Ground-state properties, excitations, and response of the 2D Fermi gas

Shiwei Zhang
Flatiron Institute
and
College of William & Mary

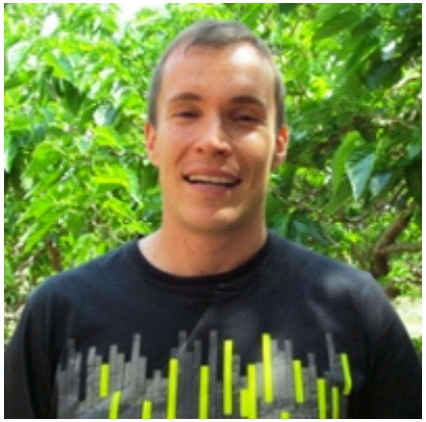
Outline

- Introduction: 2D FG and a condensed matter perspective
- Auxiliary-field quantum Monte Carlo calculations - exact* here
- Results on spin-balanced system:
  - ground-state properties
  - pairing gaps, spectral information, response
- Comment on (e.g. spin-imbalance) cases with sign problem
- Results on optical lattices with SOC
- Summary

Collaborators:

Hao Shi ->
Flatiron

Peter Rosenberg ->
FSU MagLab



Ettore Vitali ->
Cal State Fresno

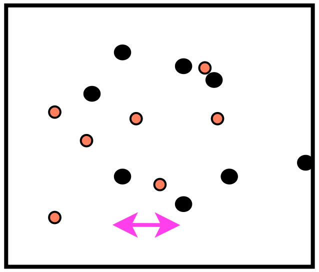
Mingpu Qin ->
Shanghai
Jiaotong U

Simone Chiesa
(Citi group)

Support:

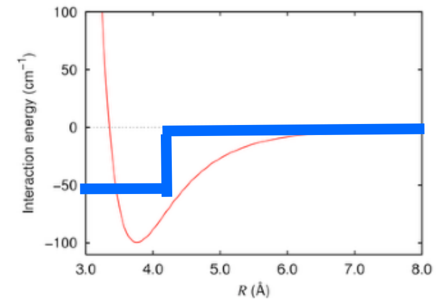
- NSF
- Simons Foundation
- DOE -- SciDAC; ThChem

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



In 3-dimensitons, 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

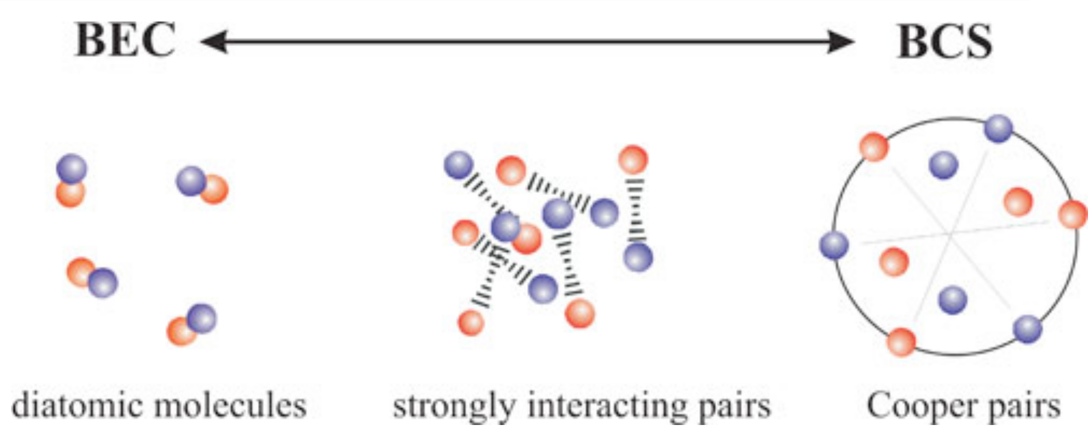
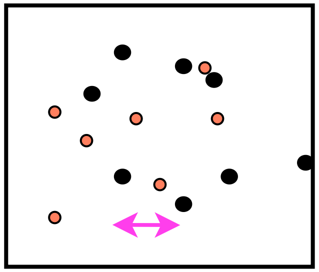


Image from D. Jin group

Ultracold atomic Fermi gas - 2D



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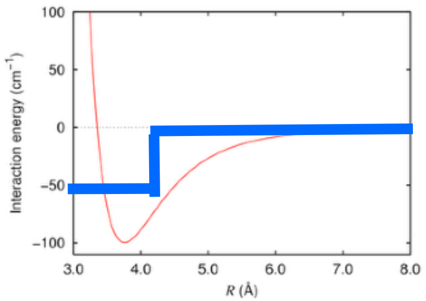

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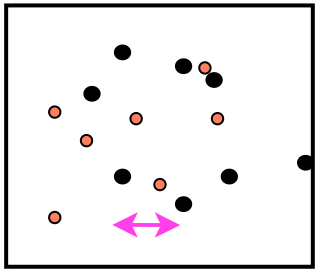

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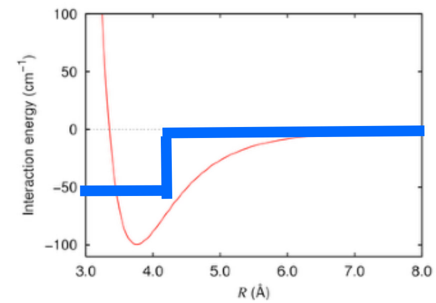
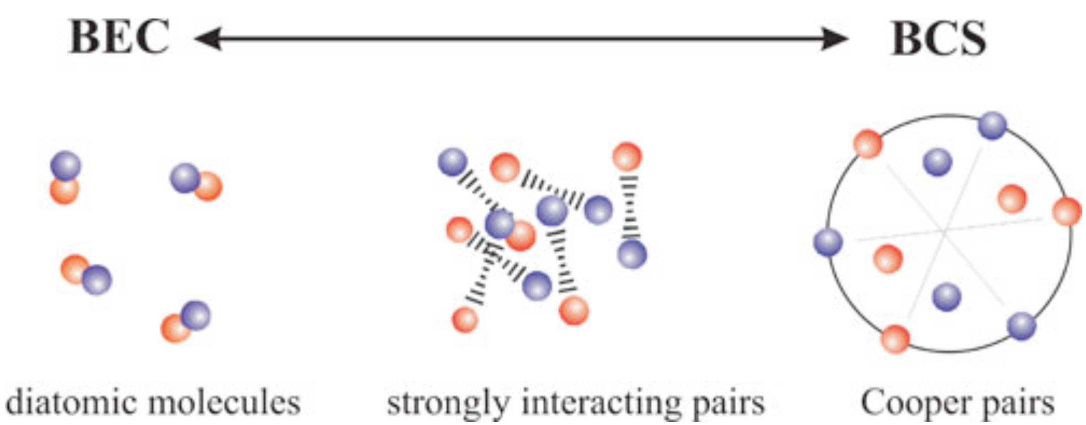


In **2-dimensions**, always bound state -- no unitarity

Pair size vs. d:



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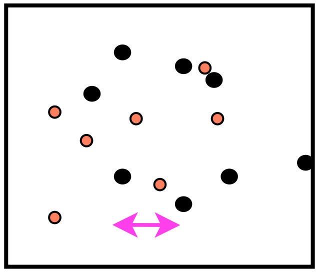

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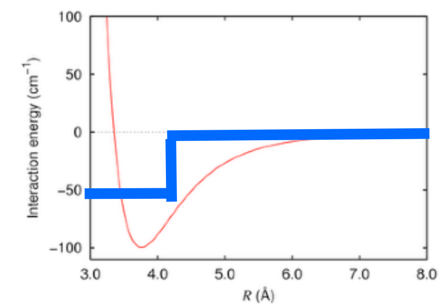

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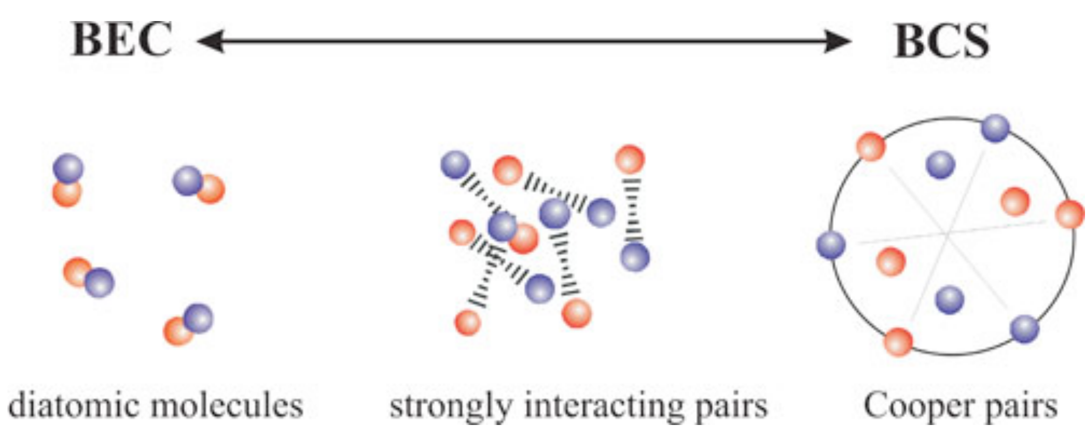

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Expt realized (recall tremendous precision in 3D)

-- 2D important in condensed matter: cuprates, ...

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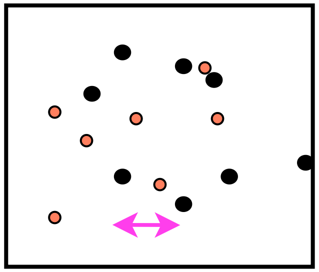

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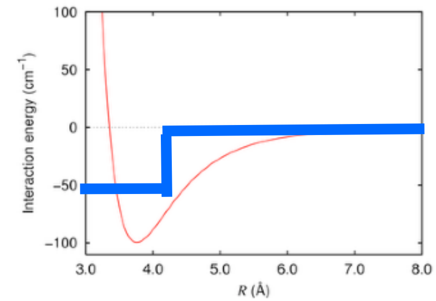

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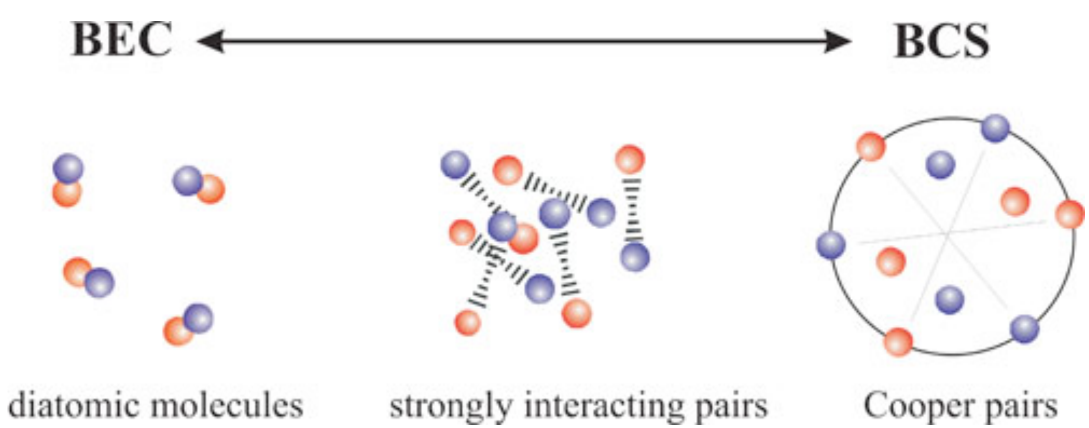

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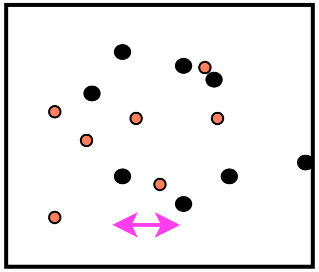
"Metric": $x \equiv \ln(k_F a)$ basically, scattering length/d

Ultracold atomic Fermi gas -- 2D



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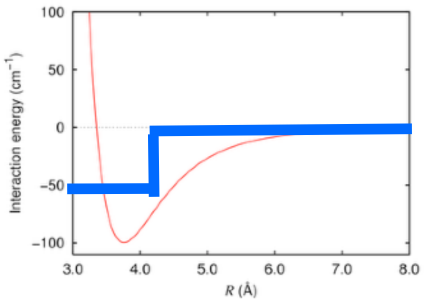
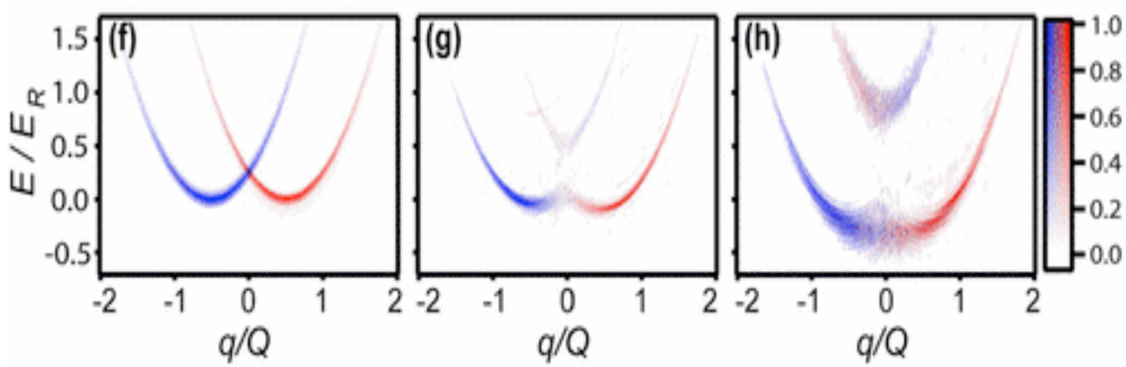
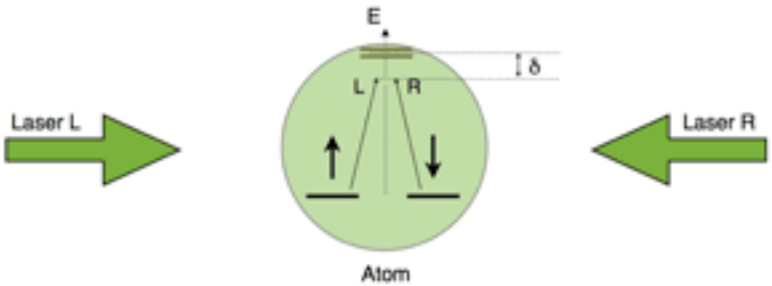


