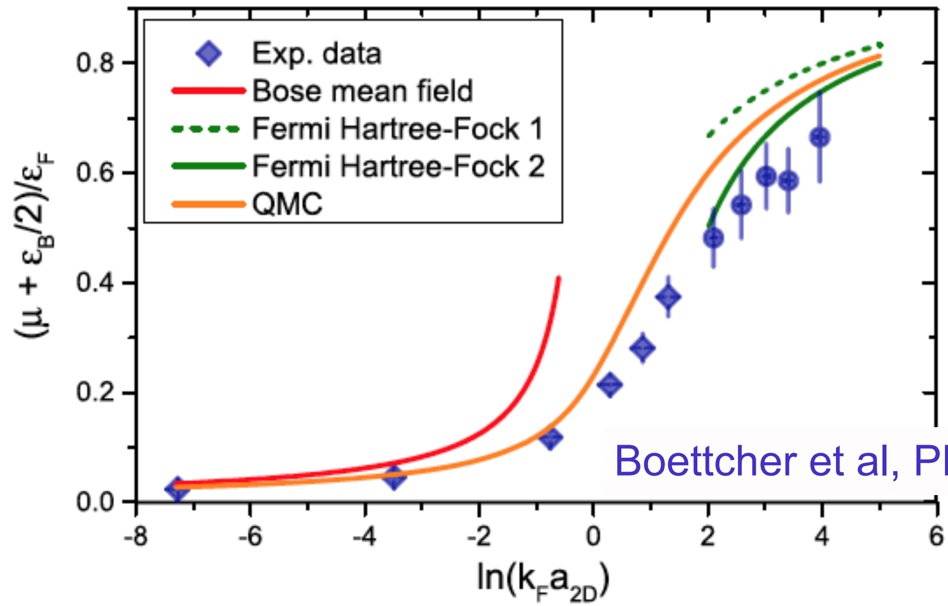
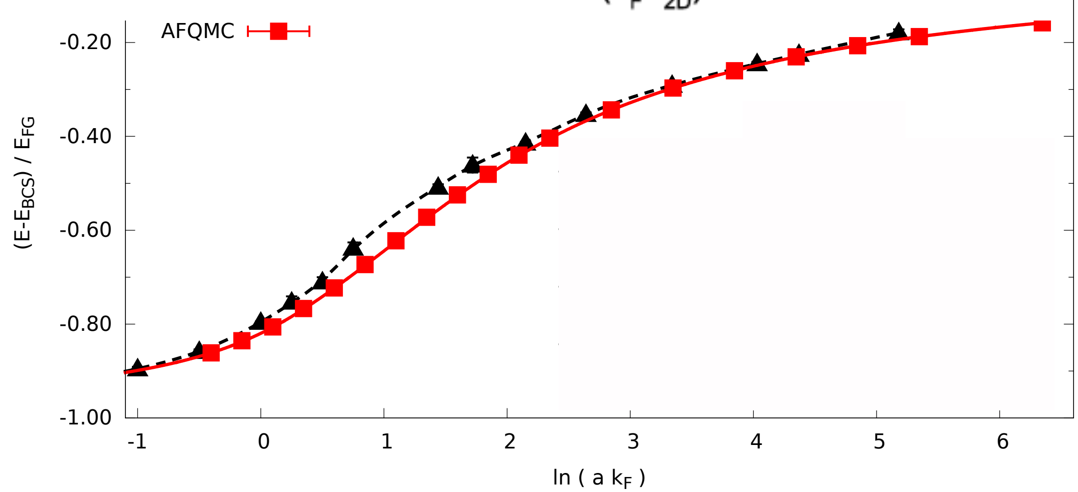
New expt and comparison



Boettcher et al, PRL '16



Shi, Chiesa, SZ, PRA '15

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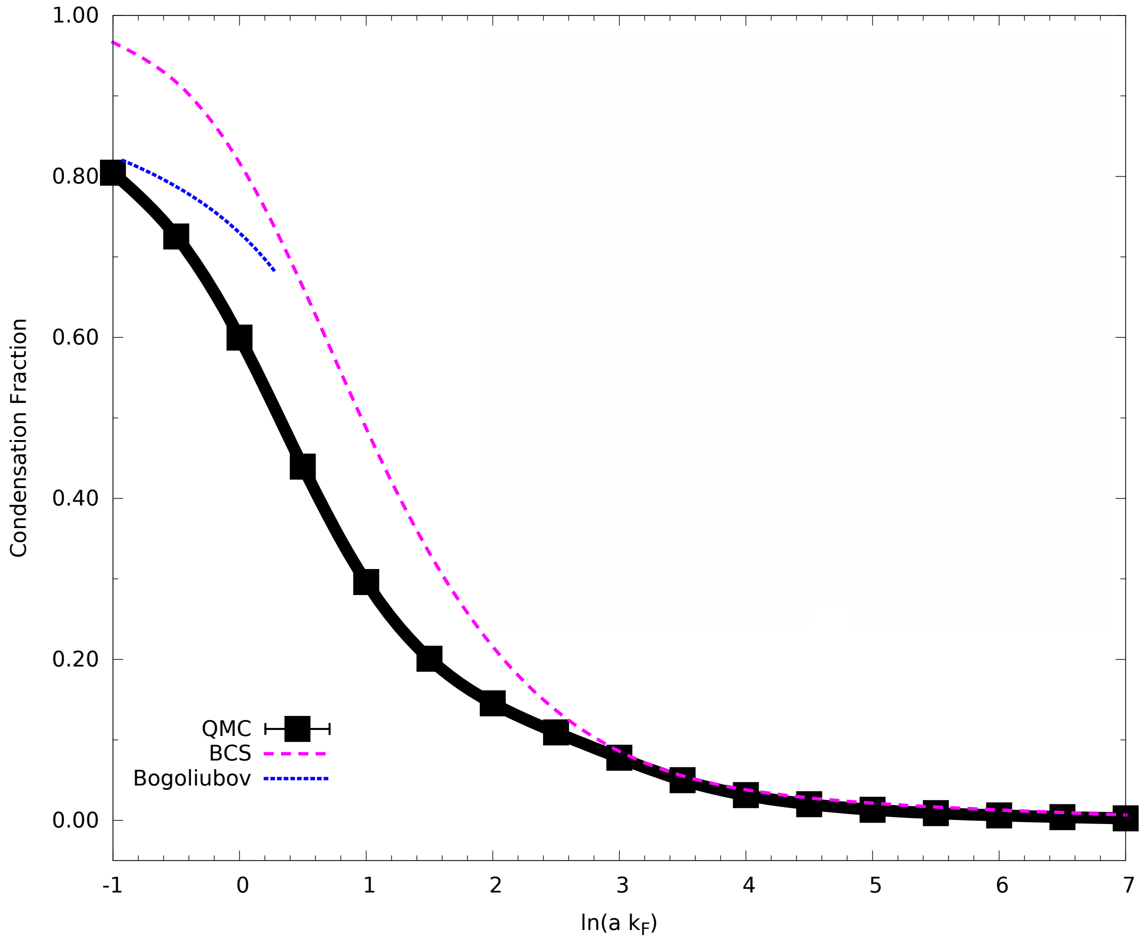
Ultracold atomic Fermi gas -- 2D

condensate fraction (diagonalize $\langle \Delta_k^\dagger \Delta_{k'} \rangle$)



Shi, Chiesa, SZ, PRA '15

Ultracold atomic Fermi gas -- 2D

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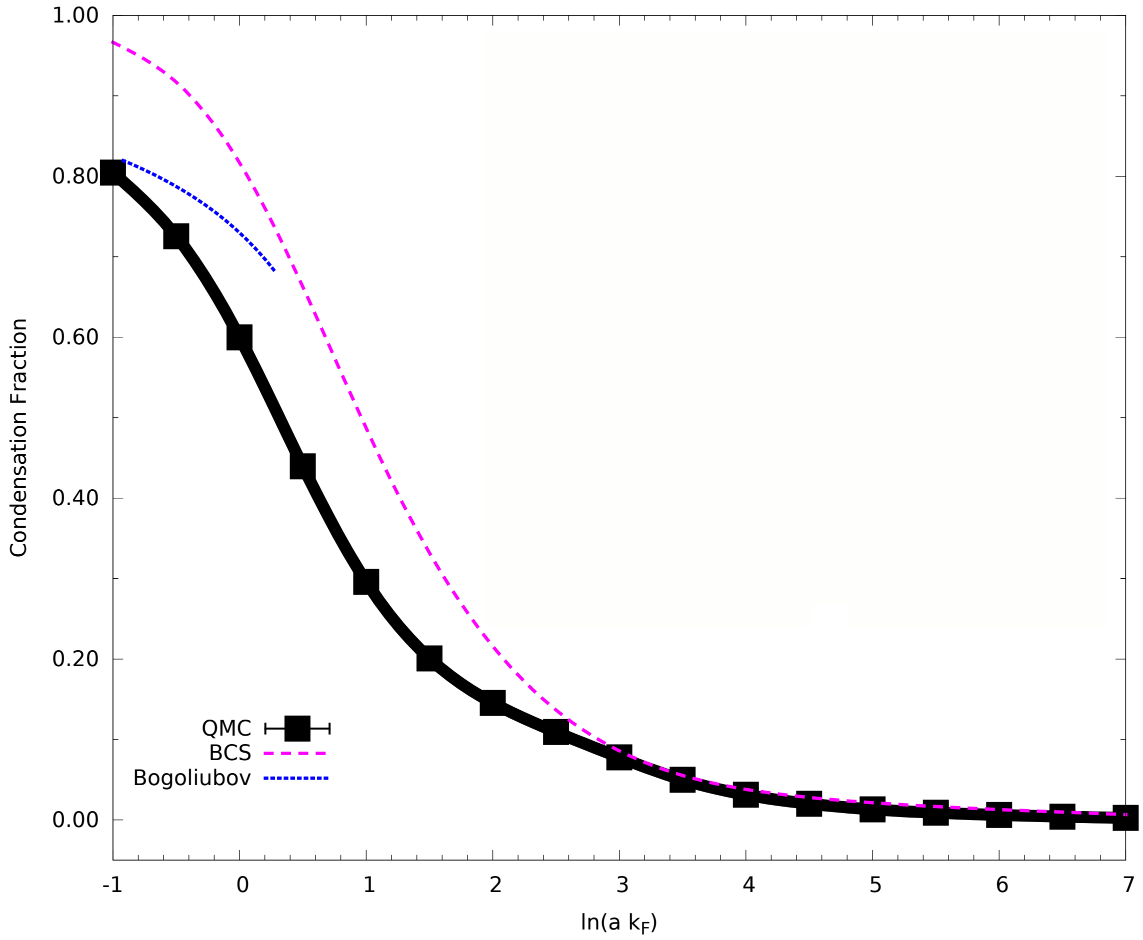
real-space 'pair wave function'



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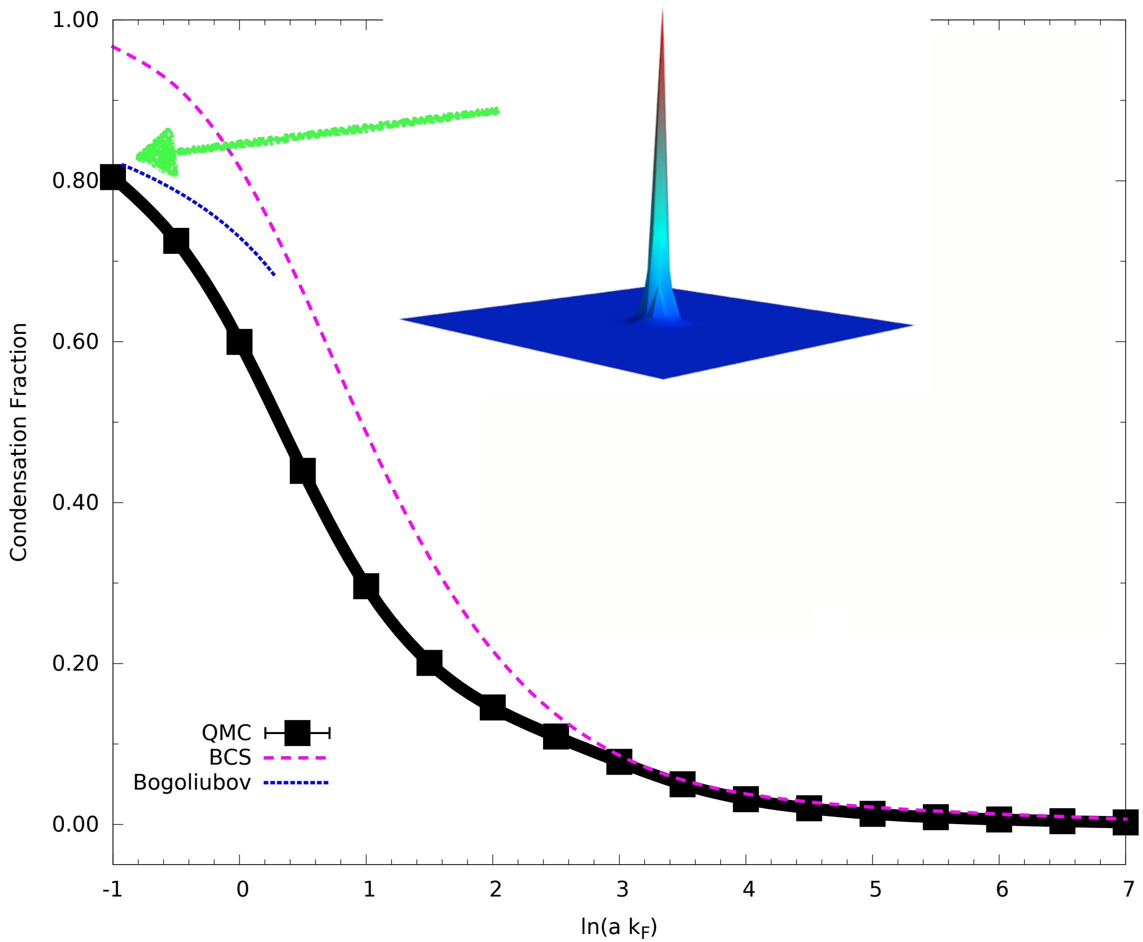