Spin-orbit coupling has been realized (PRL 109, 095301; PRL 109, 095302)





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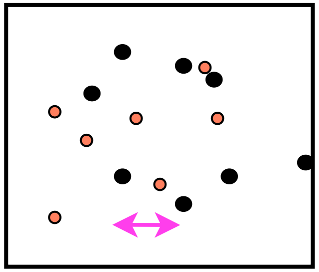

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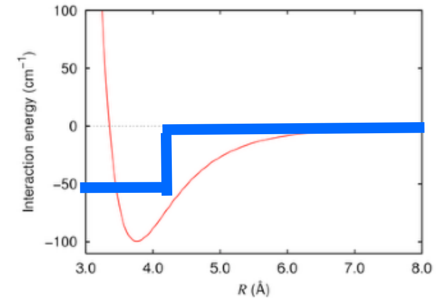

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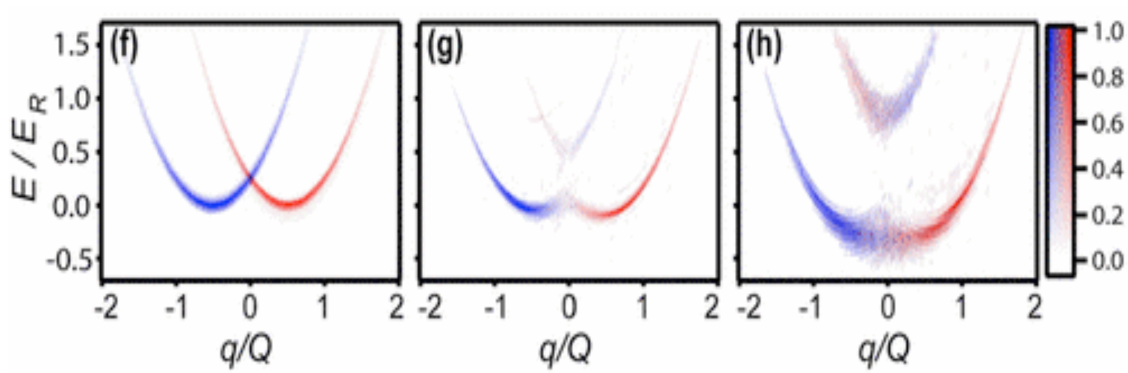
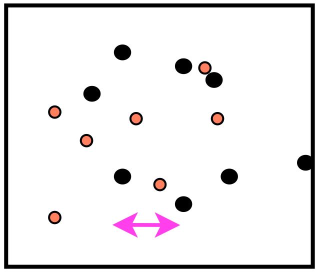


Connection to topological materials, QHE, interplay bt. SOC & pairing

Ultracold atomic Fermi gas -- 2D



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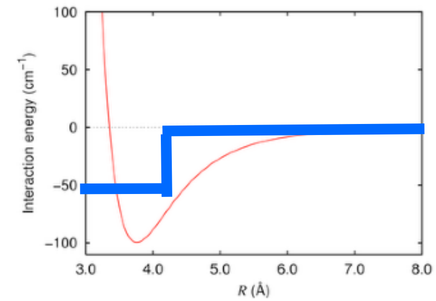

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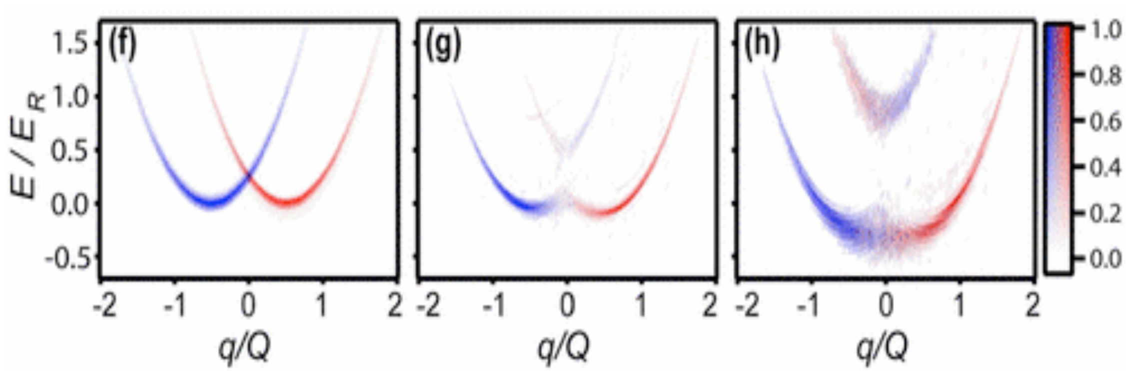

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Clean, tunable experiments

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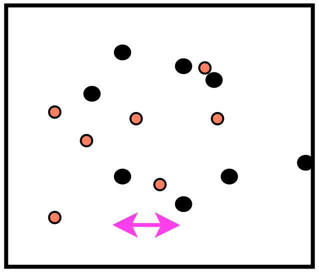

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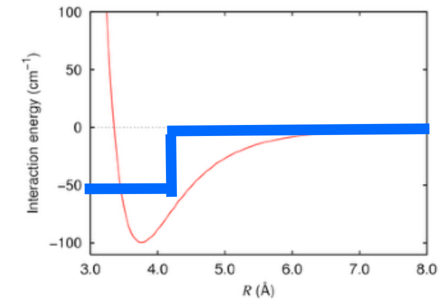

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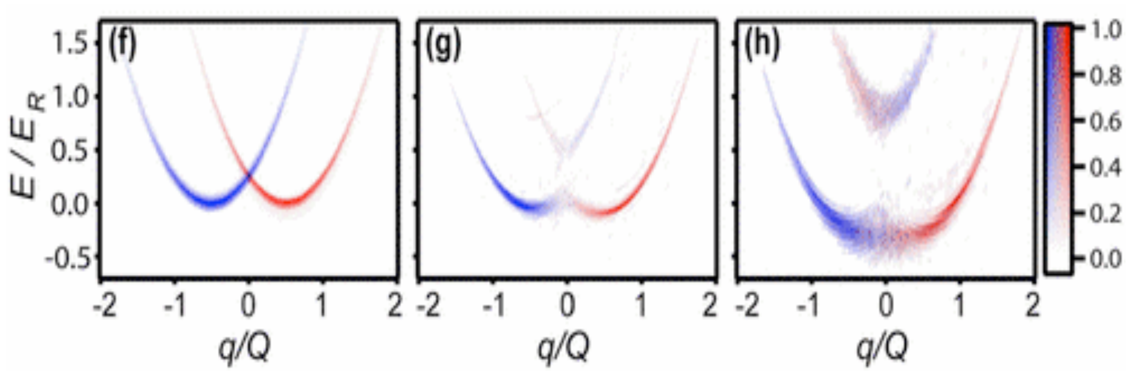

Connection to topological materials, QHE, interplay bt. SOC & pairing

Clean, tunable experiments

Theoretical work mostly at mean-field level

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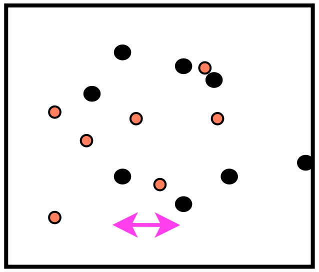

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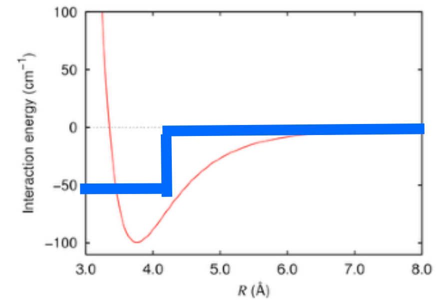

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Hamiltonian incl. synthetic Rashba SOC in dilute gas (and optic. latt. !)

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

$$\frac{U}{t} = -\frac{4\pi}{\ln(k_F a) - \ln(\mathcal{C}\, n)}, \quad n = \frac{N}{L^2}, \quad k_F = \frac{\sqrt{2\pi n}}{\Delta}$$

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An auxiliary-field perspective

To obtain **ground state**, use projection in imaginary-time:

$$\frac{\langle\Psi_T|\,H\,e^{-\tau H}\cdots e^{-\tau H}e^{-\tau H}|\Psi^{(0)}\rangle}{\langle\Psi_T|\,e^{-\tau H}\cdots e^{-\tau H}e^{-\tau H}|\Psi^{(0)}\rangle}$$

E.g. $\hat{H}=\sum\frac{\hat{p}_i^2}{2m}+\hat{V}$

$$e^{-\tau\hat{\mathbf{p}}_i^2/2m}=\int e^{-\sigma^2/2}\,e^{i\hat{\mathbf{p}}_i\cdot(\gamma\,\sigma)}\,d\sigma \qquad \gamma=\sqrt{\frac{\tau}{m}}$$

$$e^{-\tau\hat{H}}=\int e^{-\vec{\sigma}^2/2}\,e^{i\hat{P}\cdot(\gamma\,\vec{\sigma})}\,d\vec{\sigma}\;\;e^{-\tau\hat{V}}$$

translation op.

$$|R\rangle=|\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_M\rangle$$

$$|\Psi_0\rangle=\sum_R\Psi_0(R)|R\rangle$$

$$e^{-\tau\hat{H}}=\int p(\sigma)B(\sigma)d\sigma$$

$$B(\sigma)|R\rangle\rightarrow|R'\rangle$$

==> diffusion Monte Carlo (GFMC)
(and path-integral MC)

- initialize $\{|R\rangle\}$ from $\Psi^{(0)}(R)$
- random walks with $\{|R\rangle\}$
- distribution -> $\Psi_0(R)$

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$$e^{-\tau \hat{H}} = \int p(\sigma) B(\sigma) d\sigma$$

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use basis

$$|\Psi_0\rangle = \sum_\phi \Psi_0(\phi)|\phi\rangle$$

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Like a TDDFT propagator

use basis

$$|\Psi_0\rangle = \sum_{\phi} \Psi_0(\phi) |\phi\rangle$$

Many-body propagator --> many 1-body prop's

Consider the propagator $e^{-\tau\hat{H}} \doteq e^{-\tau\hat{H}_1} e^{-\tau\hat{H}_2} + \mathcal{O}(\tau^2)$

$$\hat{H} = \sum_{i,j}^{N} T_{ij}\, c_j^\dagger c_j + \sum_{i,j,k,l}^{N} V_{ijkl} c_i^\dagger c_j^\dagger c_k c_l$$

e.g. $V_{ijkl} \doteq \sum_{\nu=1}^{J_{\max}} L_{ij}^{\nu}\, L_{kl}^{\nu}$

$$\hat{H}_2 = -\sum_{\nu} \hat{v}_\nu^2$$

$$\hat{v}_\nu = \sum_{i,j} L_{ij}^{\nu} c_i^\dagger c_j$$

Hubbard-Stratonovich transform.:

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

$$e^{-\tau\hat{H}} \;\to\; e^{-\tau\hat{H}_1} \int e^{-\sigma^2/2}\, e^{\sigma\sqrt{\tau}\,\hat{v}}\, d\sigma$$

$$e^{-\tau\hat{H}} = \int p(\sigma) B(\sigma) d\sigma$$

$$B(\sigma)|\phi\rangle \to |\phi'\rangle$$

Path integral over AF's by MC

Imaginary-time projection --> random walk:

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A **step** advances the SD by 'rotations'

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$$\begin{pmatrix} \psi_1 & \psi_1 \\ \psi_2 & \psi_2 \\ \cdot & \cdot \\ \cdot & \cdot \\ \psi_N & \psi_N \end{pmatrix}$$

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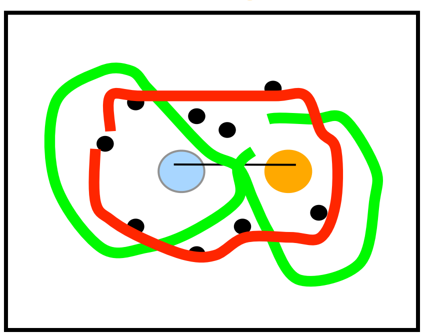
MnO



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1-body op

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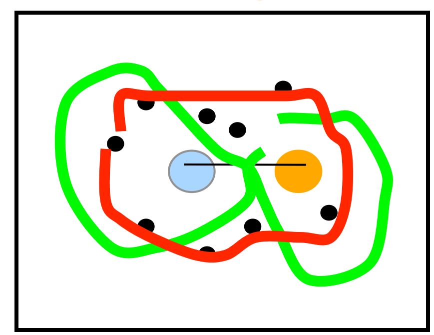

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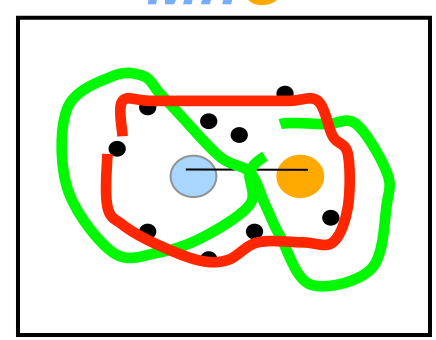
AF variable -- sample

MnO



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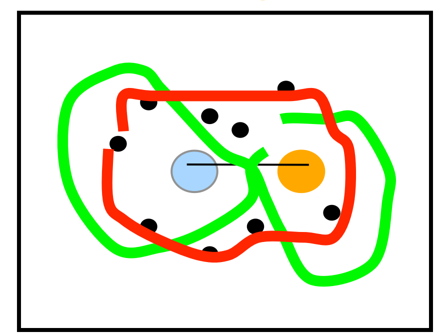
$$B(\sigma)|\phi\rangle \rightarrow |\phi'\rangle$$

A **step** advances the SD by 'rotations'

$$e^{\sigma \hat{v}} \begin{pmatrix} \psi_1 & \psi_1 \\ \psi_2 & \psi_2 \\ \cdot & \cdot \\ \cdot & \cdot \\ \psi_N & \psi_N \end{pmatrix}$$

N is size of 'basis'

MnO



Path integral over AF's by MC

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NxN matrix

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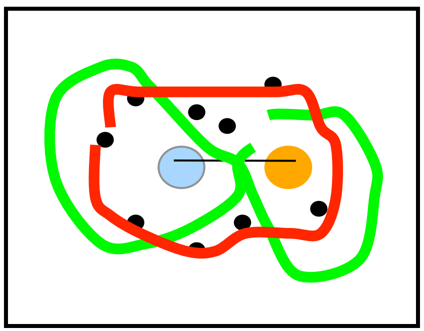

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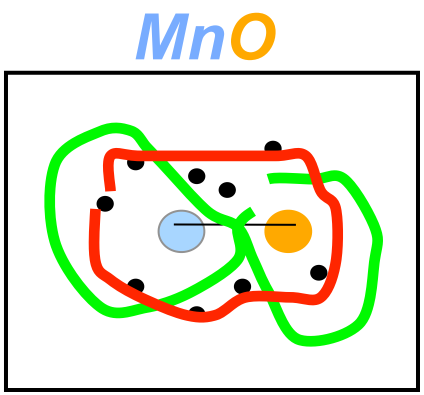

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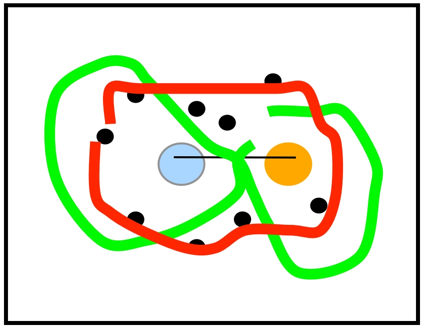
MnO



The sign problem

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$$B(\sigma)|\phi\rangle \to |\phi'\rangle$$

The sign problem

- happens whenever $B \ldots B|\phi\rangle \to -|\phi\rangle$ exists
- symmetry can prevent this - sign-problem-free cases:
  - attractive interaction, spin-balanced (det[ ])^2
  - repulsive half-filling bipartite (particle-hole)
  - attractive, spin-balanced, w/ spin-orbit coupling
  - a more general formulation w/ Majorana fermions

PRL 116, 250601 (2016)

Equal-time correlations and observables

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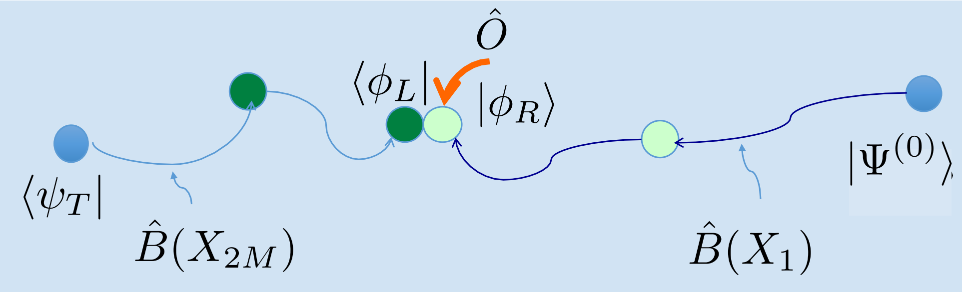

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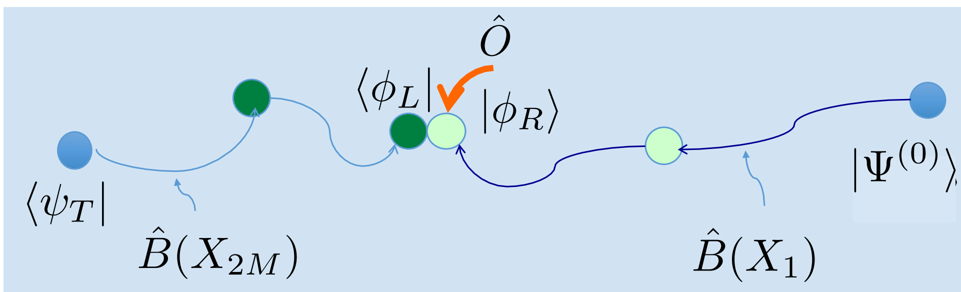

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Note

- Apply force bias - importance sampling - much more efficient than "standard algorithm"

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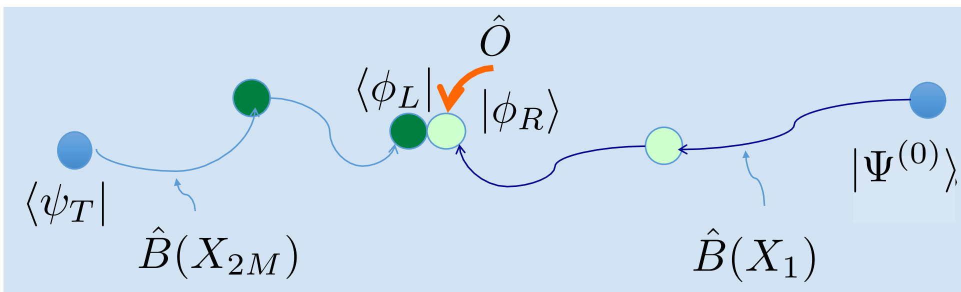

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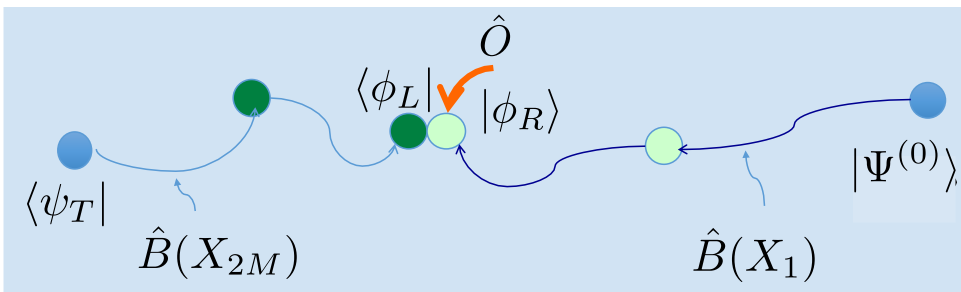

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Note

- Apply force bias - importance sampling - much more efficient than "standard algorithm"
- Infinite variance for sign-problem-free cases (Hao Shi talk)
- If sign problem, apply constraint in forward direction. In that case back-propagation is required

Imaginary-time correlations

Imaginary-time projection --> random walk:

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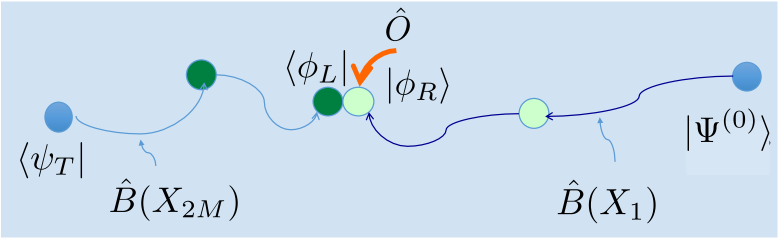

Vitali et al, PRB '16

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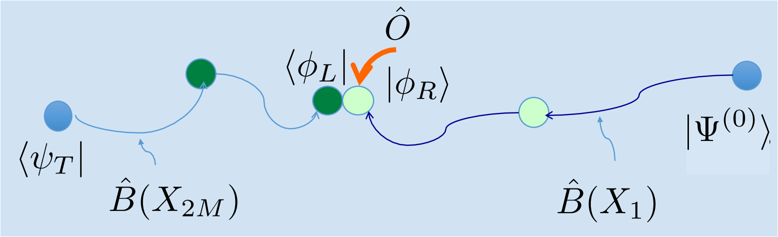

Imaginary-time GFs: $G(k, \tau) = \langle \Psi_0 | c_k e^{-\tau \hat{H}} c_k^\dagger | \Psi_0 \rangle$

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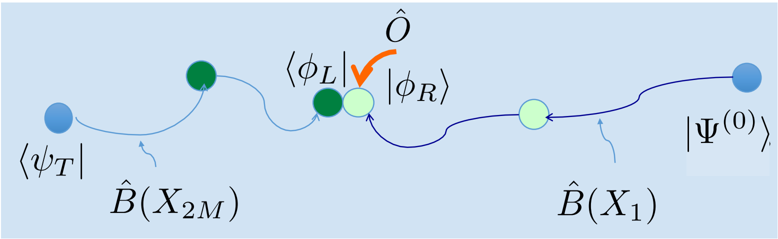

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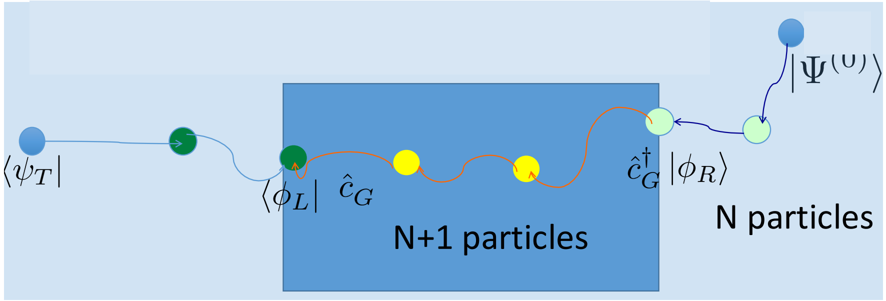

Standard algorithm: commutators, (basis size)^3

Vitali et al, PRB '16

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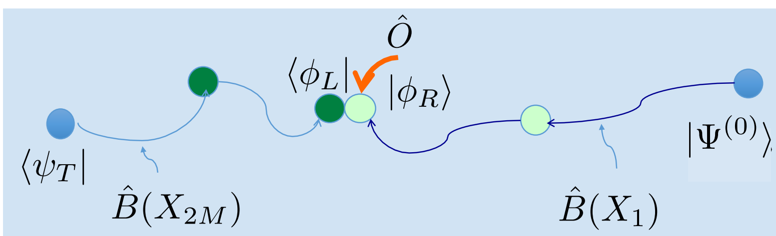

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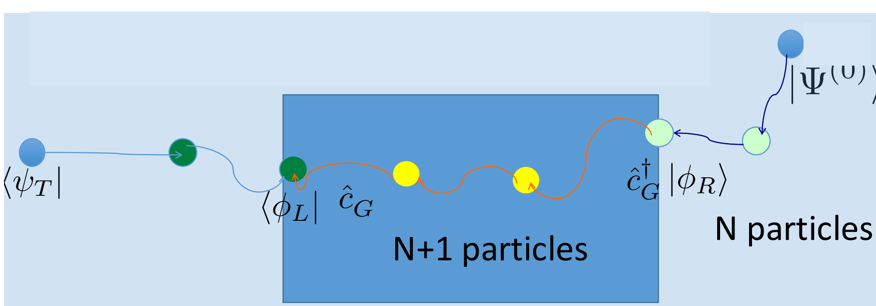

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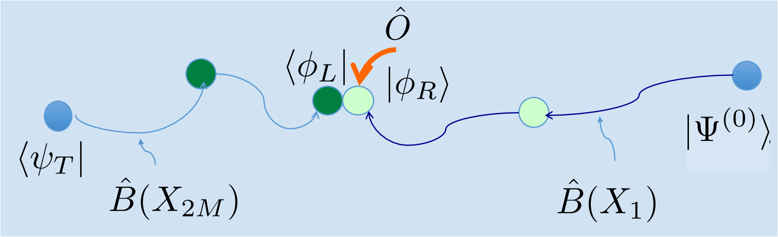

Imaginary-time density/spin corr:

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Vitali et al, PRB '16

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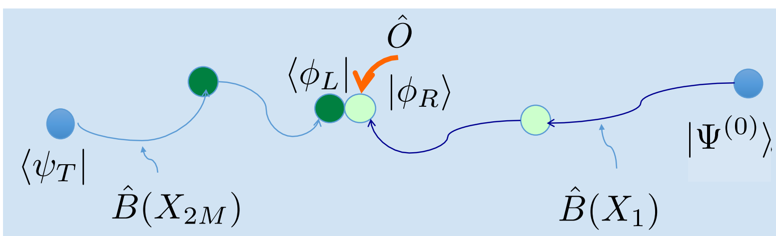

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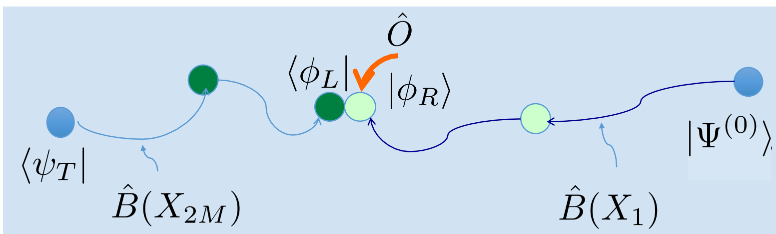

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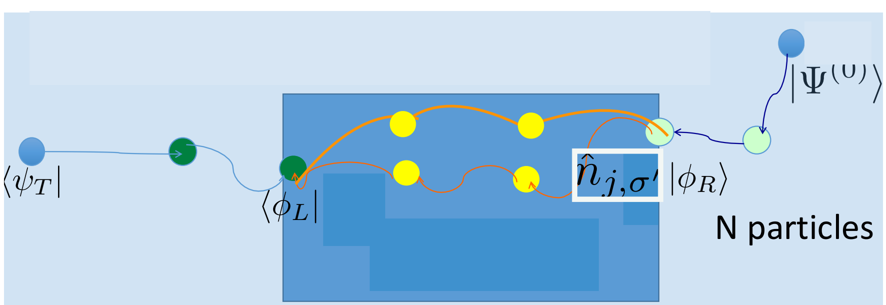