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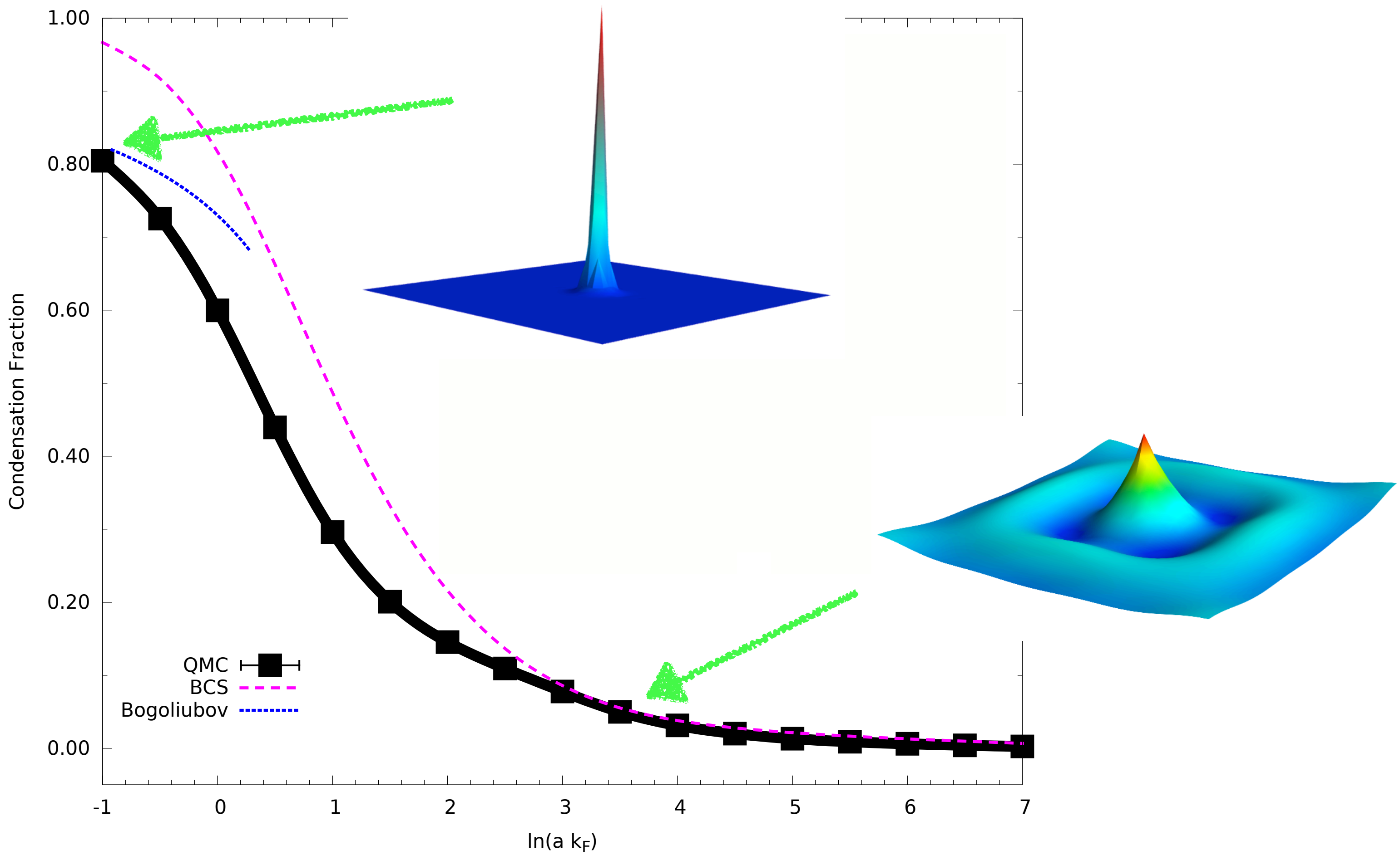

Shi, Chiesa, SZ, PRA '15

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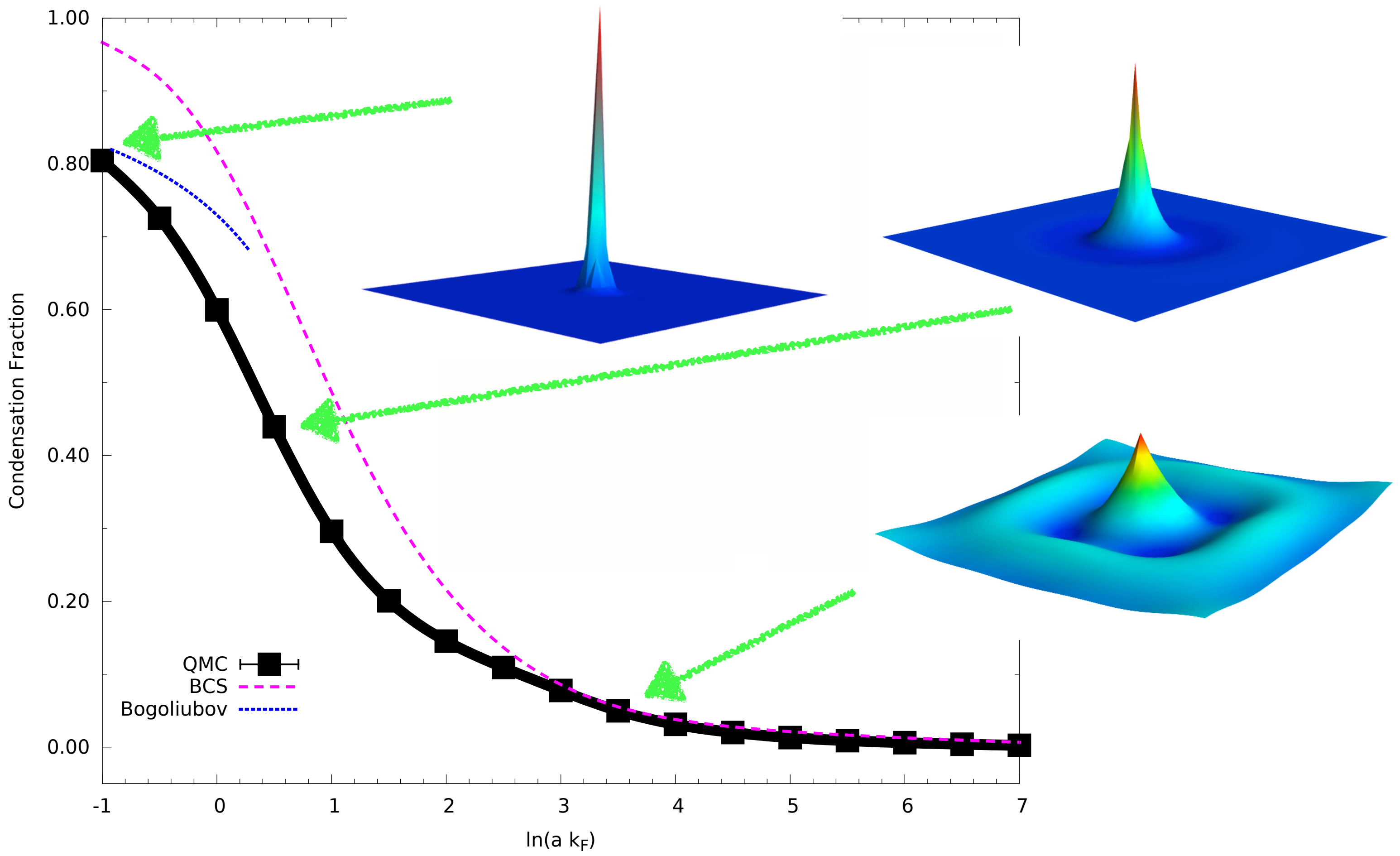

Shi, Chiesa, SZ, PRA '15

Pairing gap

$$G^p(\mathbf{k},\tau) = \langle \hat{c}_{\mathbf{k}}\, e^{-\tau(\hat{H}-\mu\hat{N})}\, \hat{c}^\dagger_{\mathbf{k}} \rangle \longrightarrow \omega^+(\mathbf{k}) = -\lim_{\tau\to+\infty} \frac{\log\left(G^p(\mathbf{k},\tau)\right)}{\tau}$$

quasi-particle dispersion

Vitali et al PRA '17

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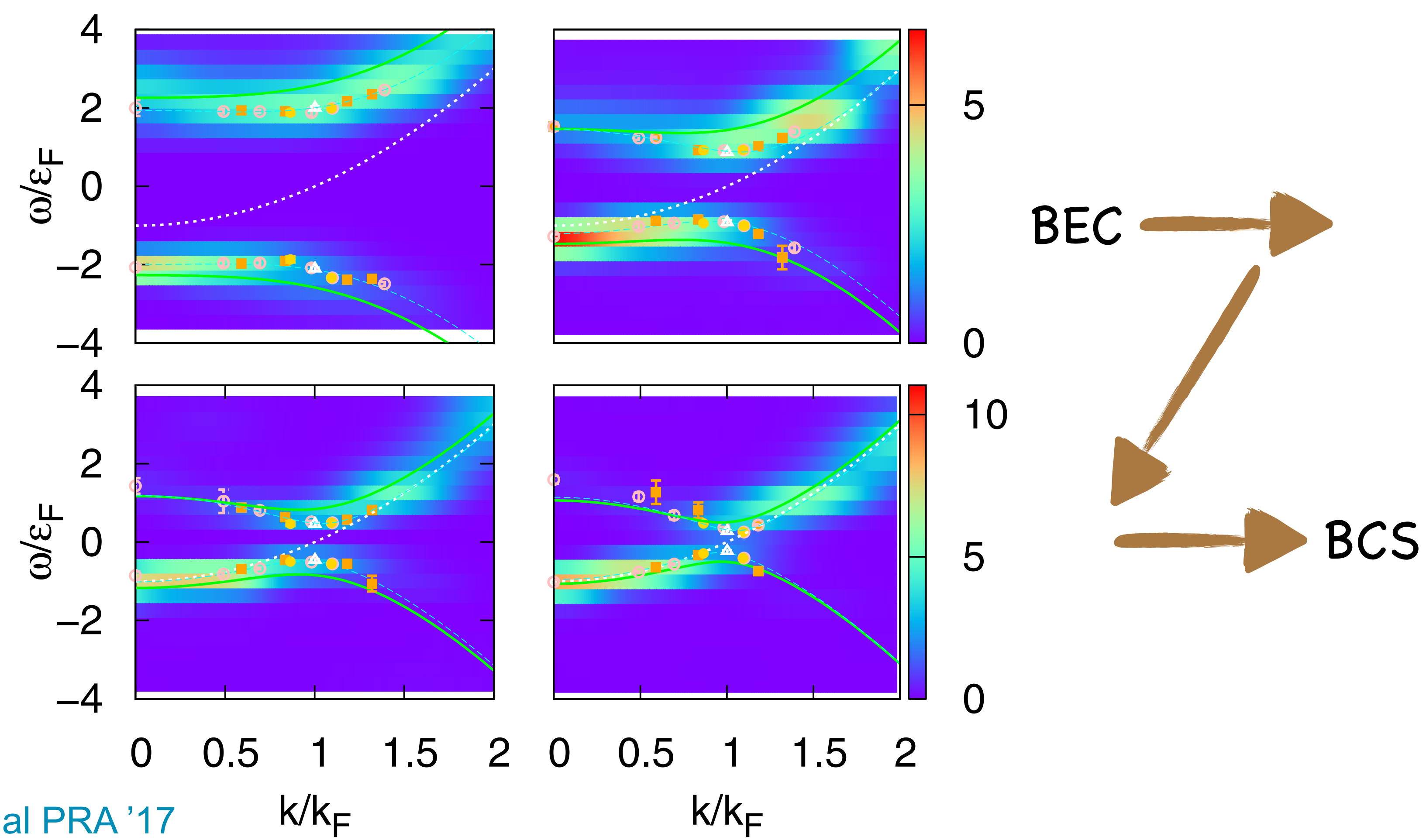

Vitali et al PRA '17

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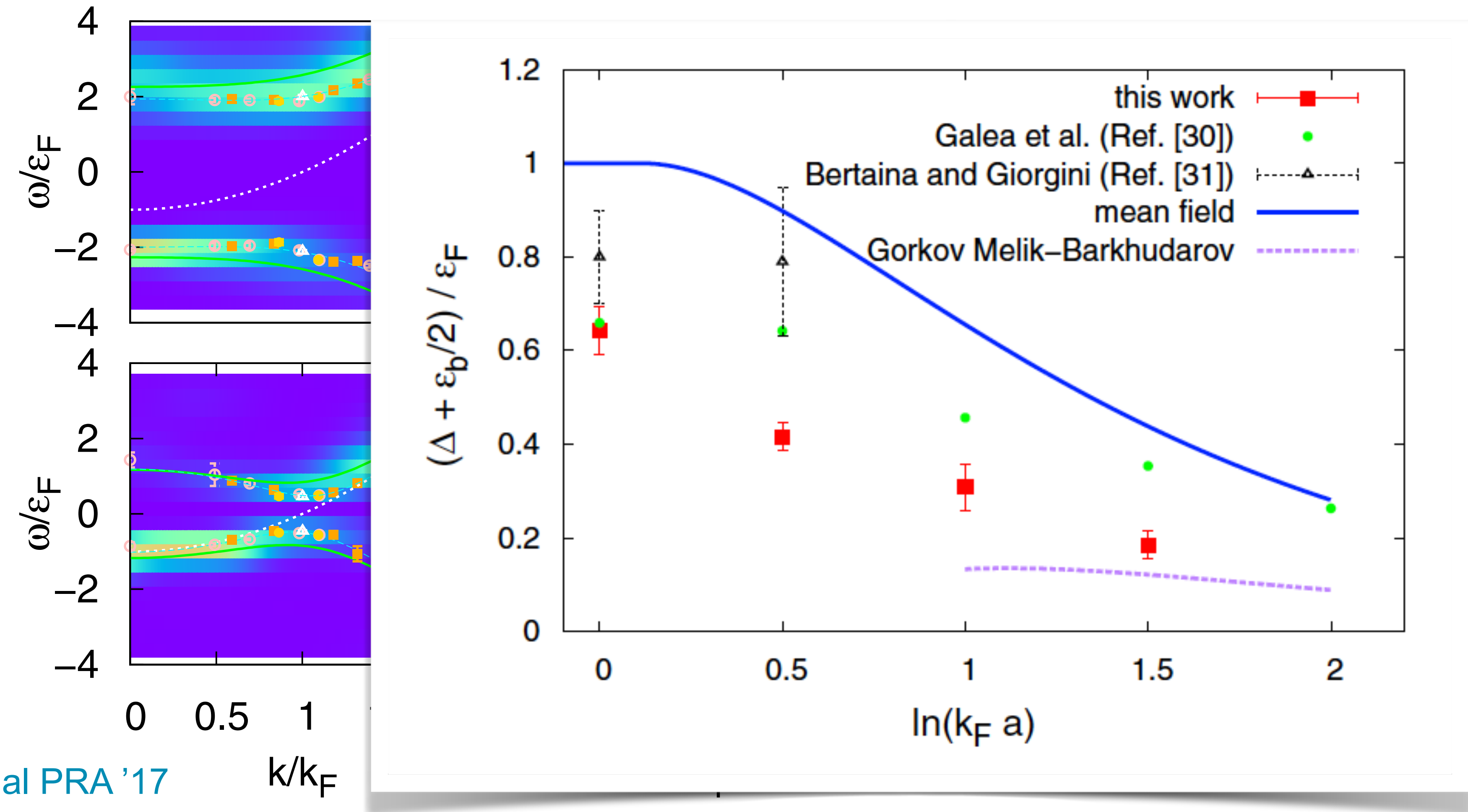

Vitali et al PRA '17

Response functions

Dynamical structure factors $S^{\hat{O}}(\vec{k},\omega) = \langle\, \hat{O}_{\vec{k}}\, \delta(\omega - \hat{H})\, \hat{O}_{-\vec{k}}\, \rangle$

scattering experiment

Vitali et al PRA '17

Response functions

Dynamical structure factors

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scattering experiment

$$\langle \Psi_0 | \hat{n}_{i,\sigma} e^{-\tau \hat{H}} \hat{n}_{j,\sigma'} | \Psi_0 \rangle$$

Vitali et al PRA ’17

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scattering experiment

Analytic cont. *

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Vitali et al PRA '17

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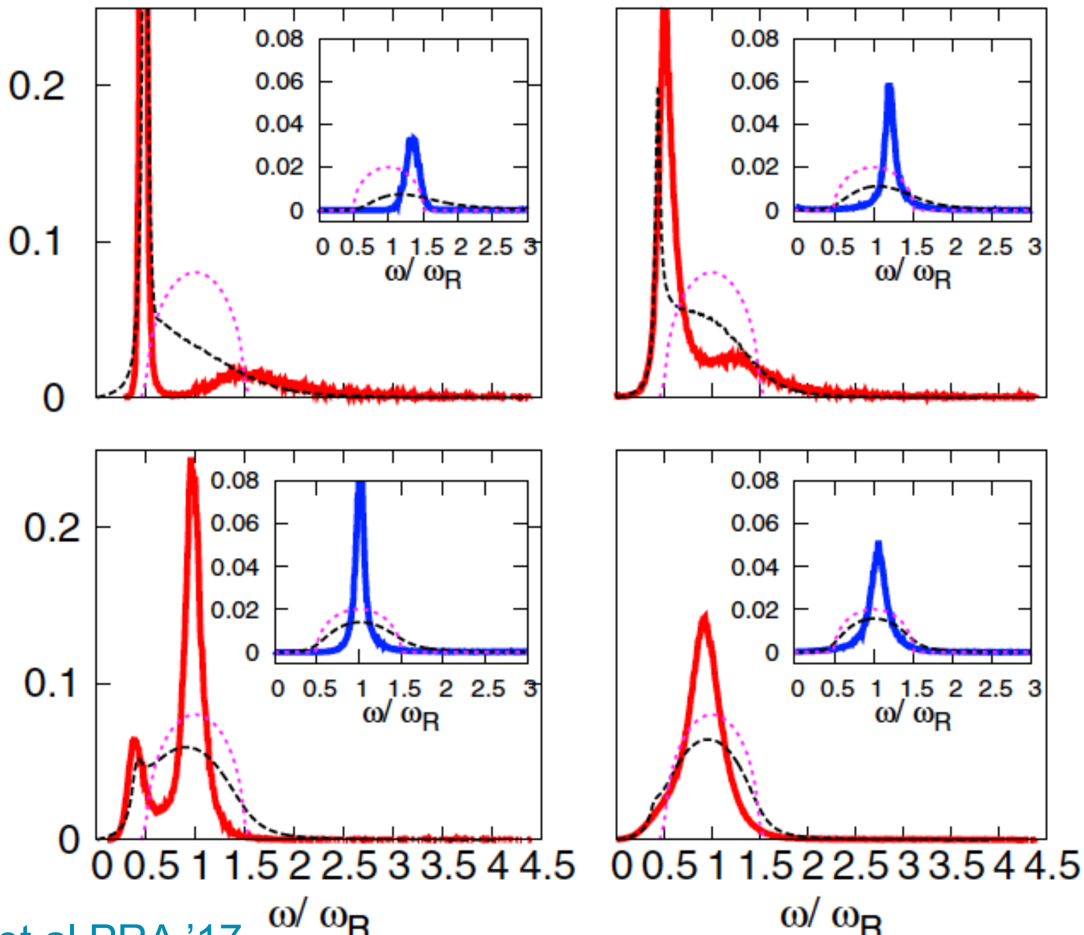

- *k*=4*k_F
- main: density
  inset: spin

Vitali et al PRA '17

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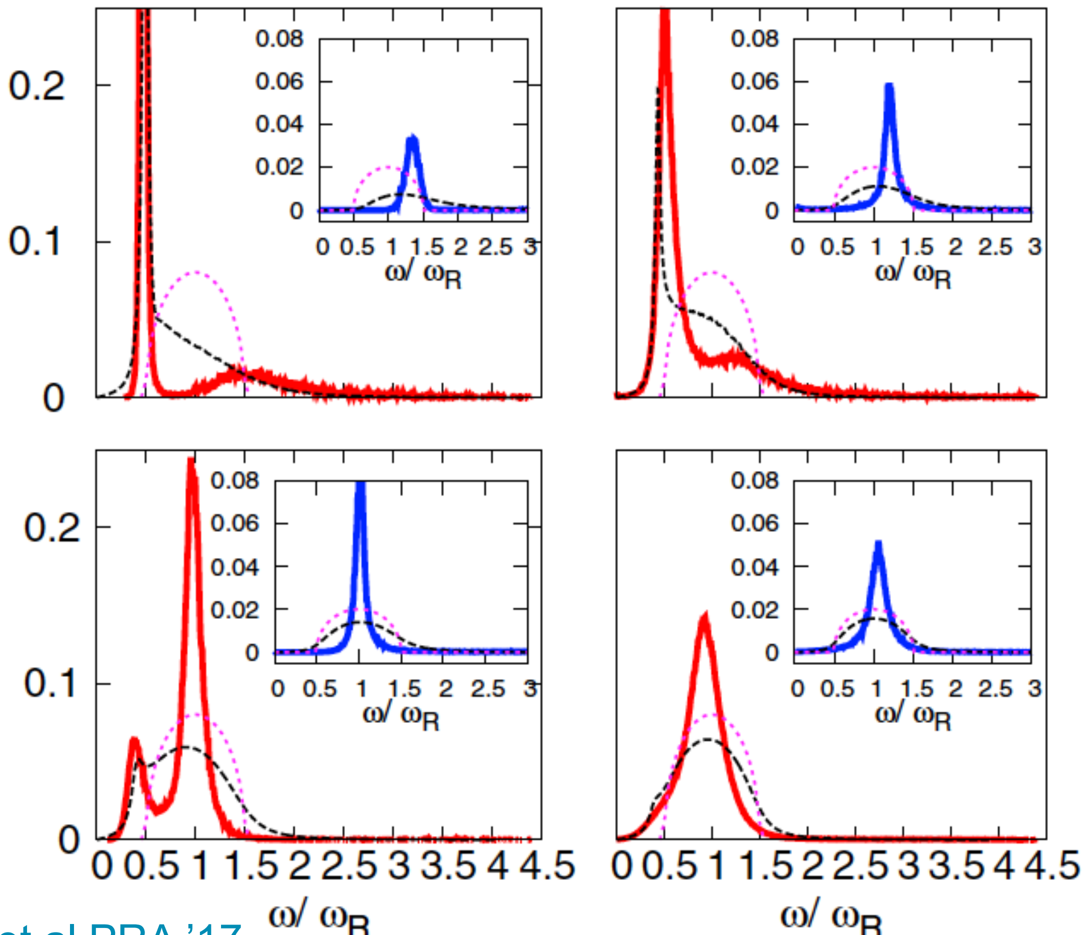

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- $\omega_R = \dfrac{\hbar^2 \vec{k}^2}{2m}$: atom recoil

Vitali et al PRA ’17

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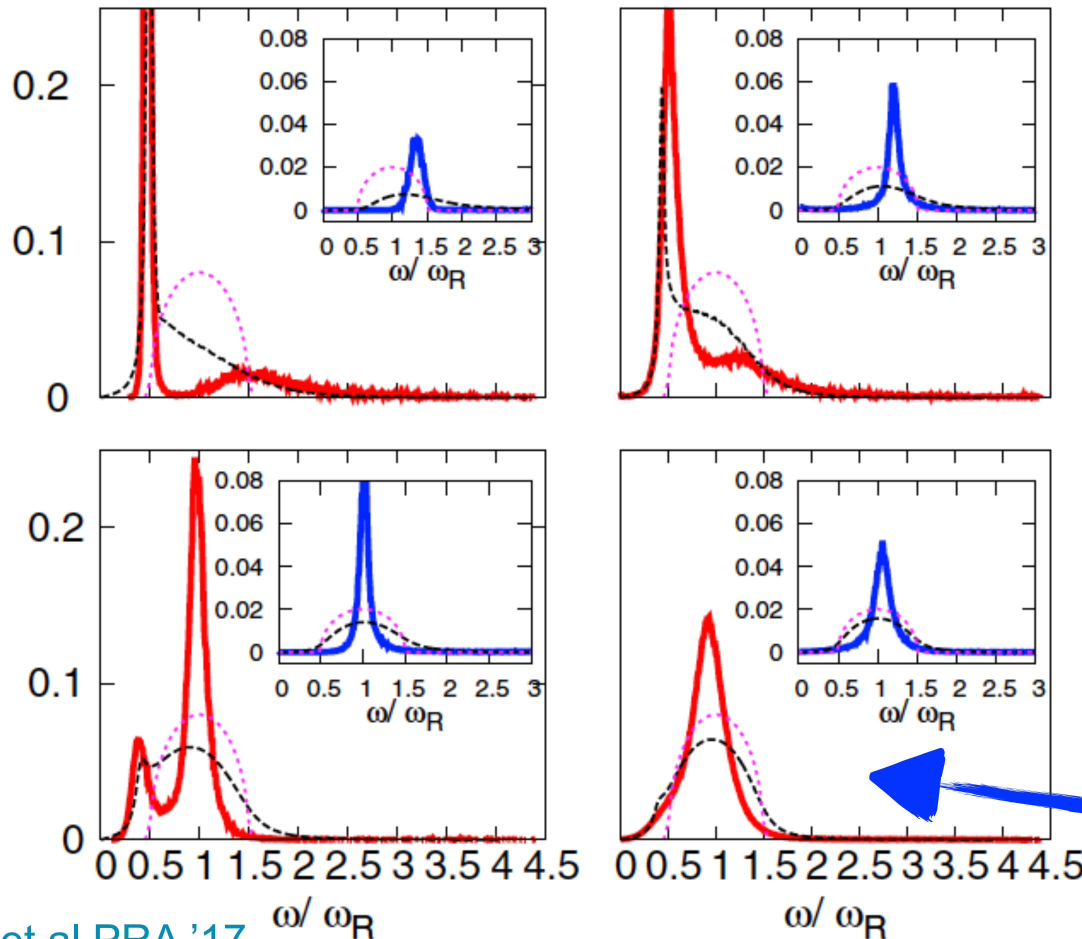

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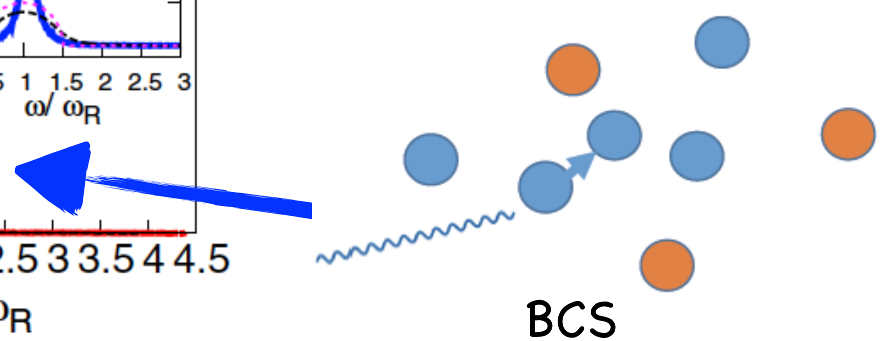