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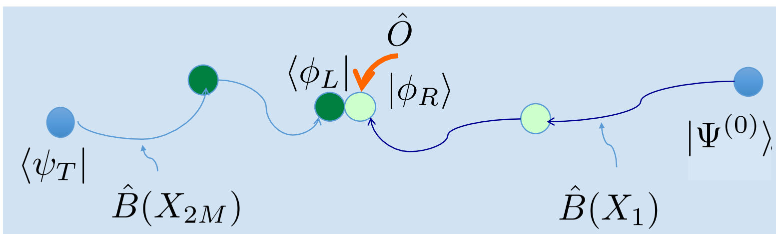

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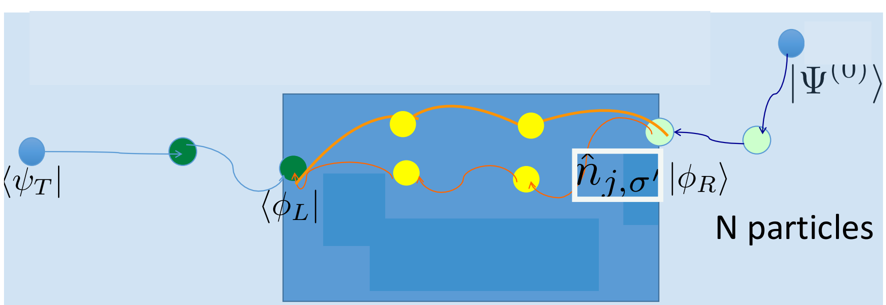

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Vitali et al, PRB '16

Ground-state properties, excitations, and response of the 2D Fermi gas

Shiwei Zhang
Flatiron Institute
and
College of William & Mary

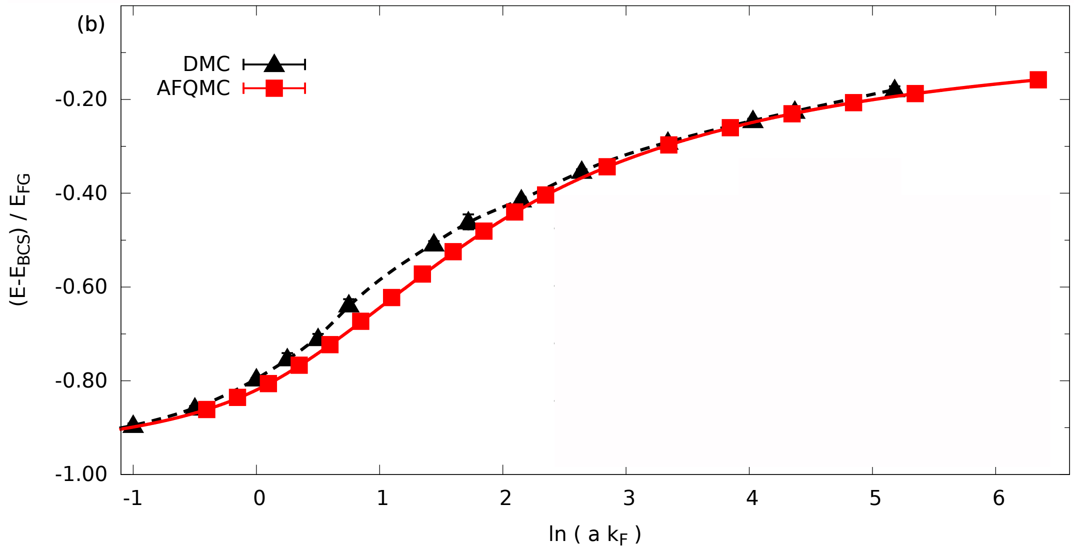
Outline

- Introduction: 2D FG and a condensed matter perspective
- Auxiliary-field quantum Monte Carlo calculations - exact* here
- Results on spin-balanced system:
  - ground-state properties
  - pairing gaps, spectral information, response
- Comment on (e.g. spin-imbalance) cases with sign problem
- Results on optical lattices with SOC
- Summary

Ultracold atomic Fermi gas -- 2D

Exact EOS obtained, fit provided

- BCS trial wf;
  Variance control;
  sampling tricks;



DMC: prev. best (var)

Bertaina & Giorgini, PRL '11

Shi, Chiesa, SZ, PRA '15

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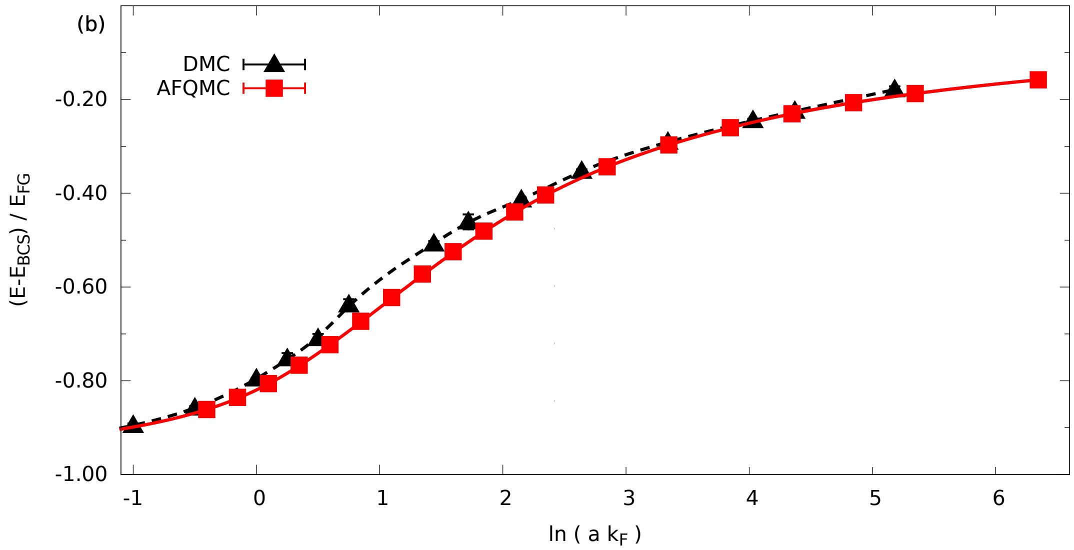

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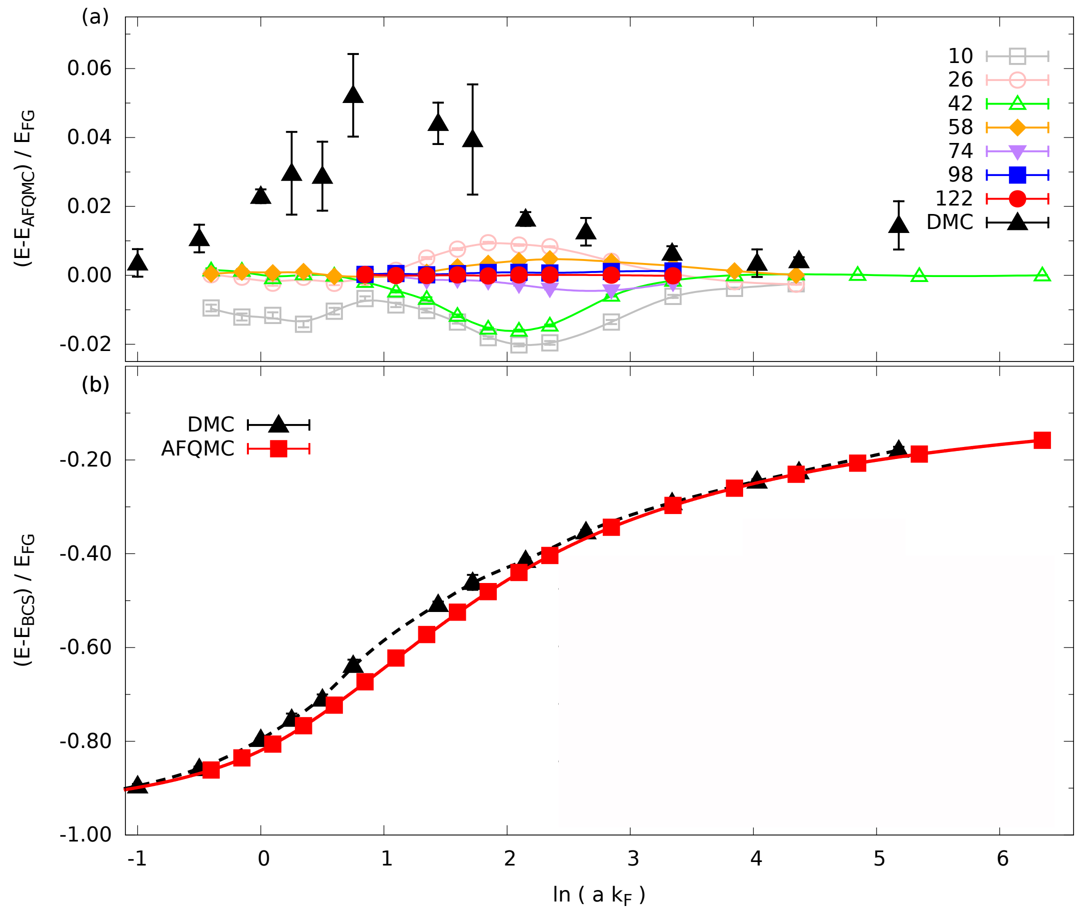

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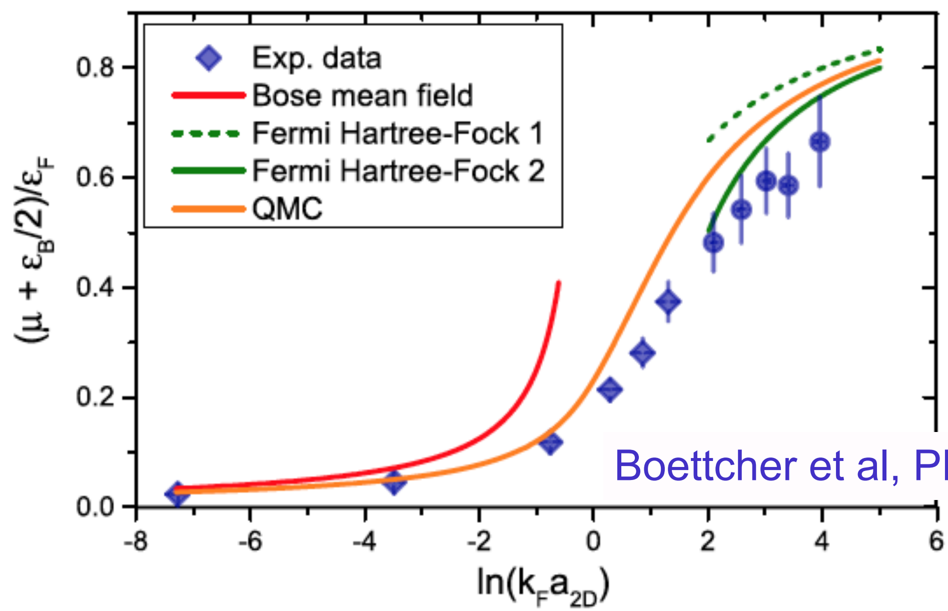
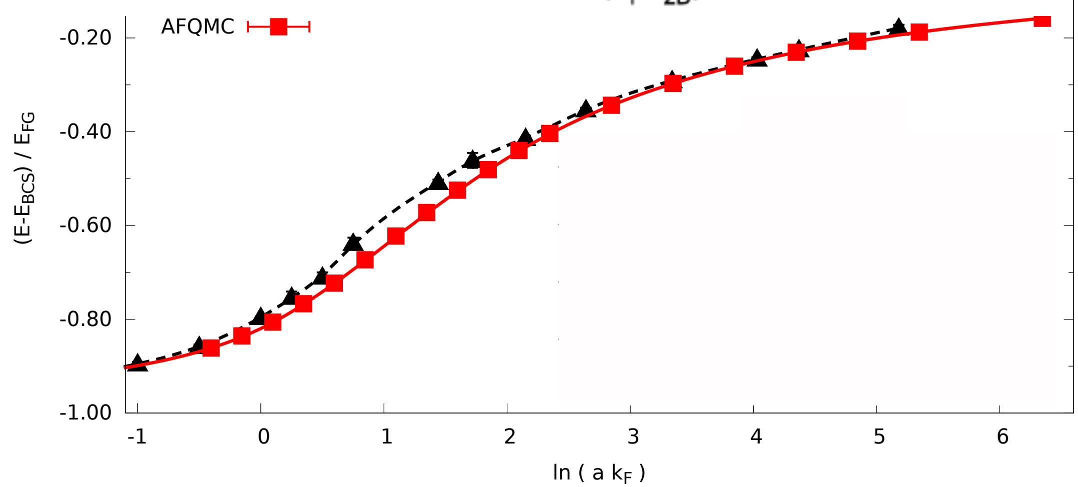