Vitali et al PRA ’17

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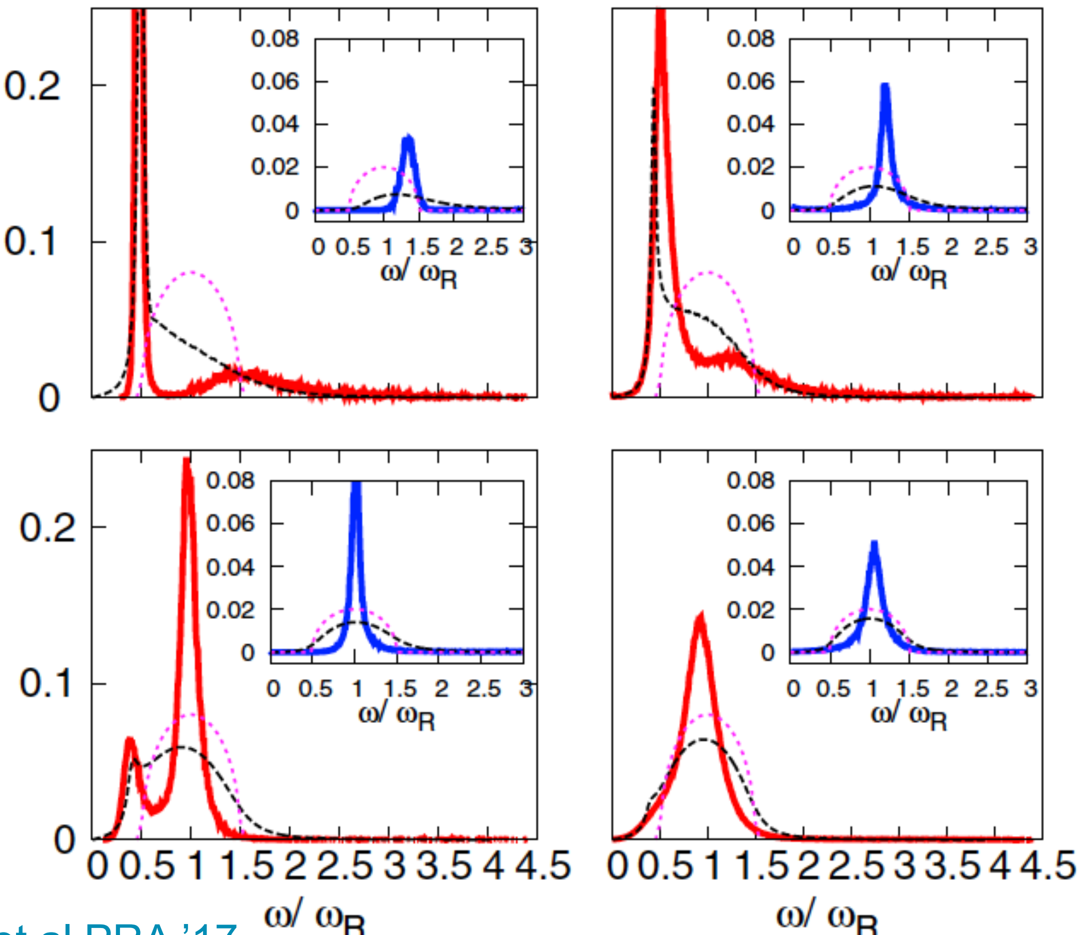

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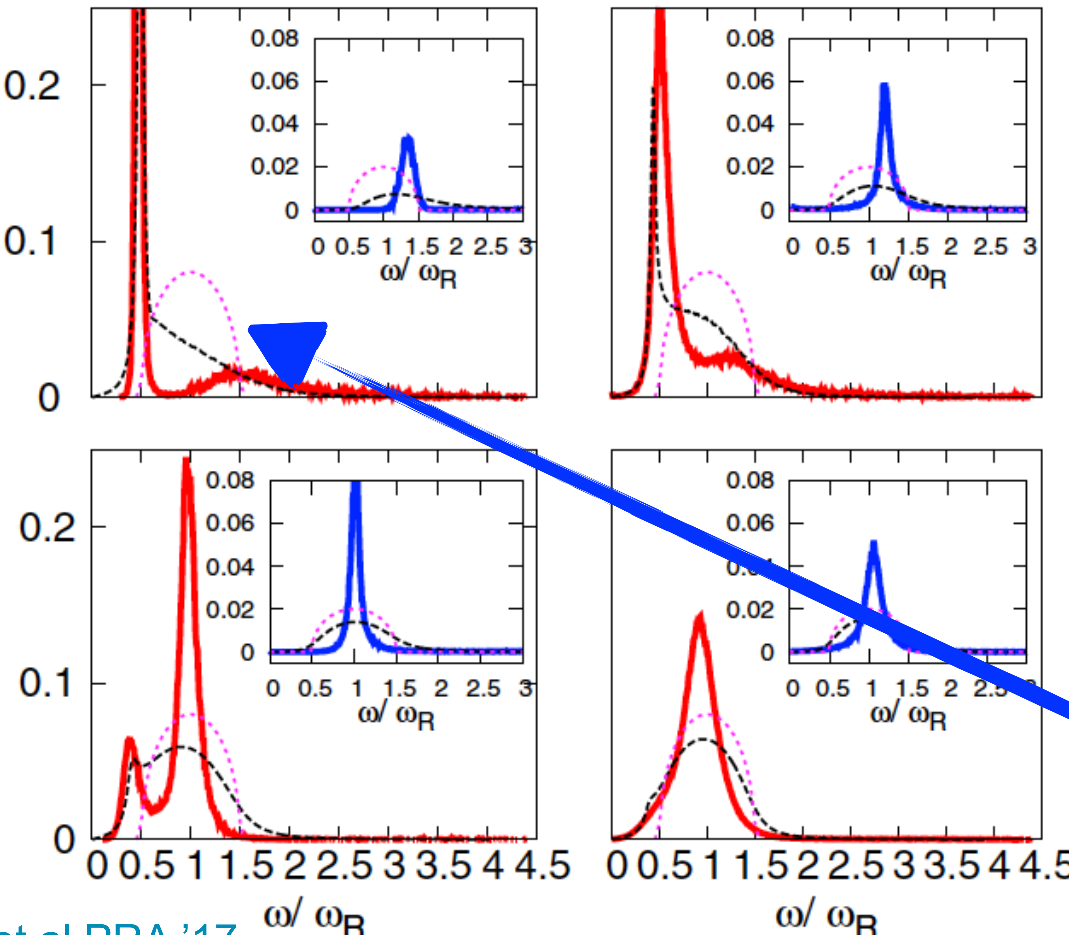
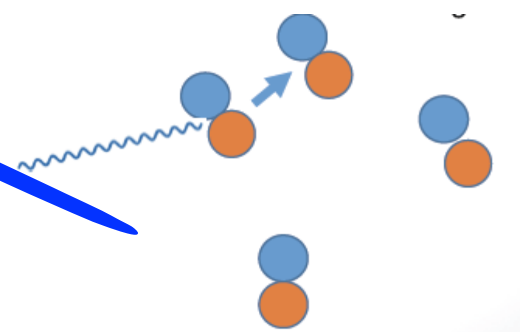
$$\langle \Psi_0 | \hat{n}_{i,\sigma} e^{-\tau \hat{H}} \hat{n}_{j,\sigma'} | \Psi_0 \rangle$$

scattering experiment



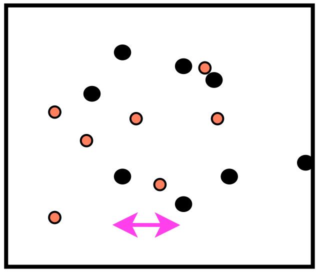
Vitali et al PRA ’17

- k=4*k_F
- main: density
  inset: spin
- $\omega_R = \frac{\hbar^2 \vec{k}^2}{2m}$: atom recoil



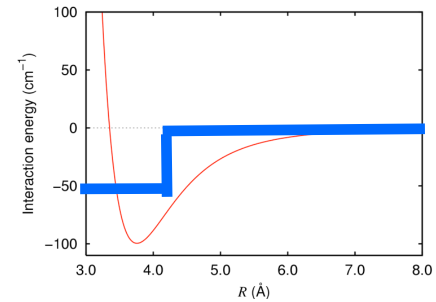
BEC

Spin-orbit coupling



$$H = -\frac{\hbar^2}{2m}\left(\sum_i^{N/2} \nabla_i^2 + \sum_j^{N/2} \nabla_j^2\right) + \sum_{i,j} V(r_{ij})$$

inter-particle spacing d >> range of V



In 2D, always bound state. Size vs. d:

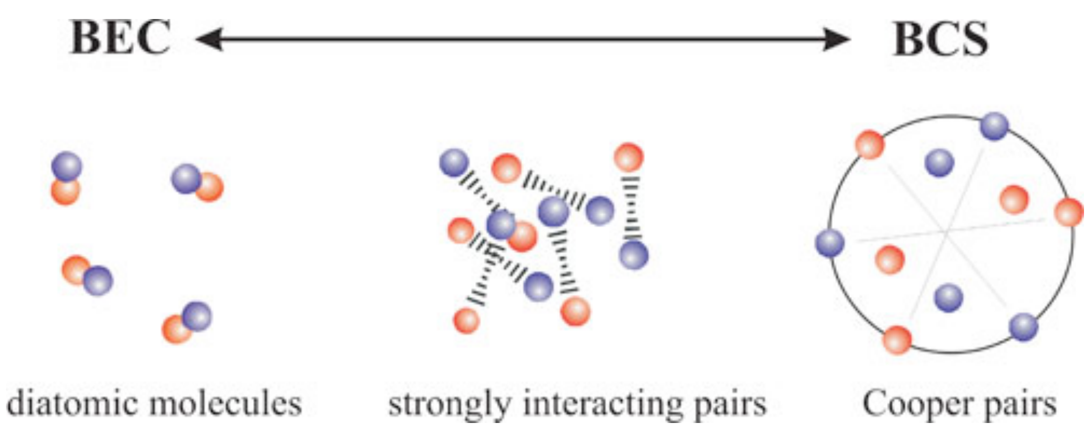
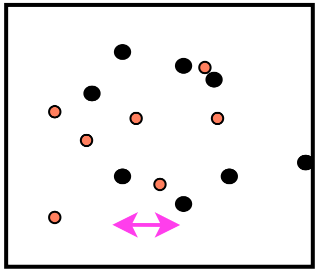


Image from D. Jin group

Spin-orbit coupling



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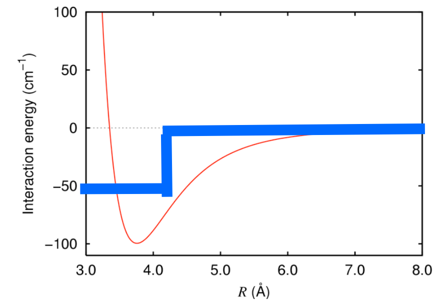

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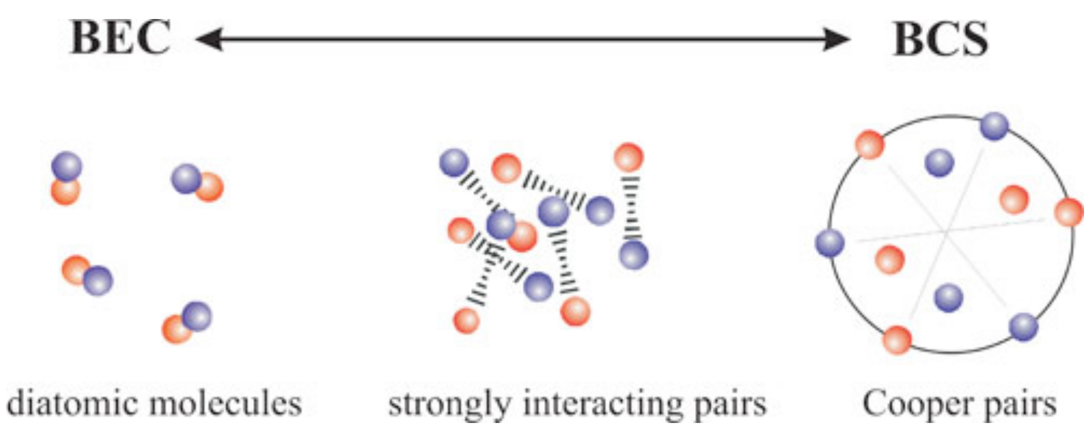
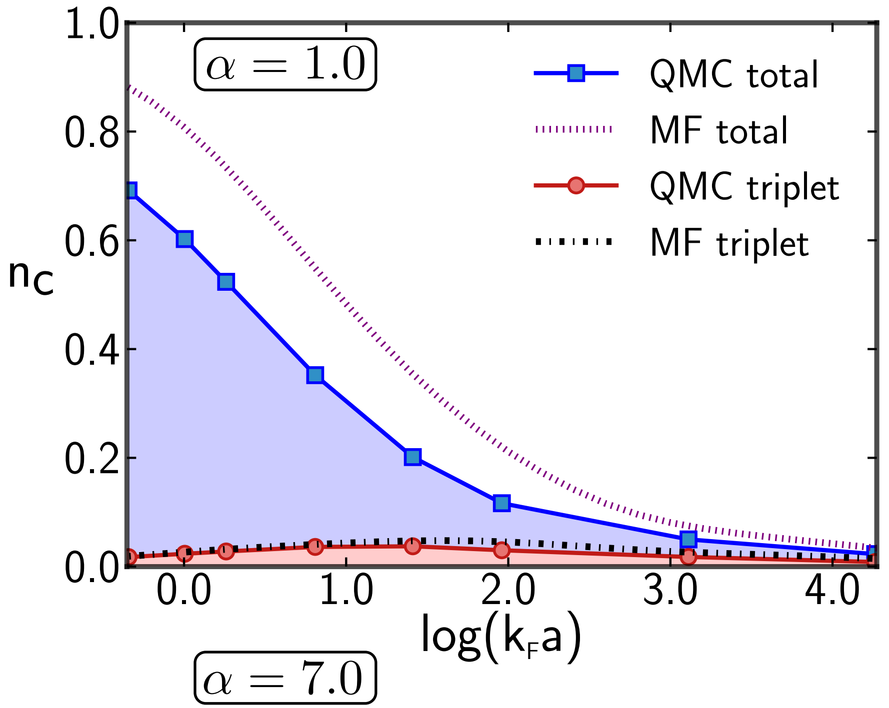


Image from D. Jin group

Expt: synthetic spin-orbit coupling realized, e.g. Rashba

$$H = \sum_{\mathbf{k}\sigma} k^2 c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow} + \sum_{\mathbf{k}} \lambda(k_y - i k_x) c^\dagger_{\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} + h.c.$$