Boettcher et al, PRL '16



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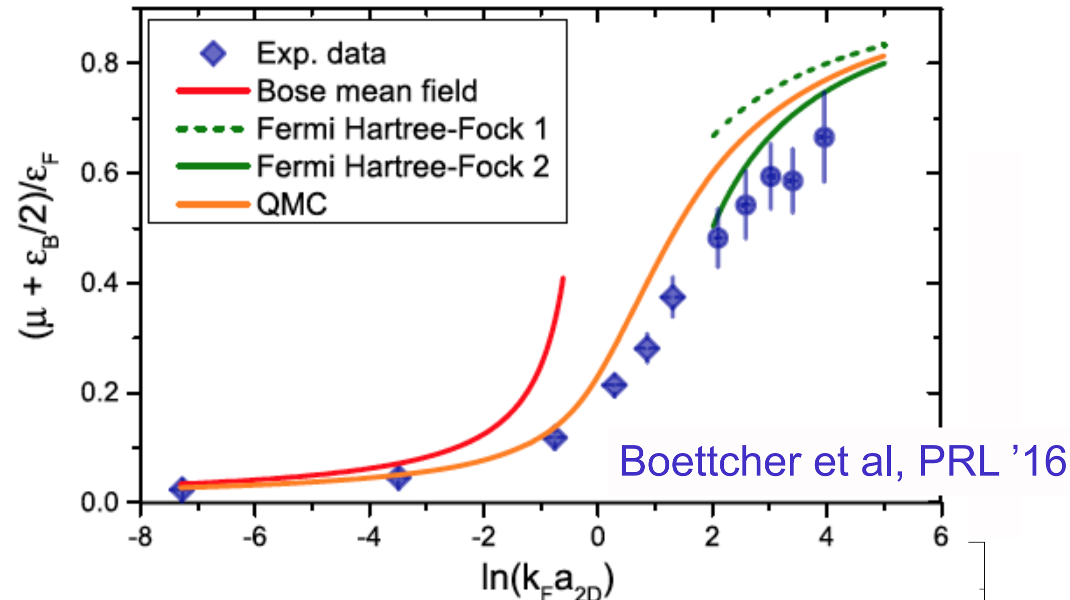

Boettcher et al, PRL '16

Precision many-body comp: benchmark thy; guide expt

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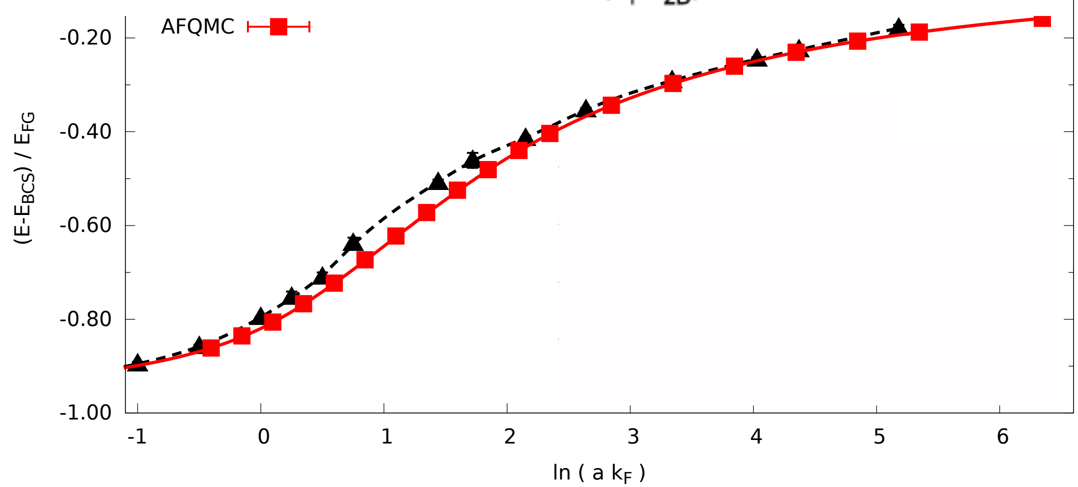

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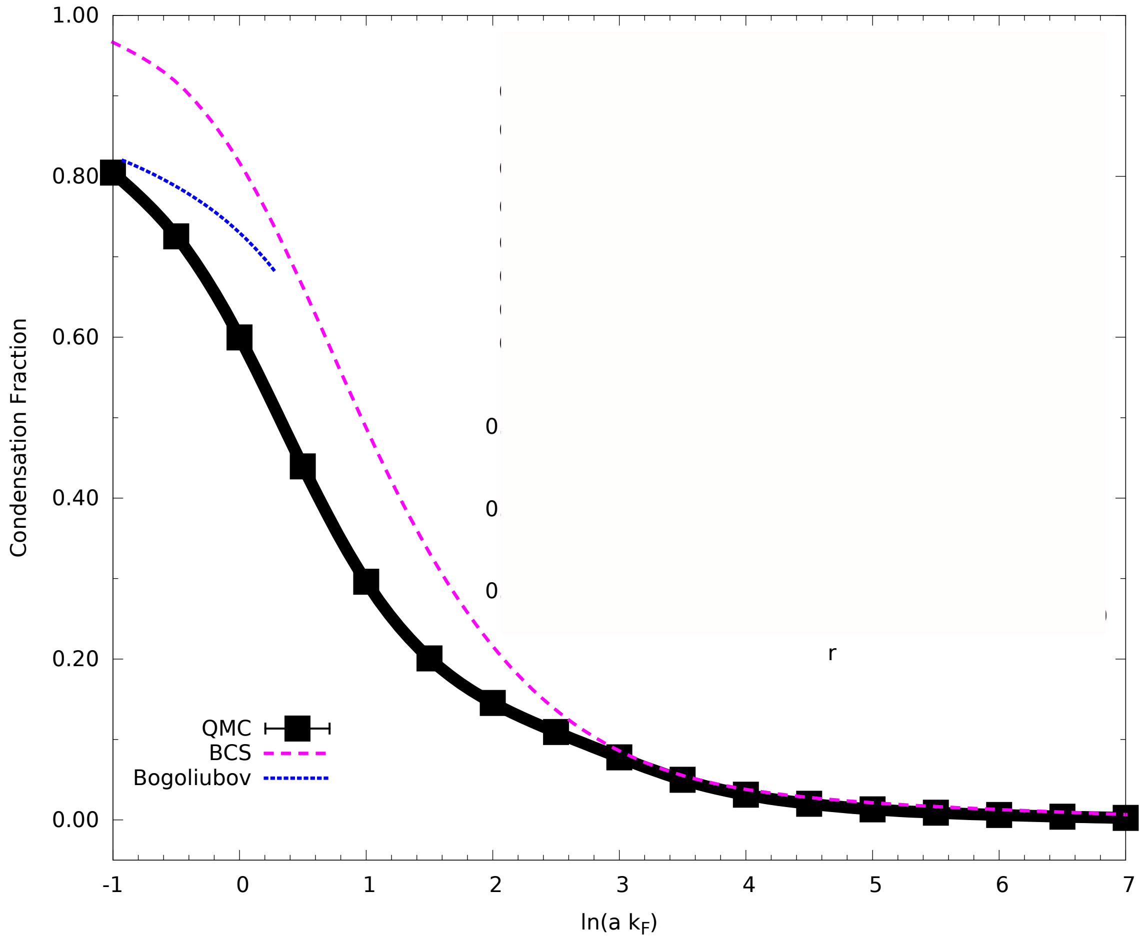
2D -- 'condensate fraction' (diagonalize $\langle \Delta_k^\dagger \Delta_{k'} \rangle$)



Shi, Chiesa, SZ, PRA '15

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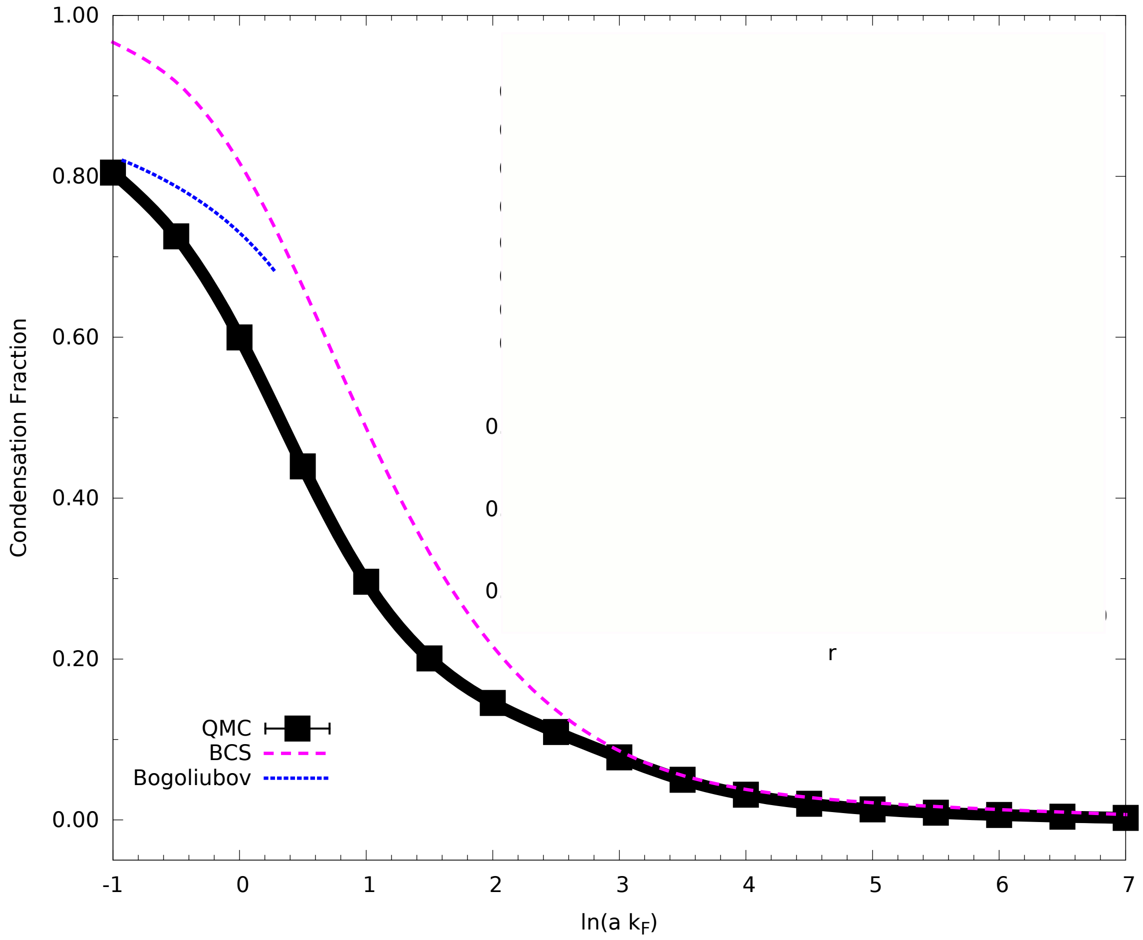
real-space 'pair wave function'



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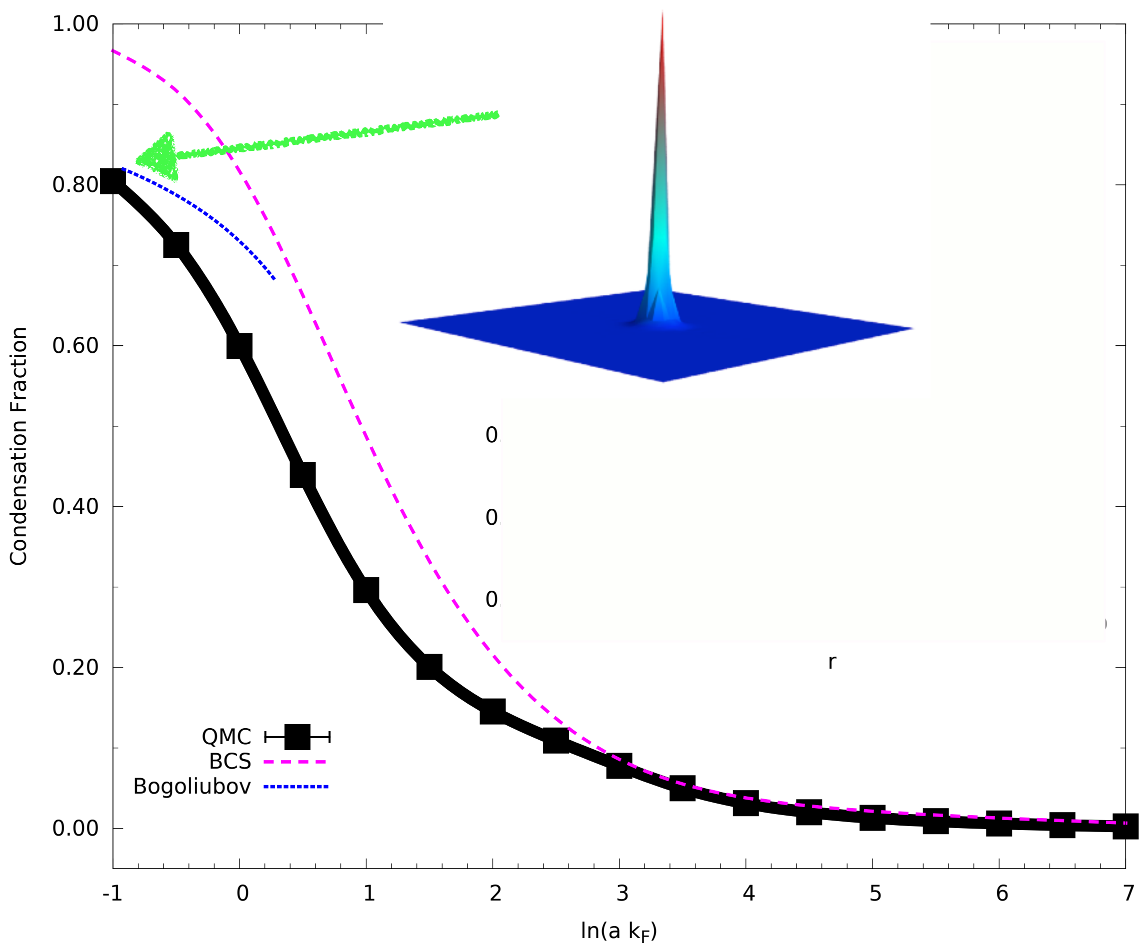

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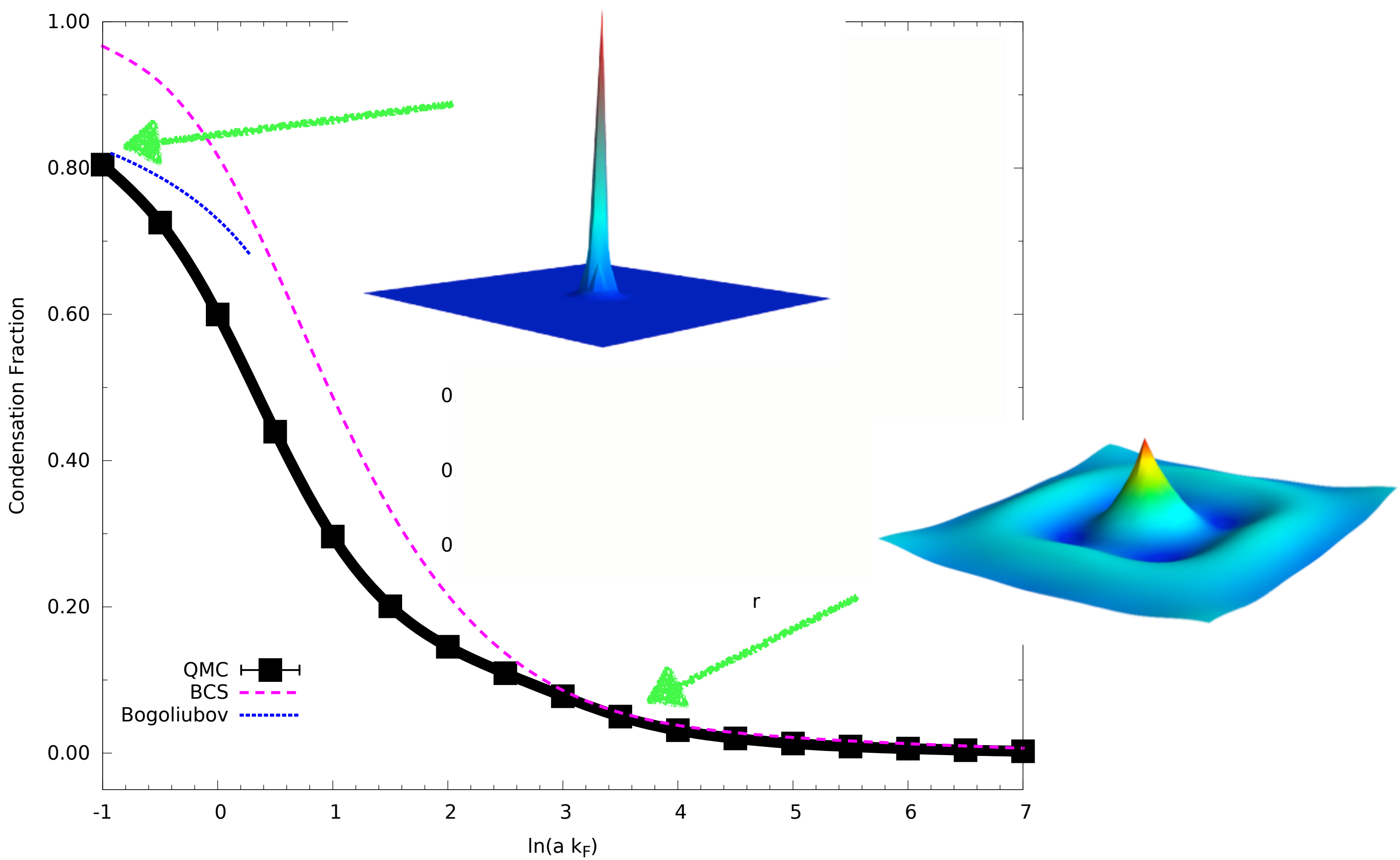

Shi, Chiesa, SZ, PRA '15

Ultracold atomic Fermi gas -- 2D

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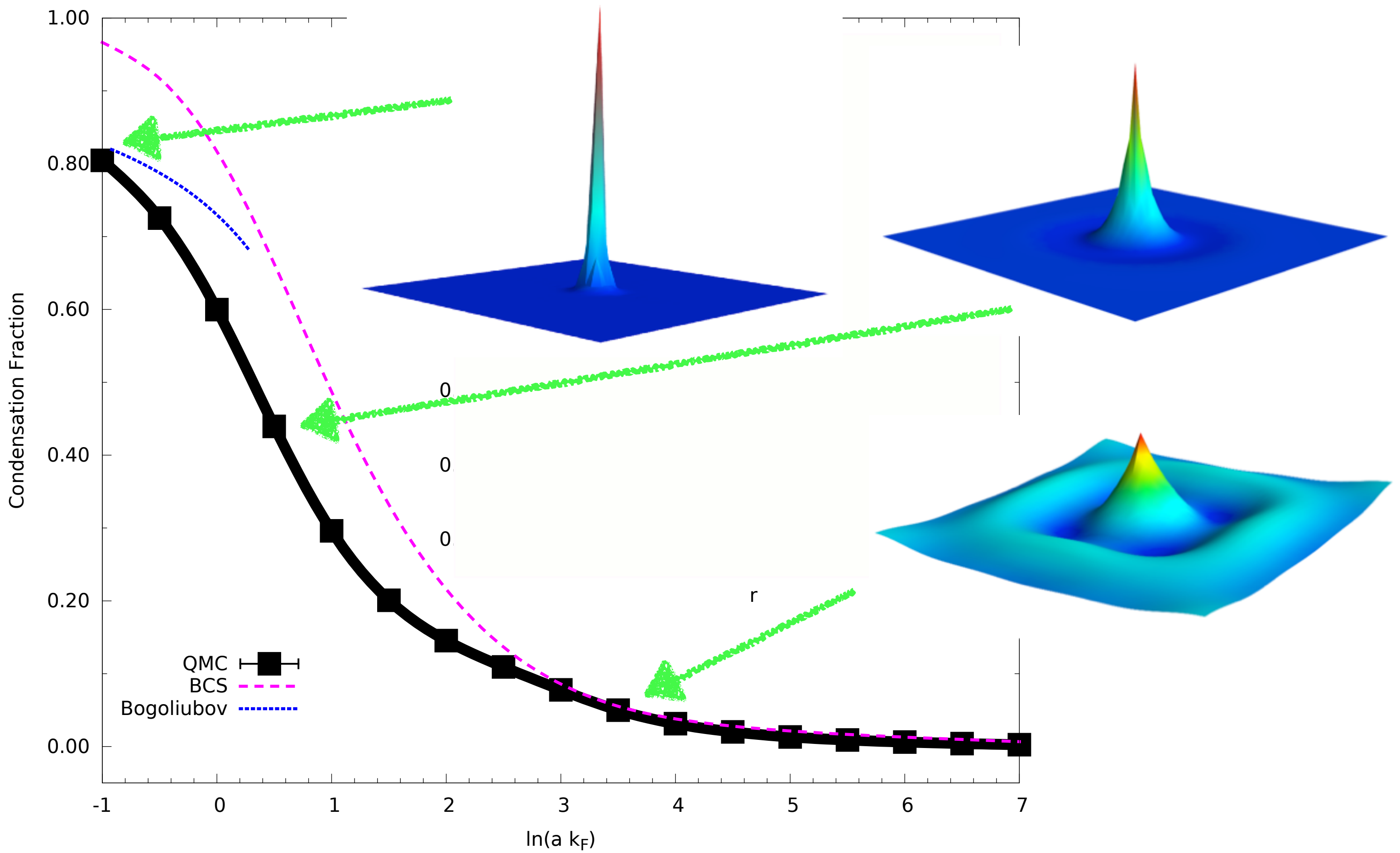

Shi, Chiesa, SZ, PRA '15

Ground-state properties, excitations, and response of the 2D Fermi gas

Shiwei Zhang
Flatiron Institute
and
College of William & Mary

Outline

- Introduction: 2D FG and a condensed matter perspective
- Auxiliary-field quantum Monte Carlo calculations - exact* here
- Results on spin-balanced system:
  - ground-state properties
  - pairing gaps, spectral information, response
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Pairing gap

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

Similarly for holes

quasi-particle dispersion

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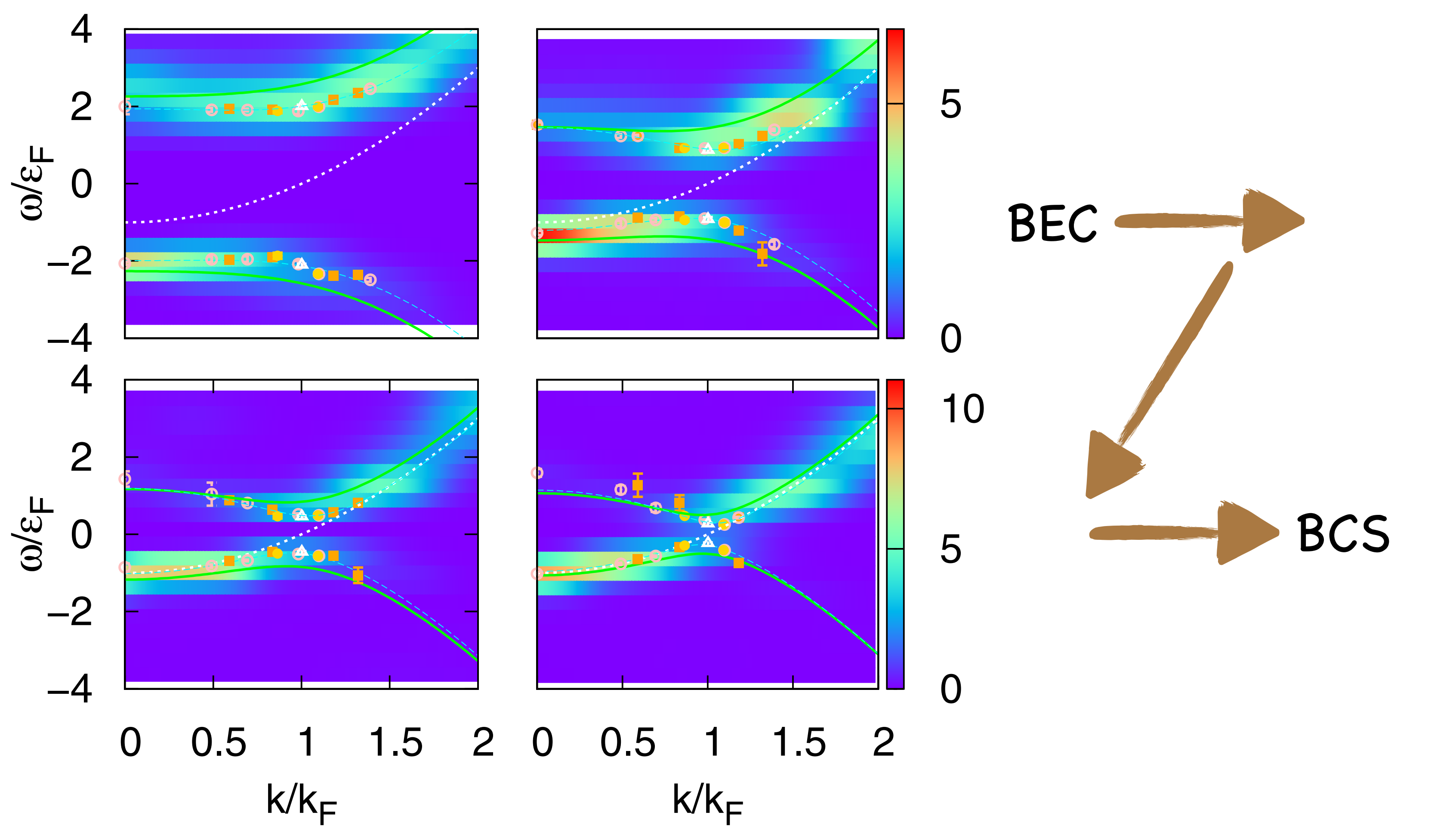

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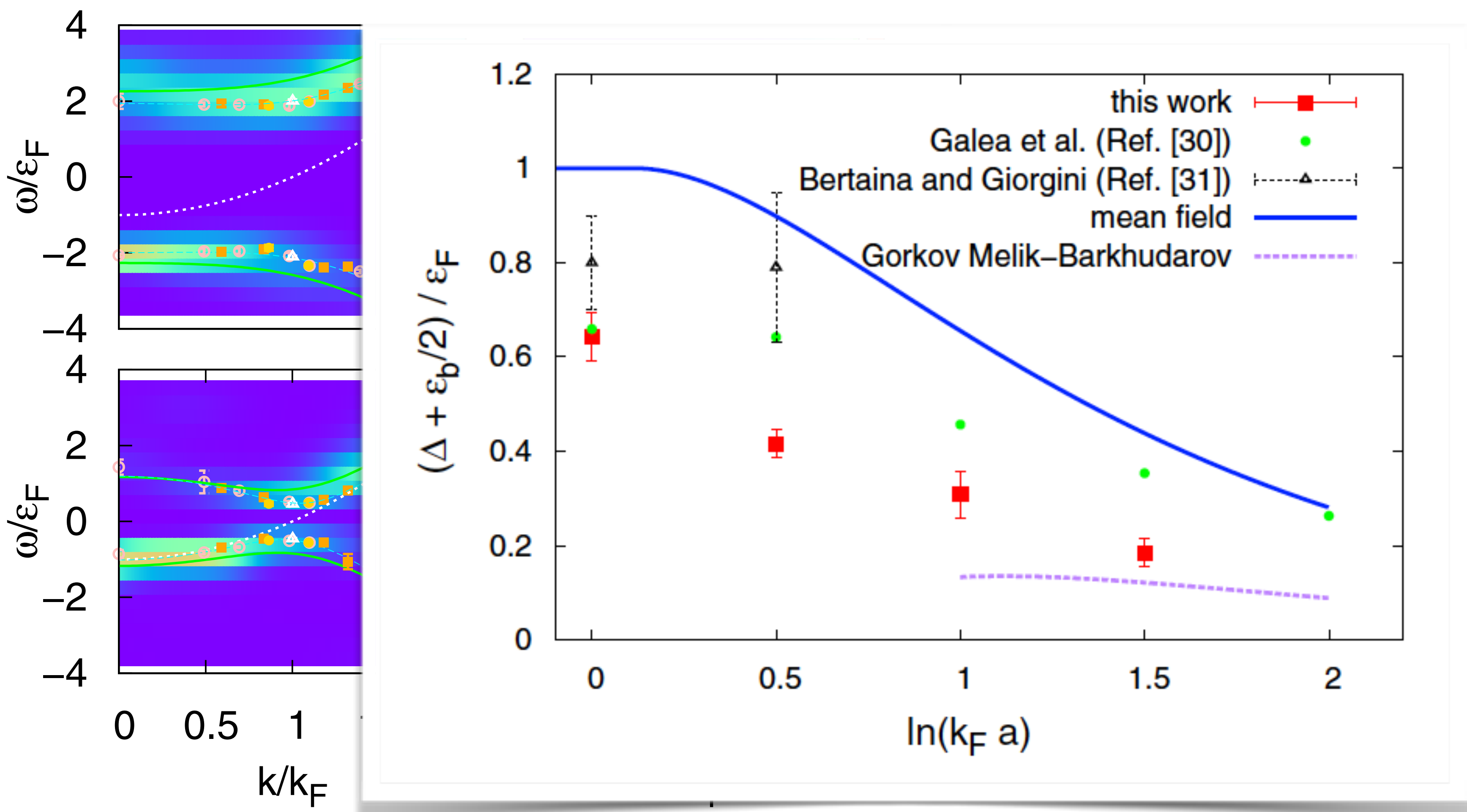