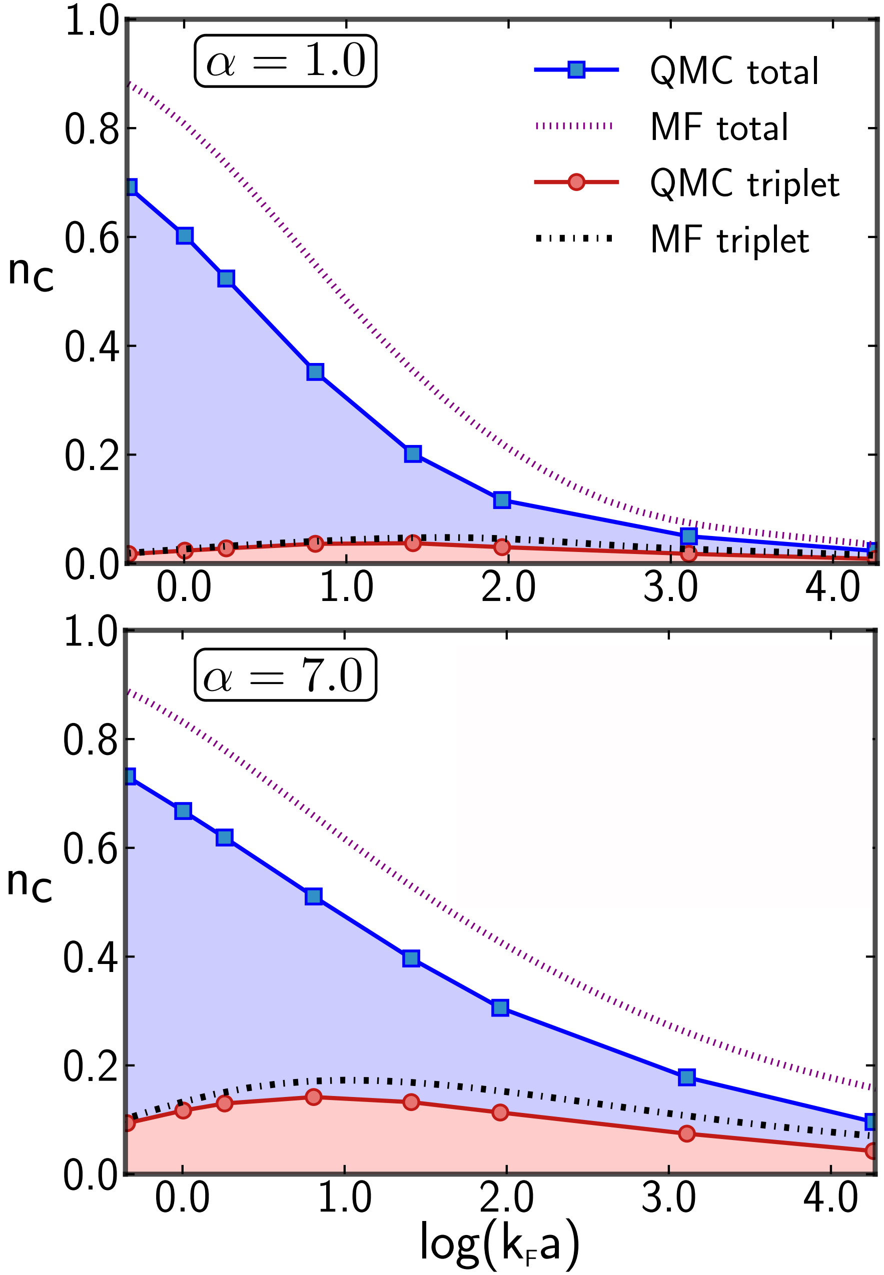
Singlet and triplet pairing --- cond frac



- Triplet pairing is maximized in the crossover regime
- MF theory tends to over-estimate, especially singlet component

Shi, Rosenberg, Chiesa, SZ, PRL ’16

Singlet and triplet pairing --- cond frac



- Triplet pairing is maximized in the crossover regime
- MF theory tends to over-estimate, especially singlet component
- Triplet pairing increases with SOC strength
- Total condensate fraction increases with SOC

Shi, Rosenberg, Chiesa, SZ, PRL ’16

Recent progress on the Fermi gas from auxiliary-field QMC

Shiwei Zhang

- Auxiliary-field QMC (AFQMC)
  - Connection with lattice methods
  - Technical advances in FG (e.g. low-rank decomp - scaling N^3 -> N)
  - Conceptual difference for general fermions: controlling the sign problem (repulsive models, real materials)
- Precision computation in the 2D Fermi gas
  - Ground state: EOS, gaps, n(k), …
  - Finite-*T*: BKT Tc , contact, response

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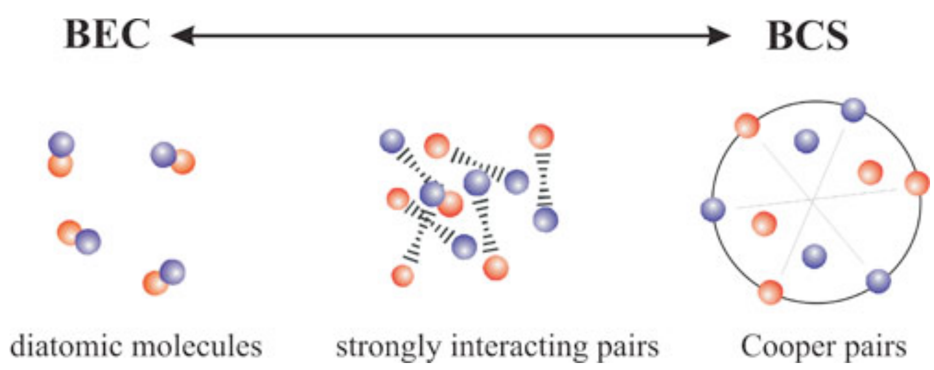
Transition *T*c in 2D Fermi gas



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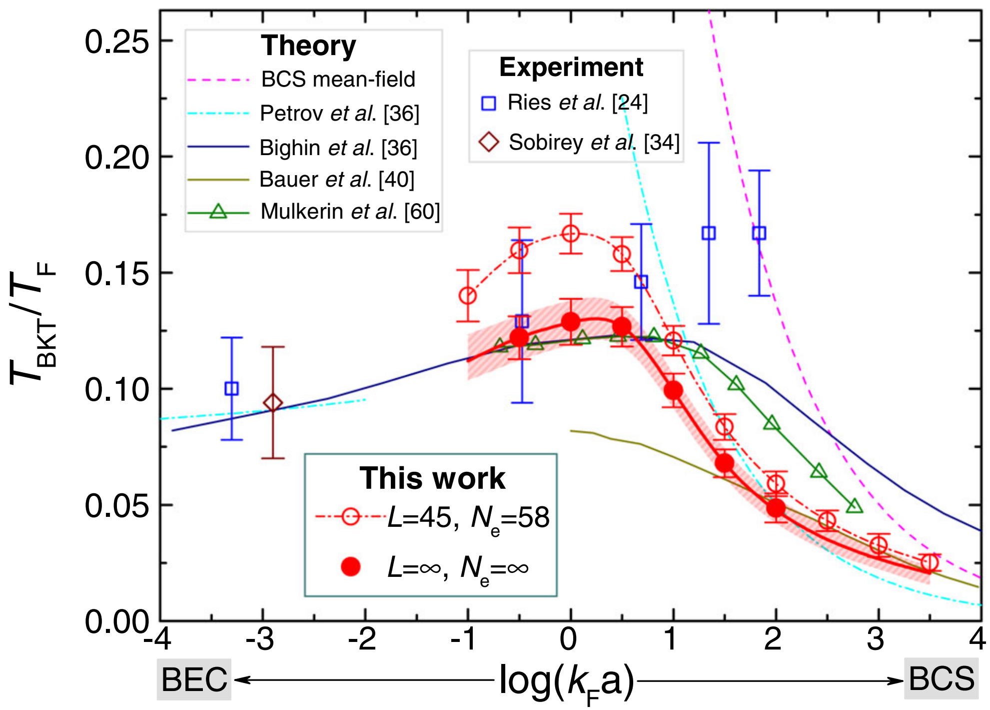

He, Shi, SZ, PRL 129, 076203 (2022)

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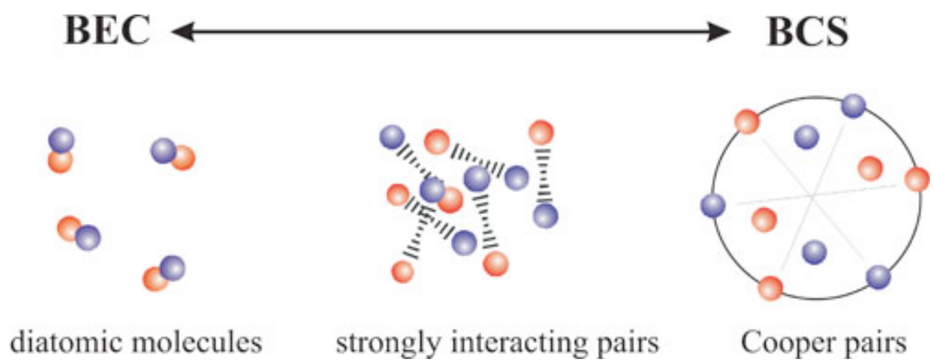

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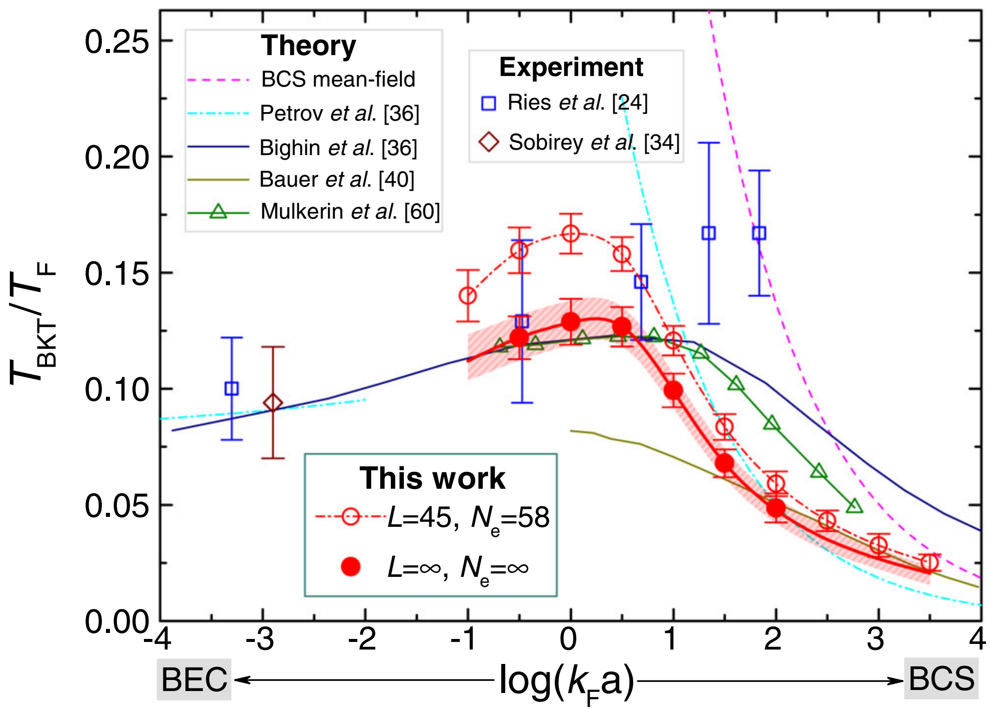

- Tour de force <= new alg.

He, Shi, SZ, PRL 129, 076203 (2022)

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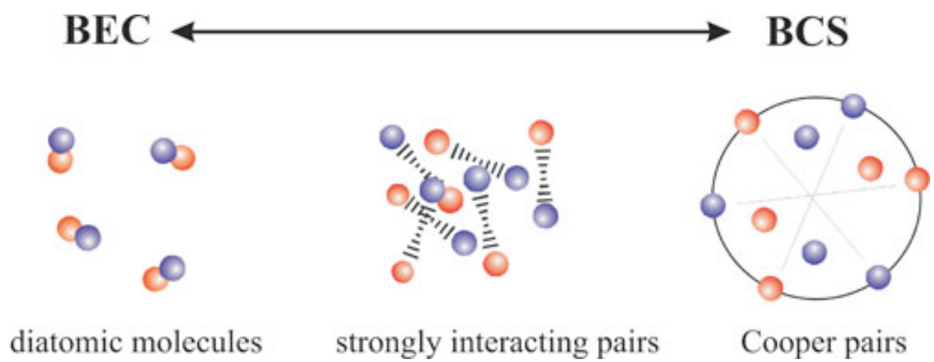

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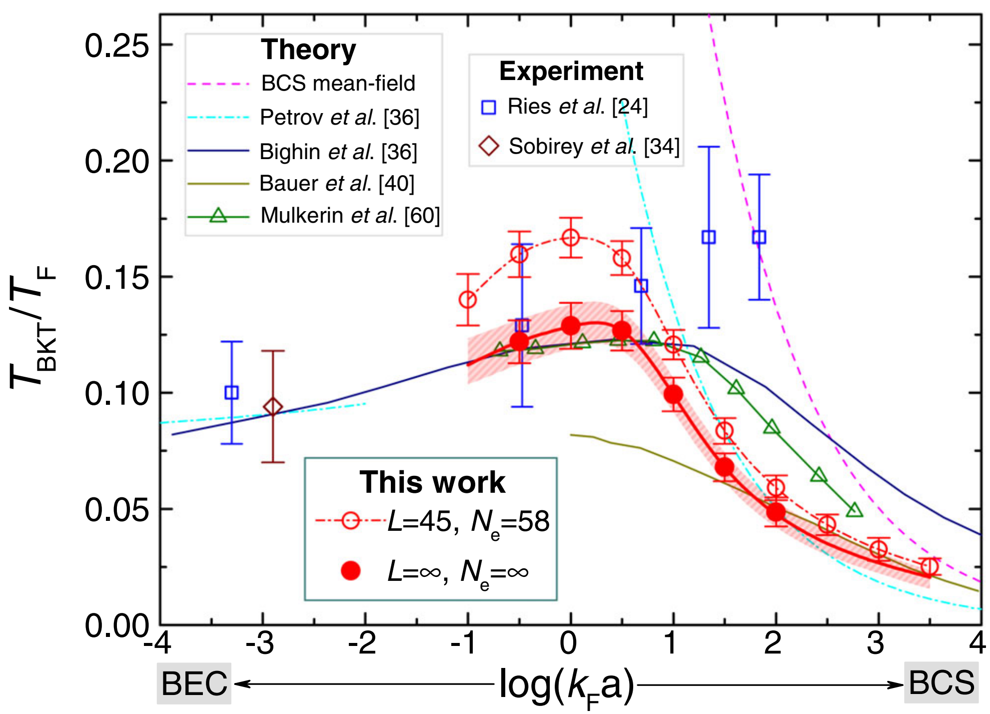

- Tour de force <= new alg.
  - low-rank decomposition (*PRL ’19*)
  - 300 -> 5000 lattice sites; $T/T_F \sim 0.2 \rightarrow 0.02$

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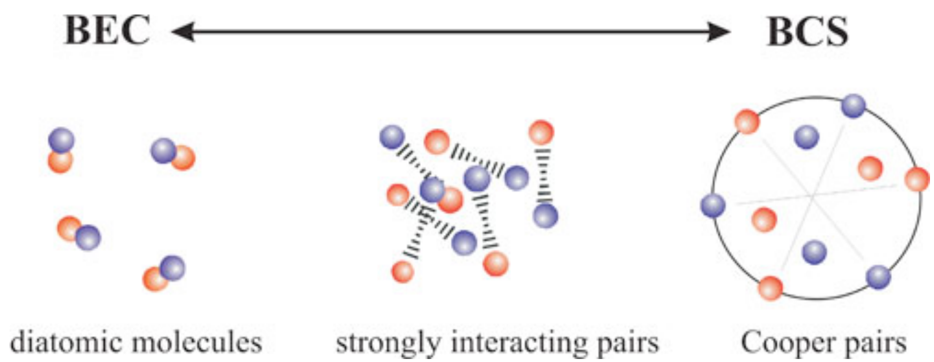

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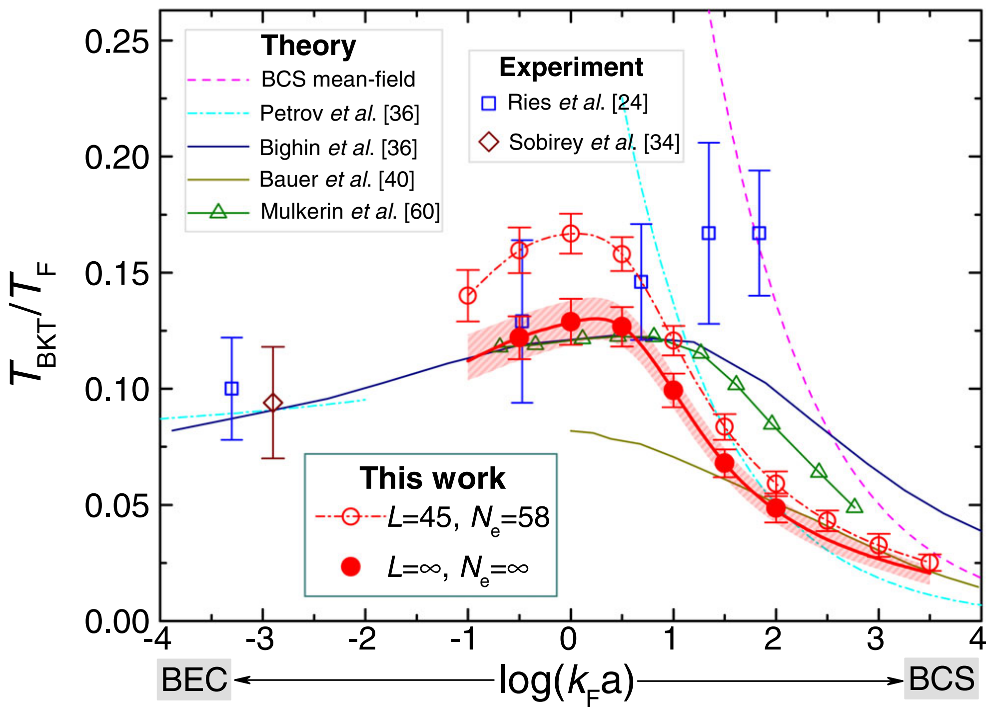

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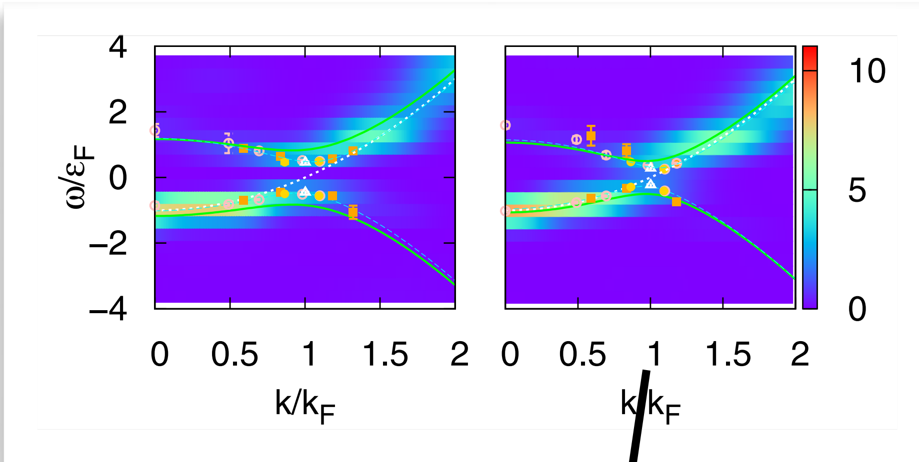
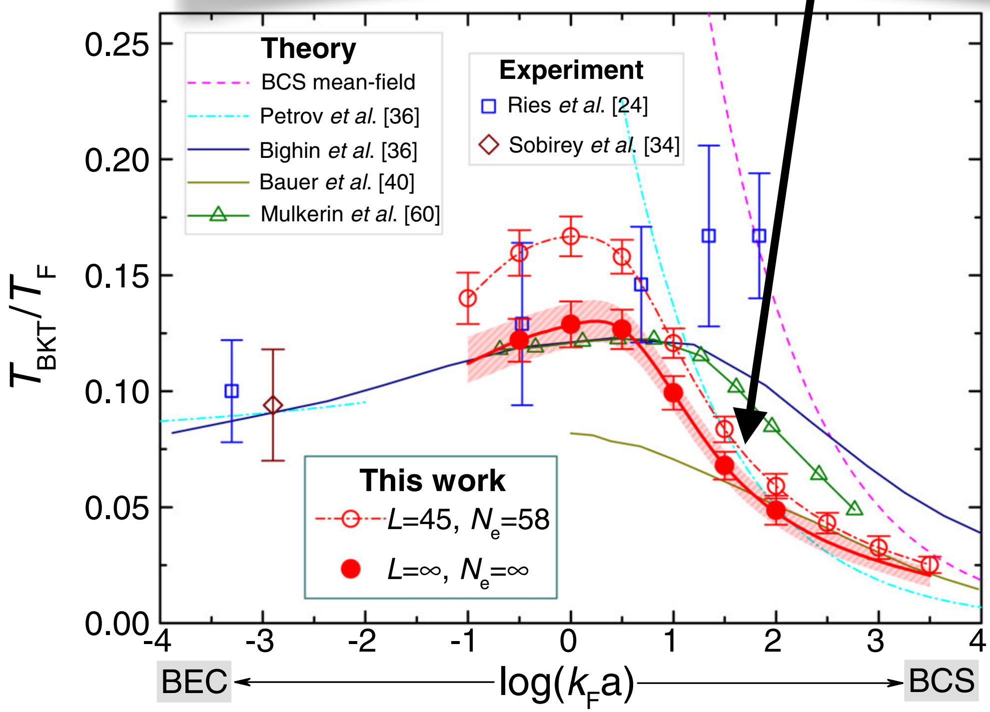
Transition *Tc* in 2D Fermi gas





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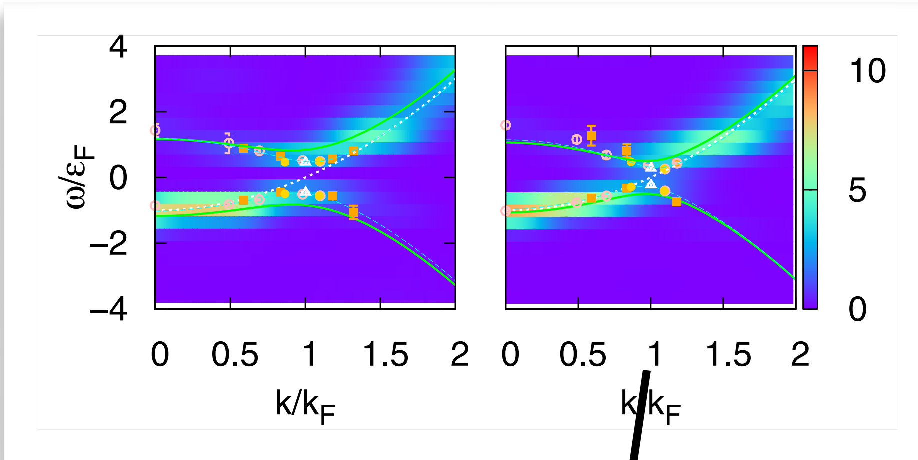
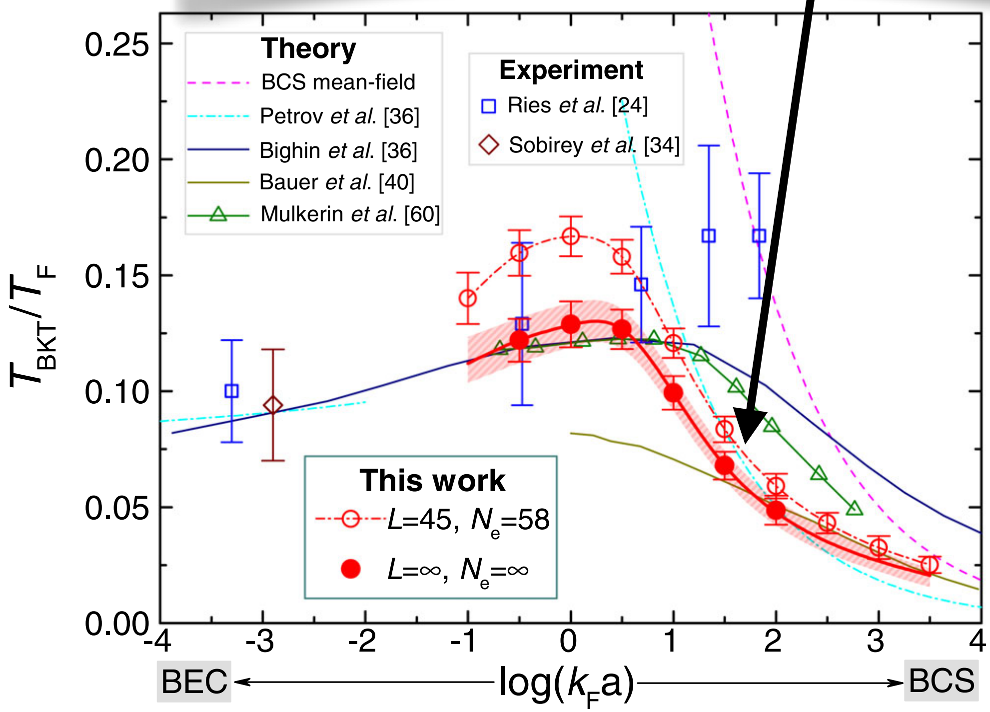
  - low-rank decomposition (*PRL '19*)
  - 300 -> 5000 lattice sites; T/T_F ~ 0.2 -> 0.02
- Problems w/ expt. in crossover and BCS ?
- Gap (*Vitali et al PRA '17*)

He, Shi, SZ, PRL 129, 076203 (2022)

Transition *Tc* in 2D Fermi gas





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$$\Delta/T_{\rm BKT} \sim 2.7$$ not so BCS!

He, Shi, SZ, PRL 129, 076203 (2022)

Fermion and pair momentum distributions

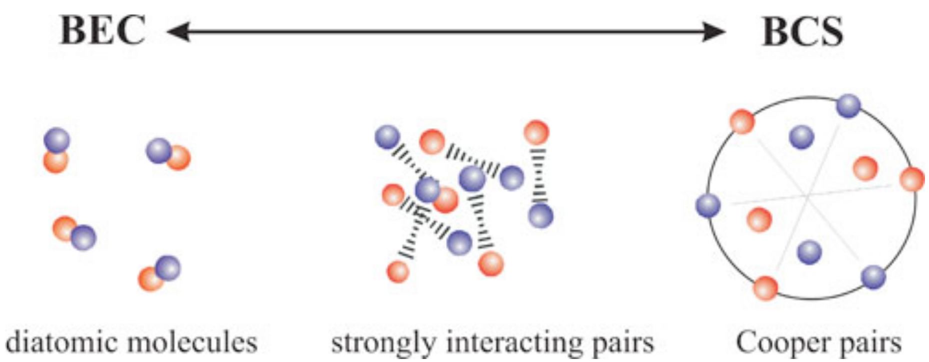
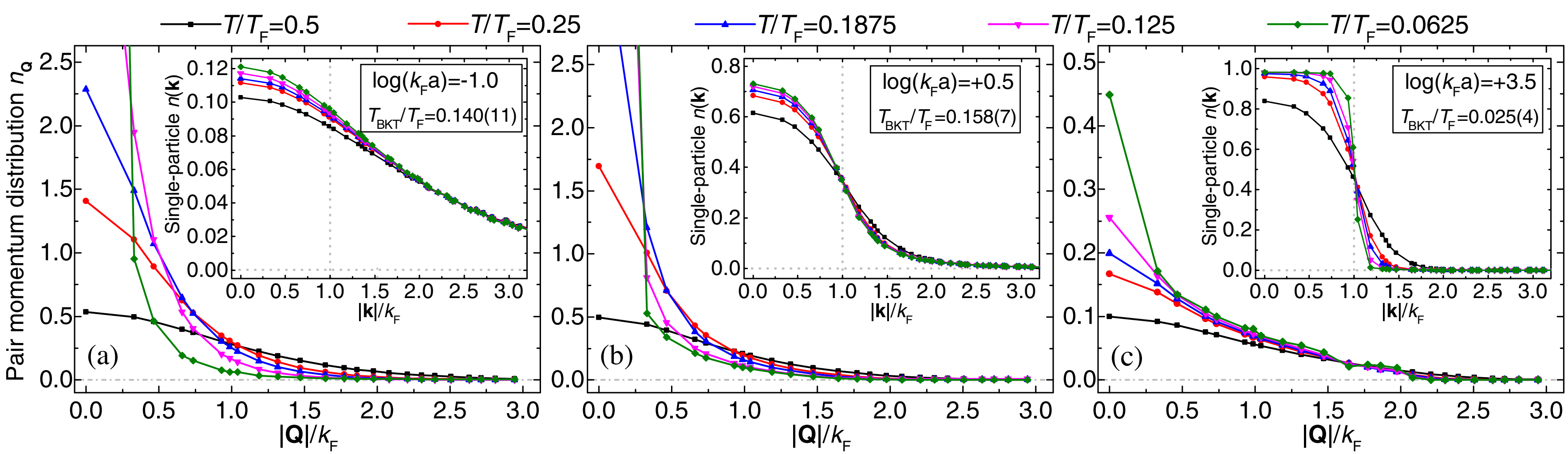