Response functions

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

can be measured by
scattering expt

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Analytic cont. *

"GIFT" (Vitali '10)

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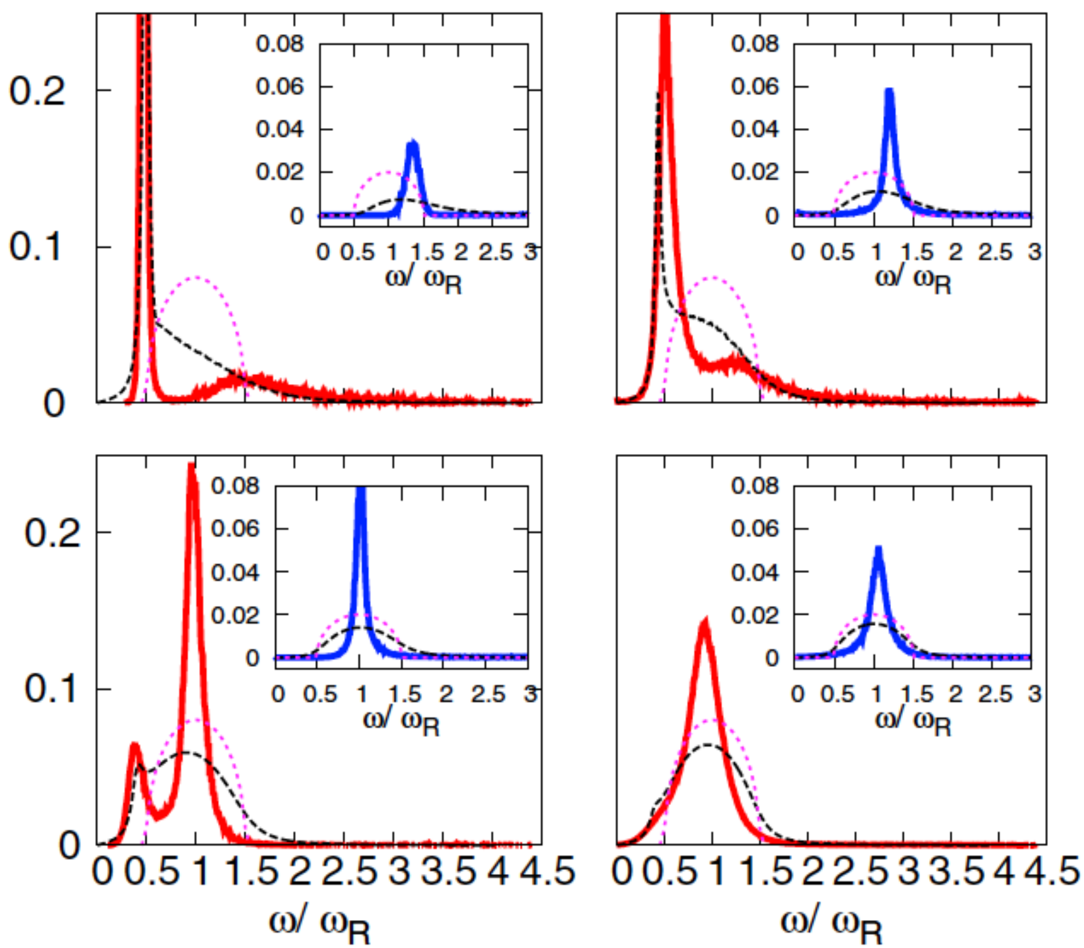

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- main: density
  inset: spin

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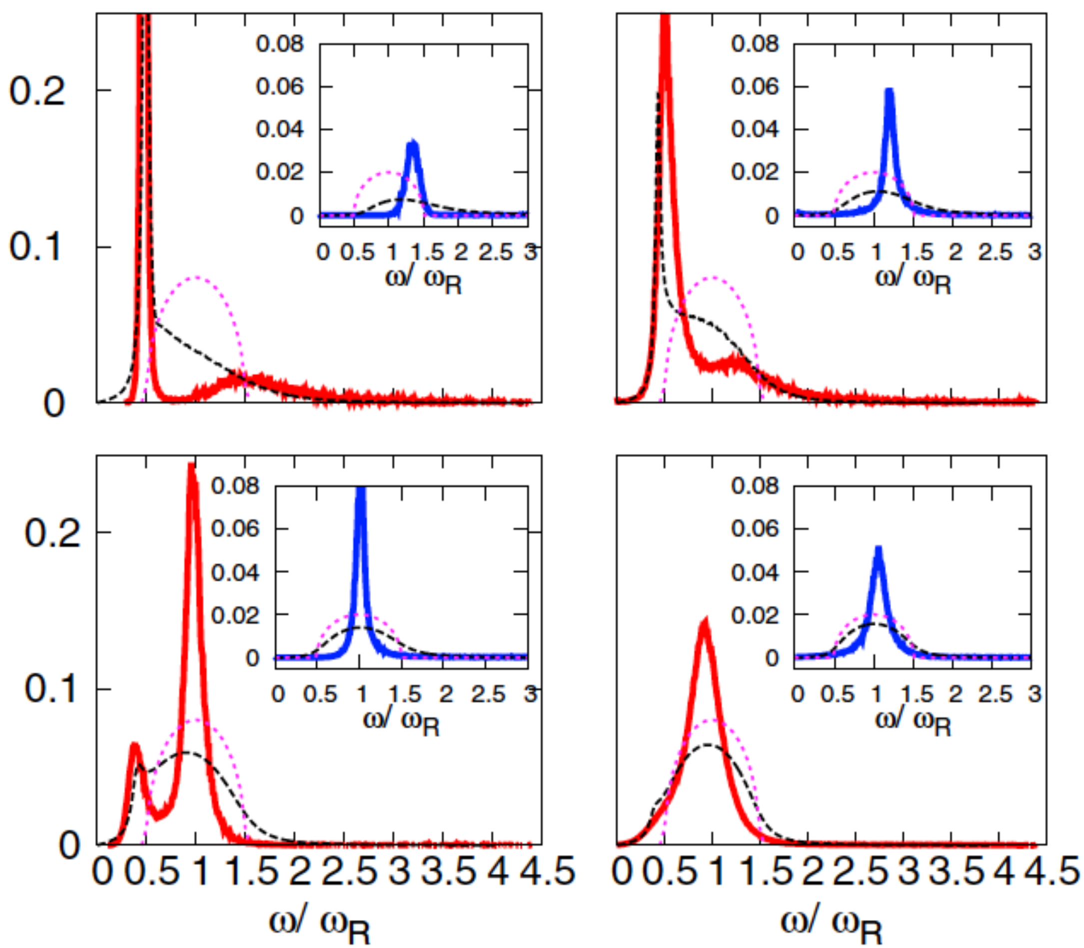

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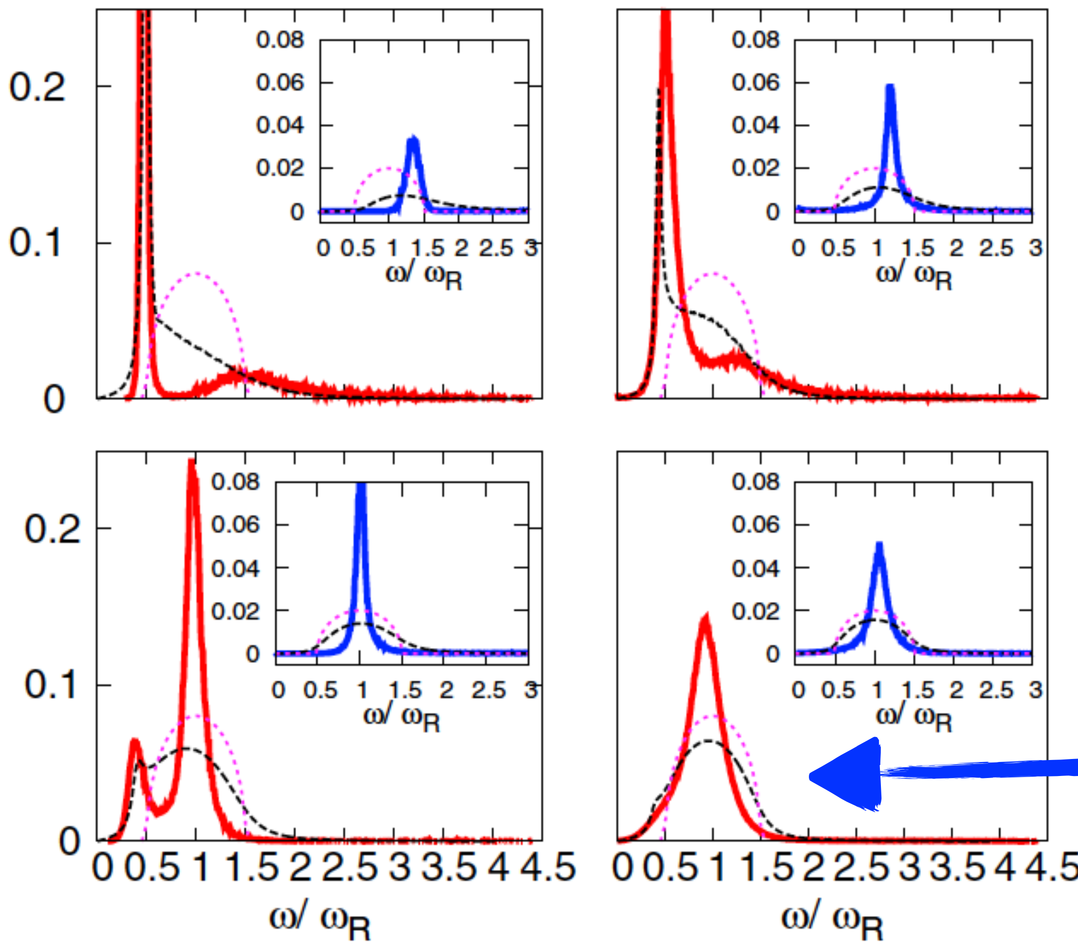

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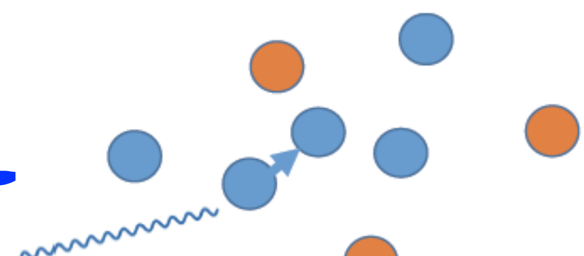

BCS

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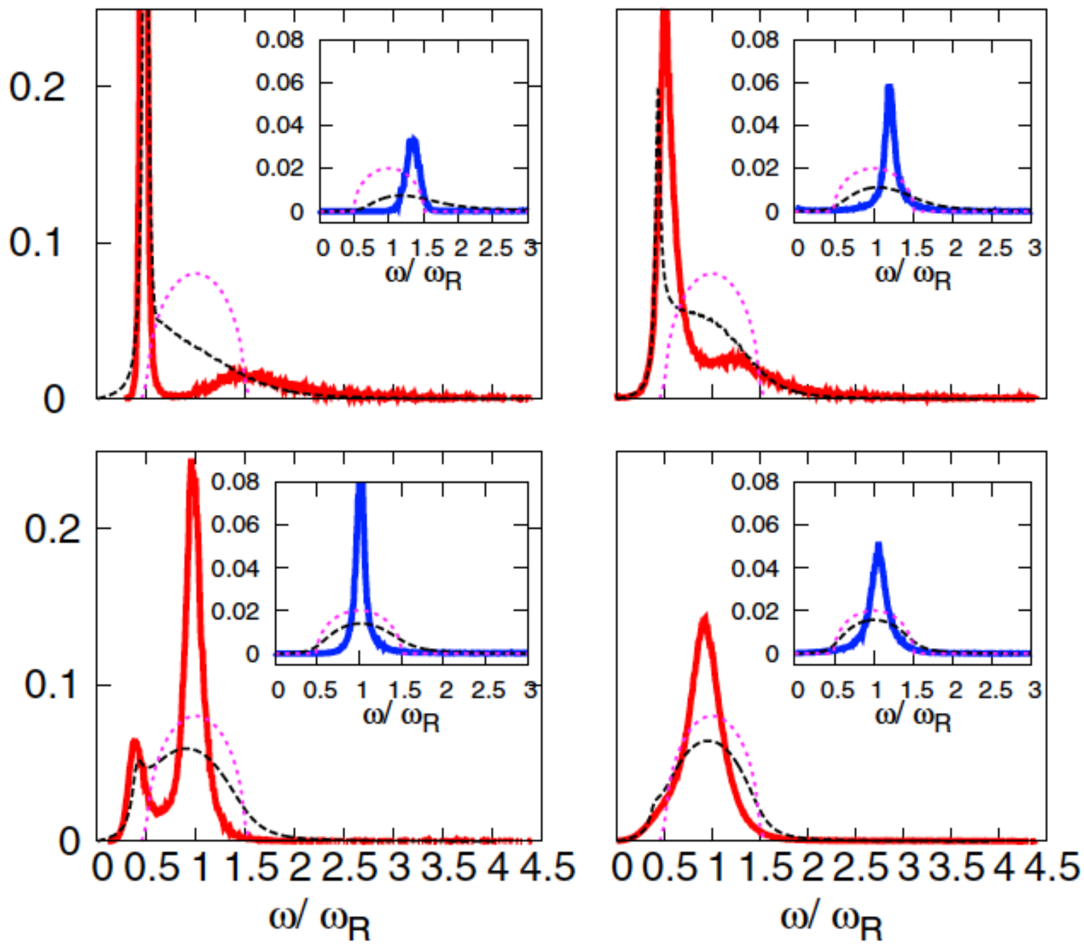