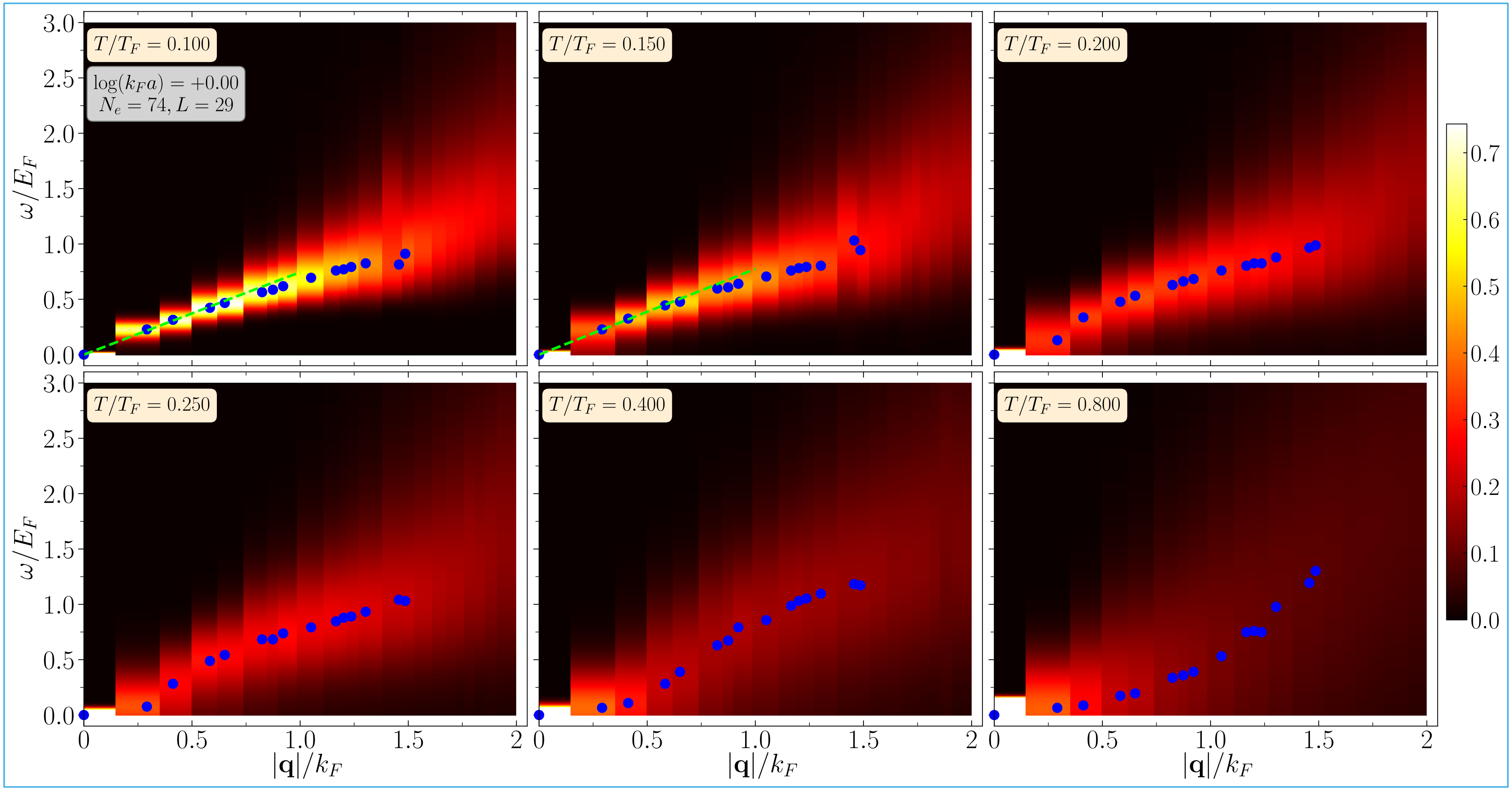
Image from D. Jin group



He, Shi, SZ, PRL 129, 076203 (2022)

Density response *Preliminary*

log(kF a)=+0.0

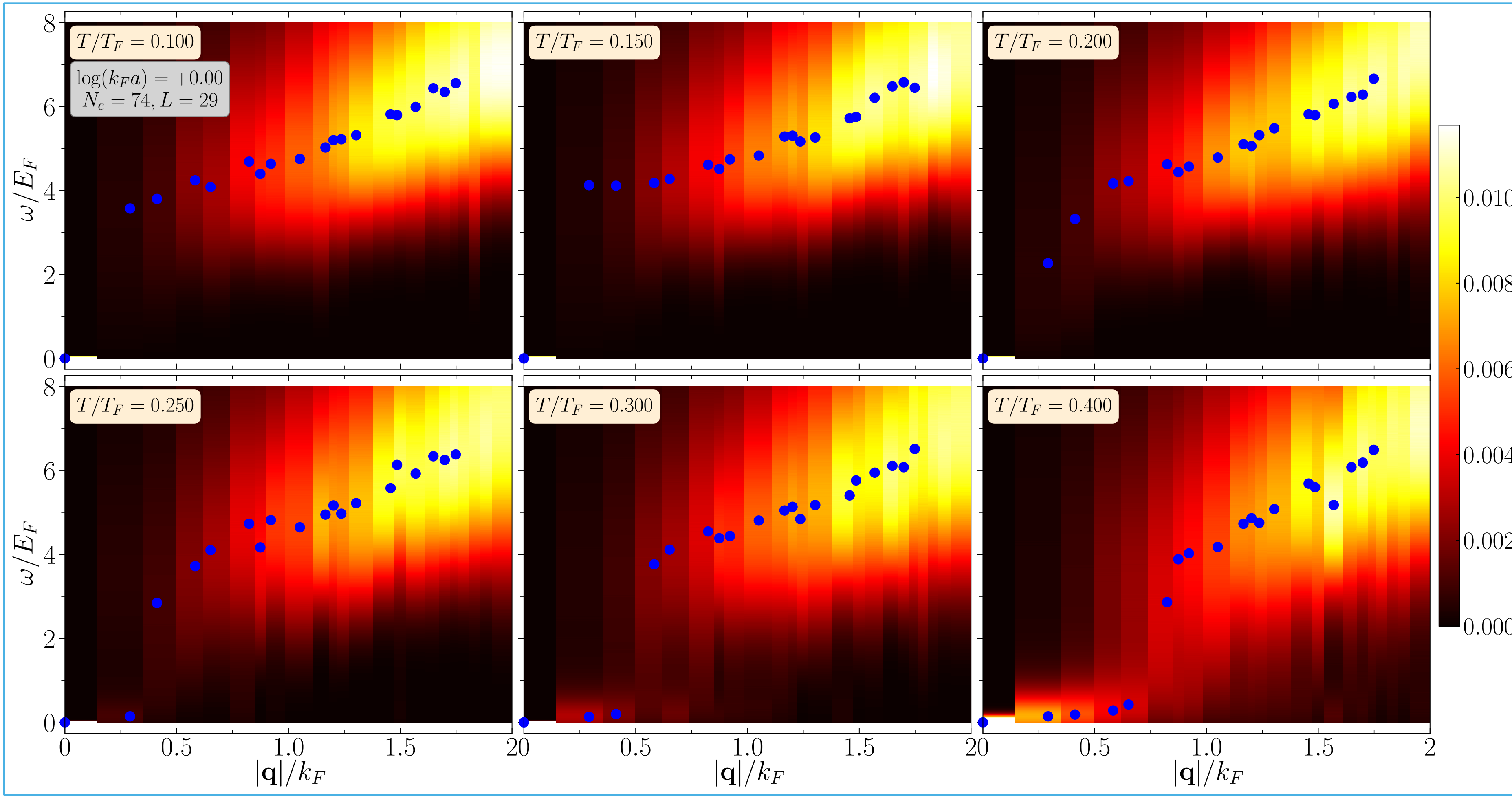


- Recall *Tc* (~ 0.125)

He & SZ, to be published

Spin response *Preliminary*

log(kF a)=+0.0



- Gap closing with increasing *T*

He & SZ, to be published

Recent progress on the Fermi gas from auxiliary-field QMC

Shiwei Zhang

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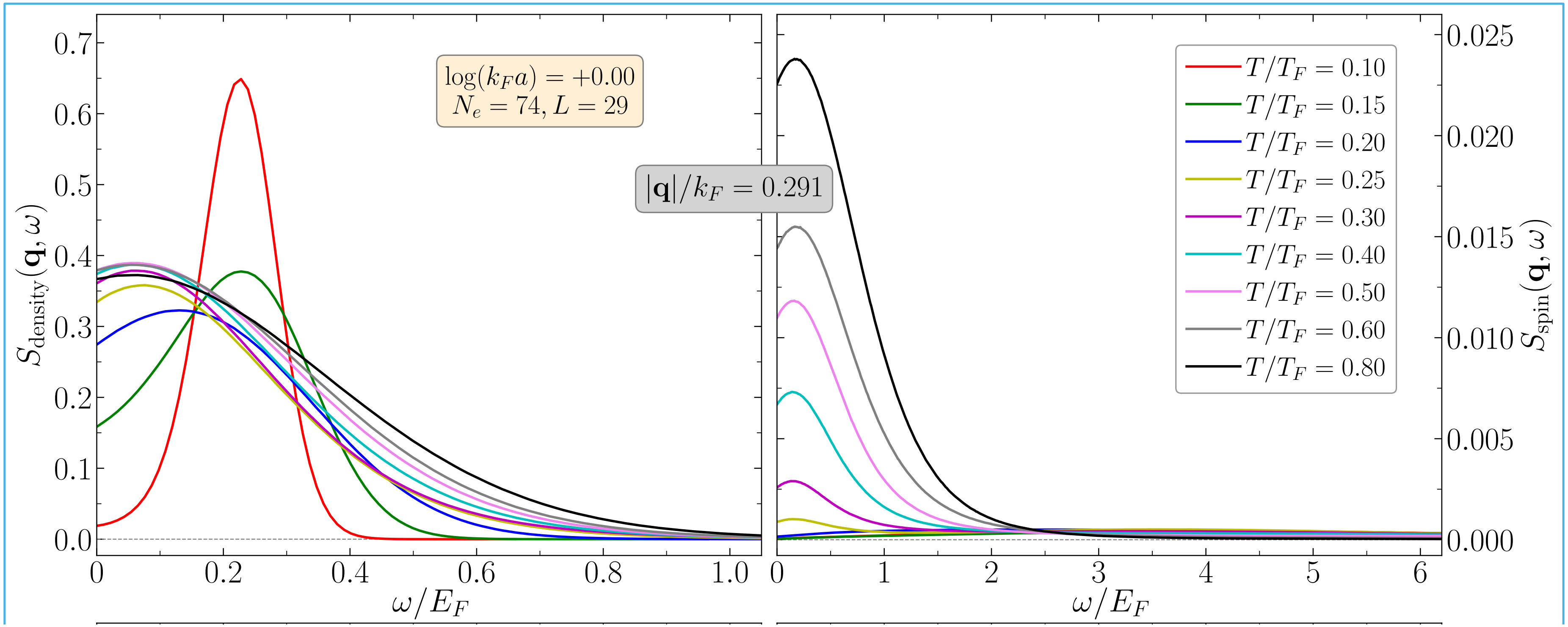
Density and spin responses



He & SZ, to be published

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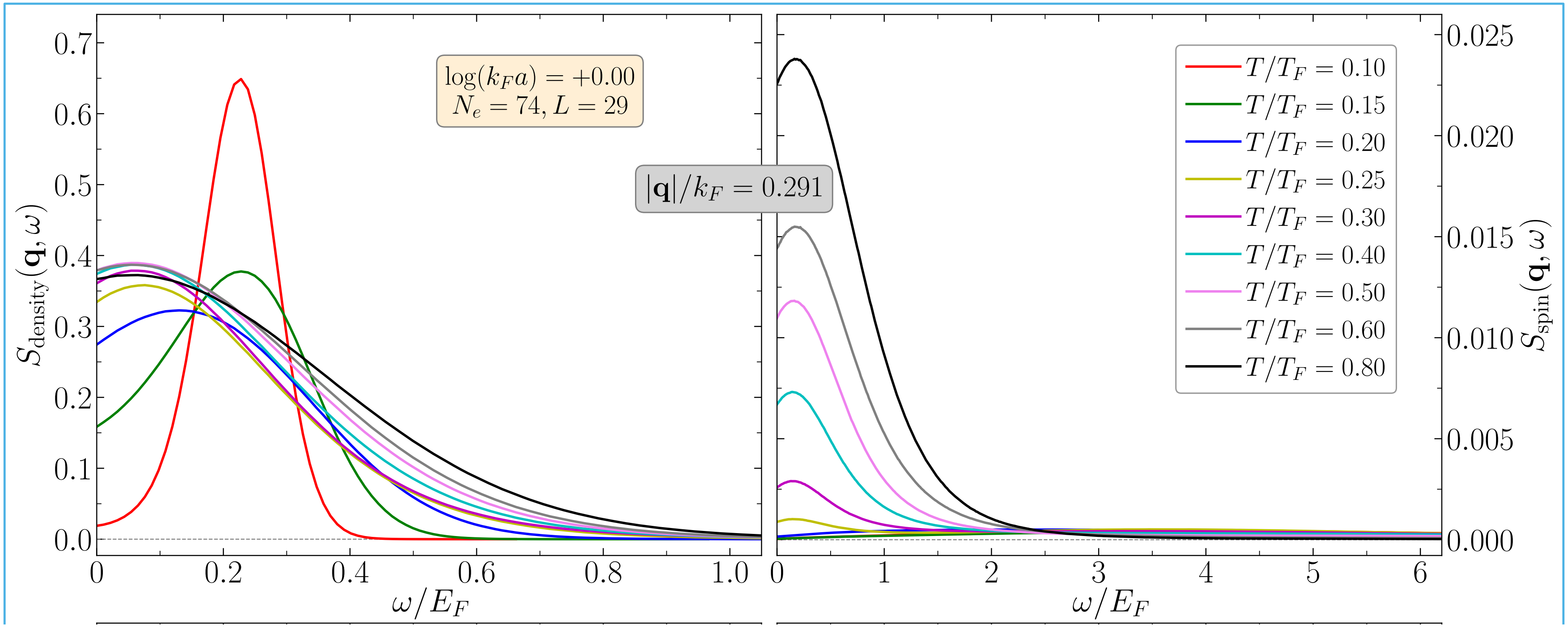
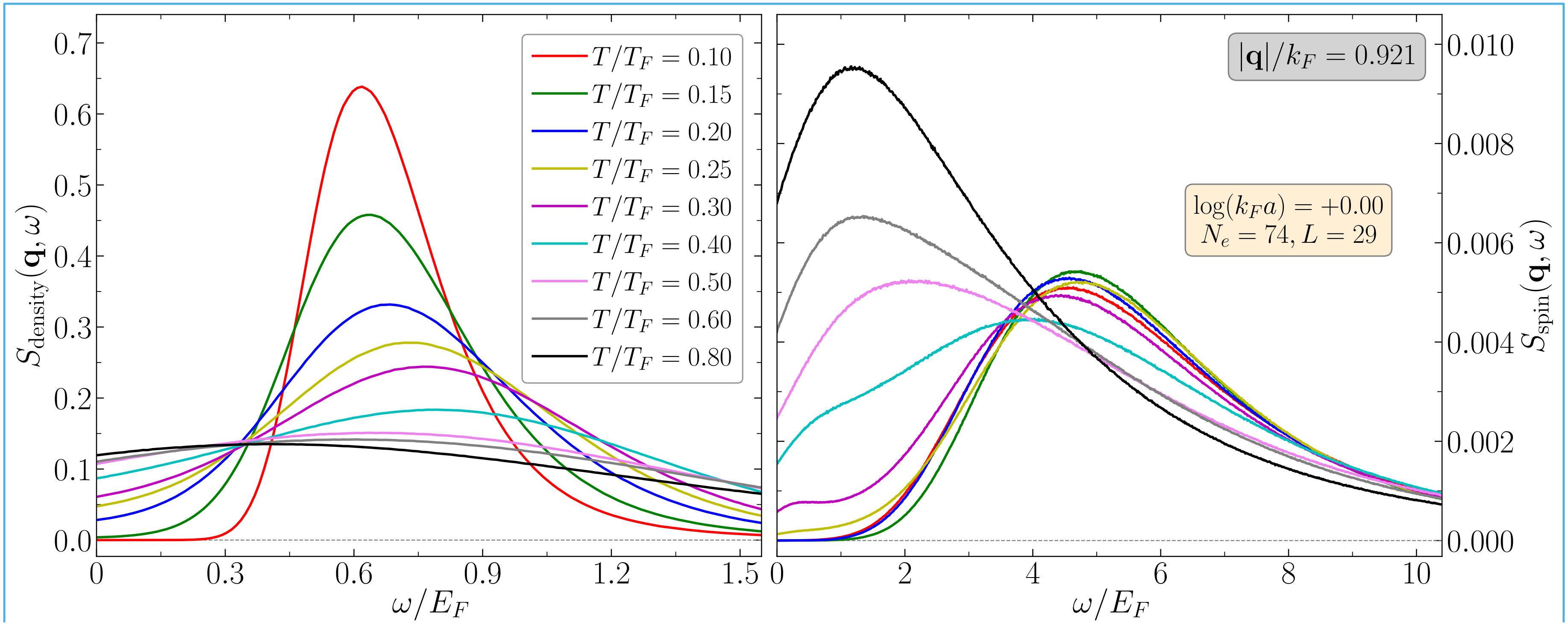


Preliminary

He & SZ, to be published

Density and spin responses



He & SZ, to be published

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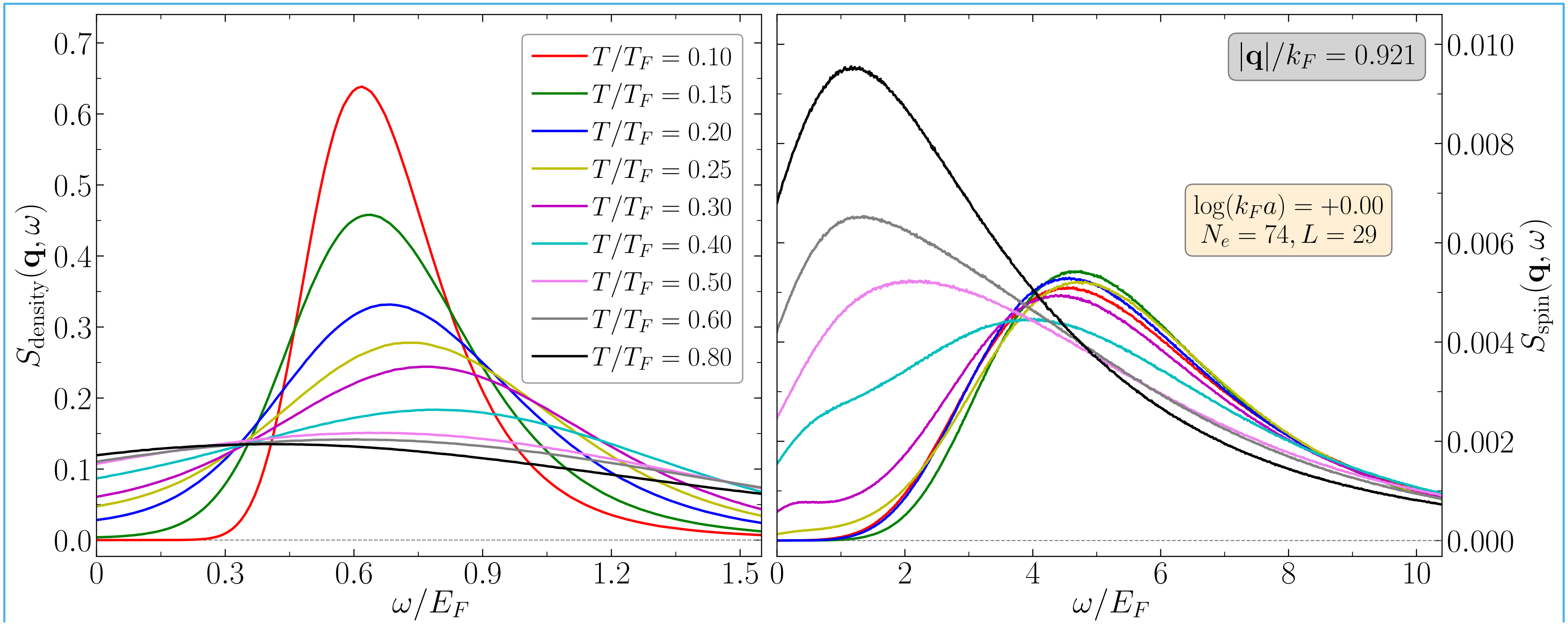
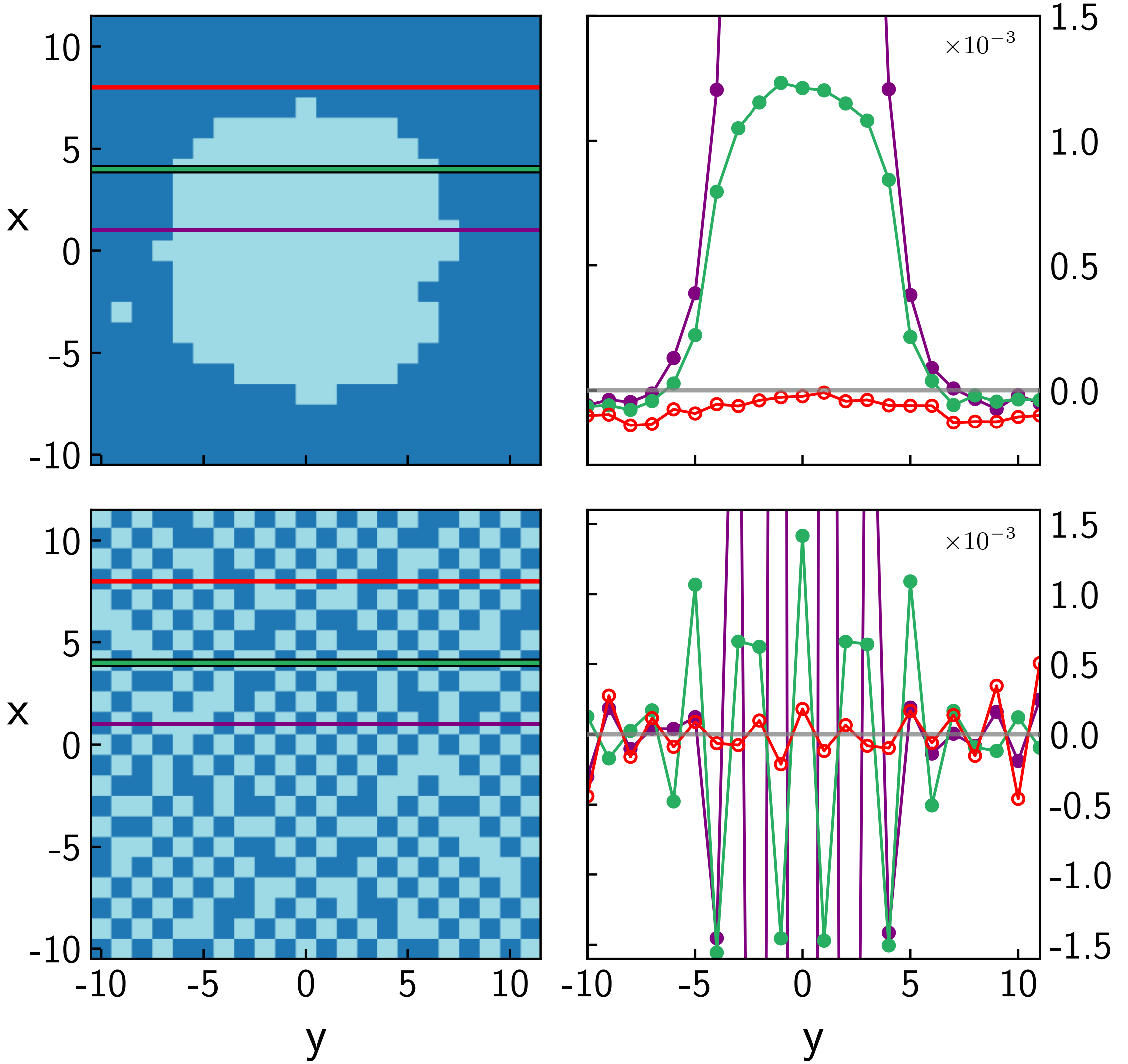


Preliminary

He & SZ, to be published

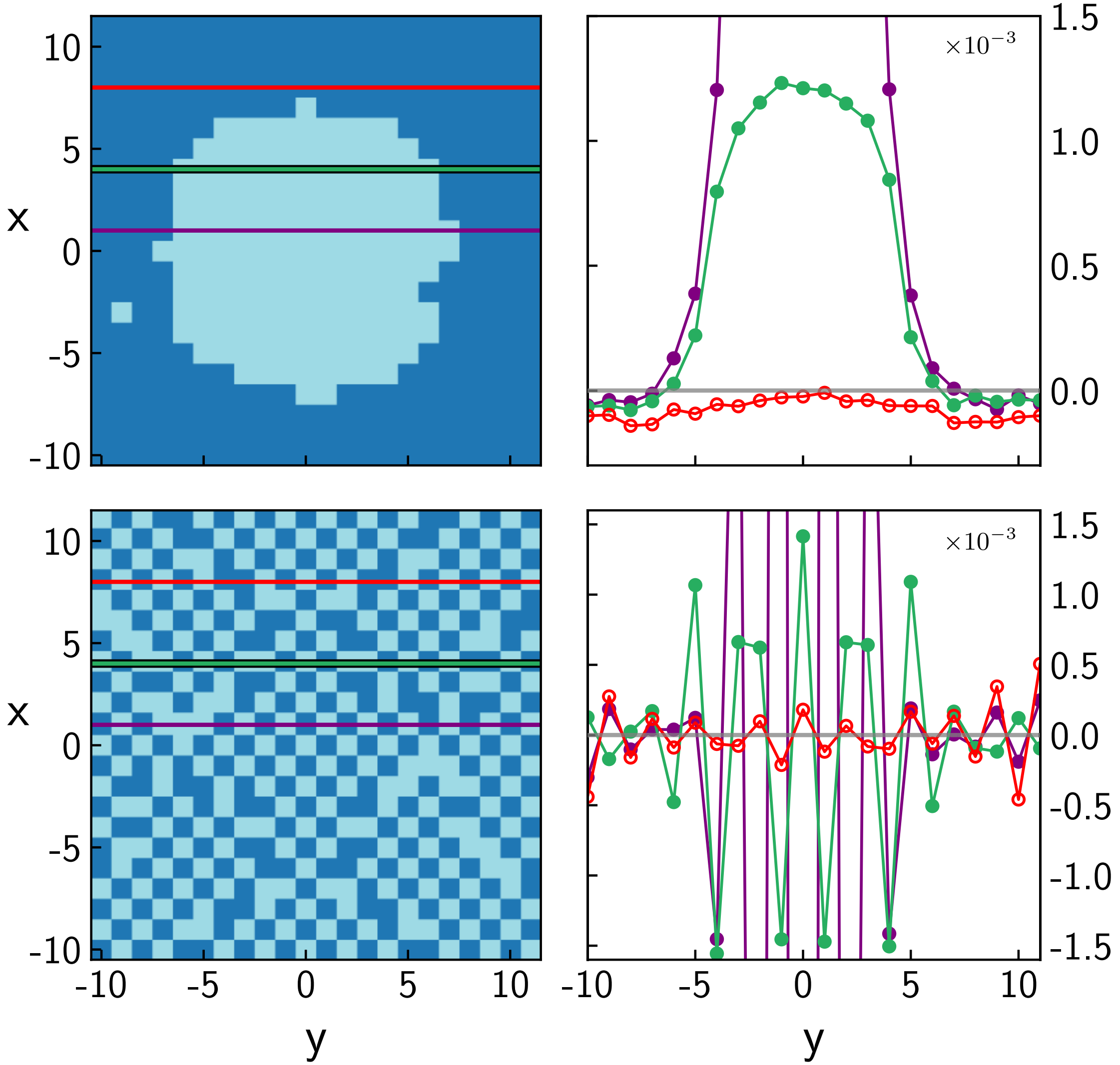
Exotic state in spin polarized systems



Vitali, Rosenberg, SZ, PRL ’22

Exotic state in spin polarized systems

optical lattice



- pairing correlation change sign - Larkin-Ovchinnikov

- Density correlation has checkerboard pattern with modulation

Vitali, Rosenberg, SZ, PRL '22