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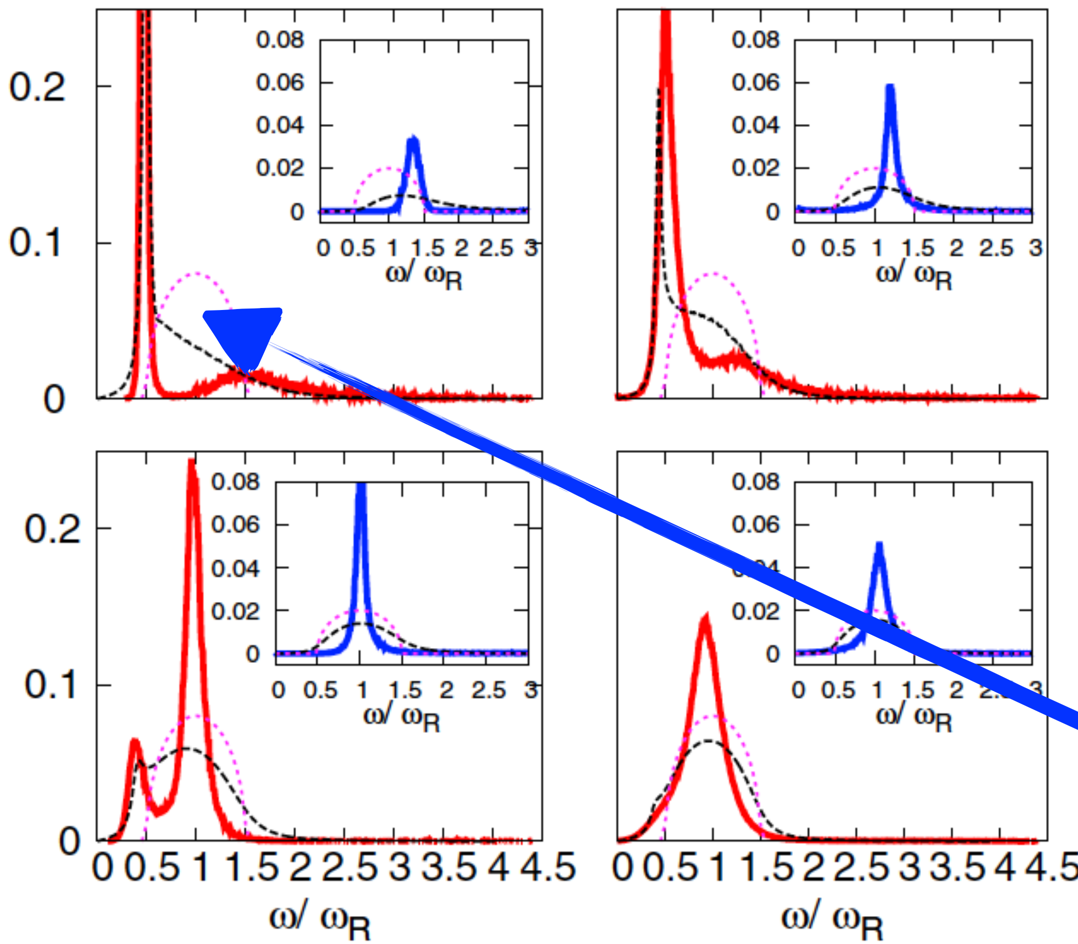

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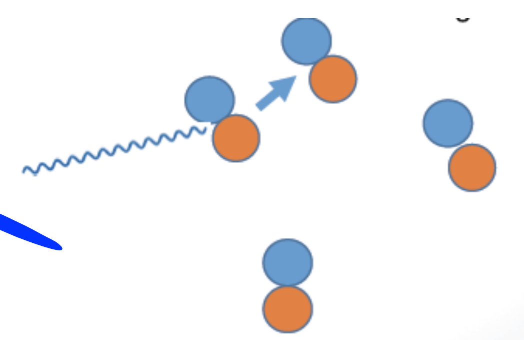

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Imaginary-time correlation under constraint

Test in repulsive Hubbard, sign problem (preliminary)

Equal-time quantities have been extensively benchmarked — high accuracy

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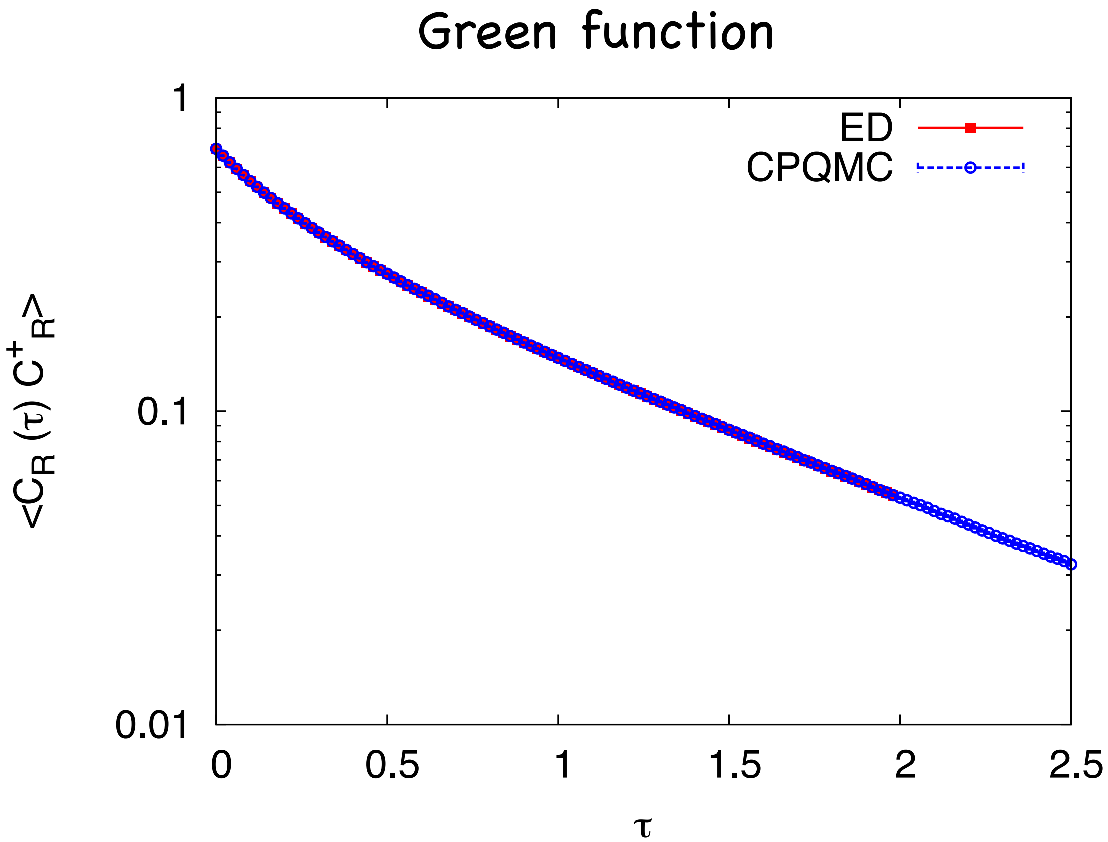

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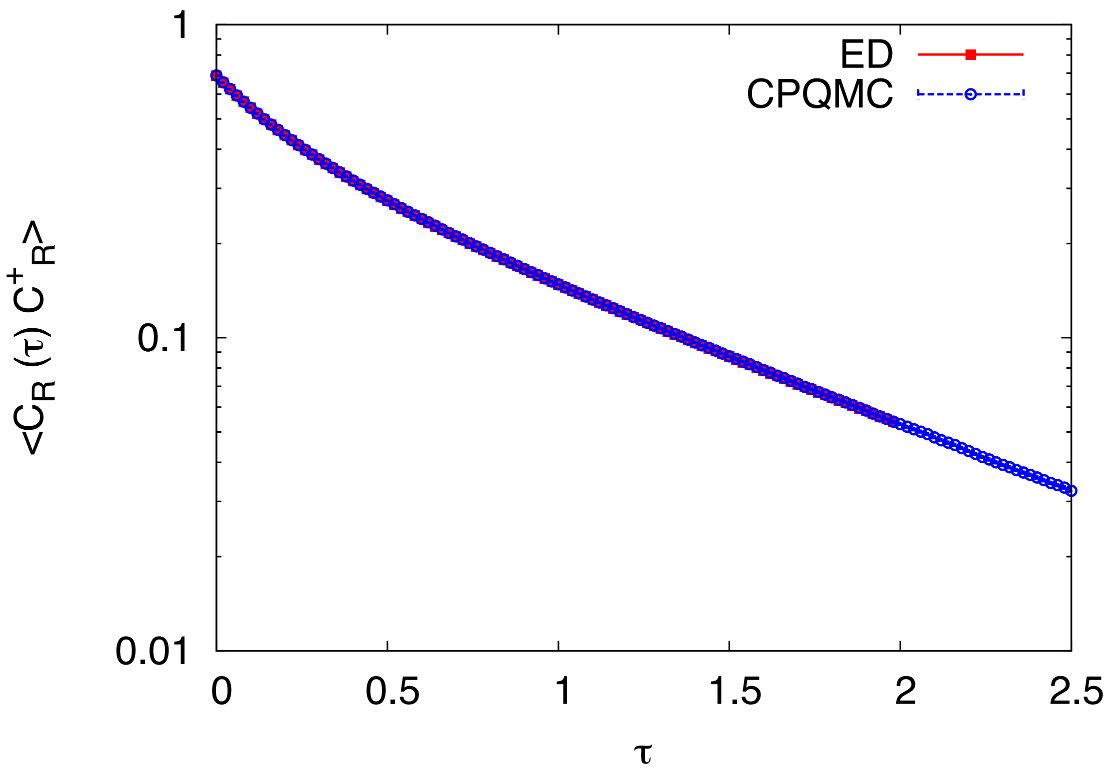

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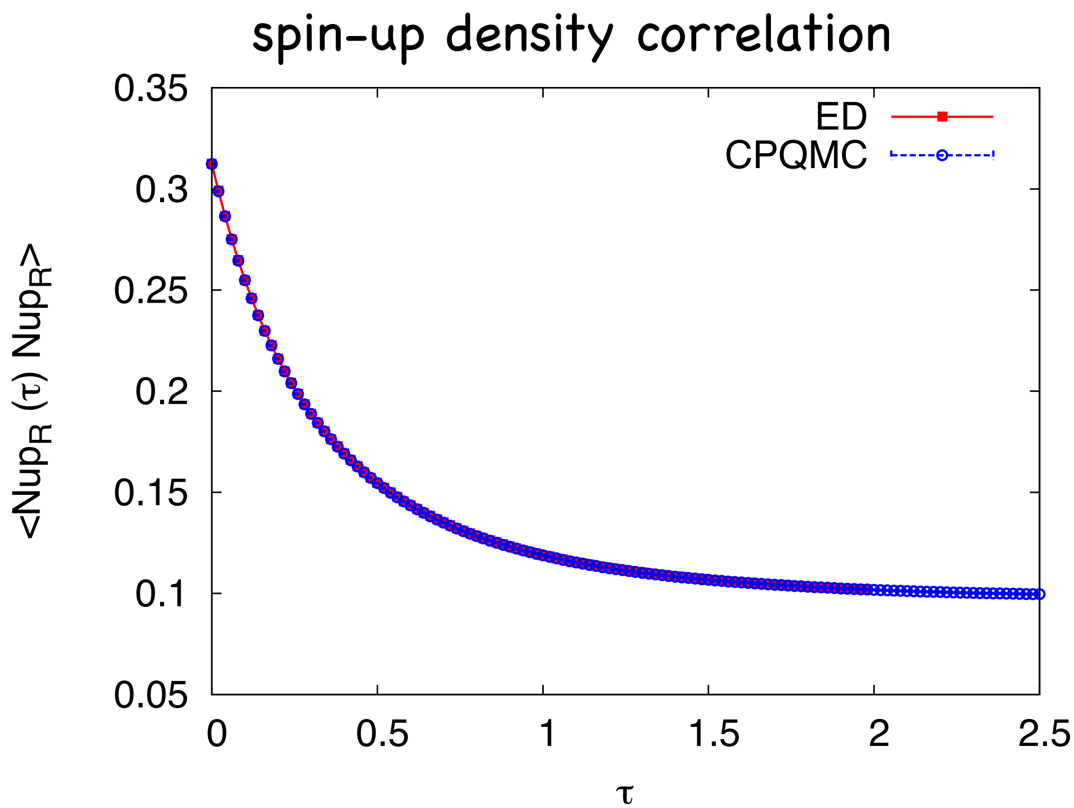

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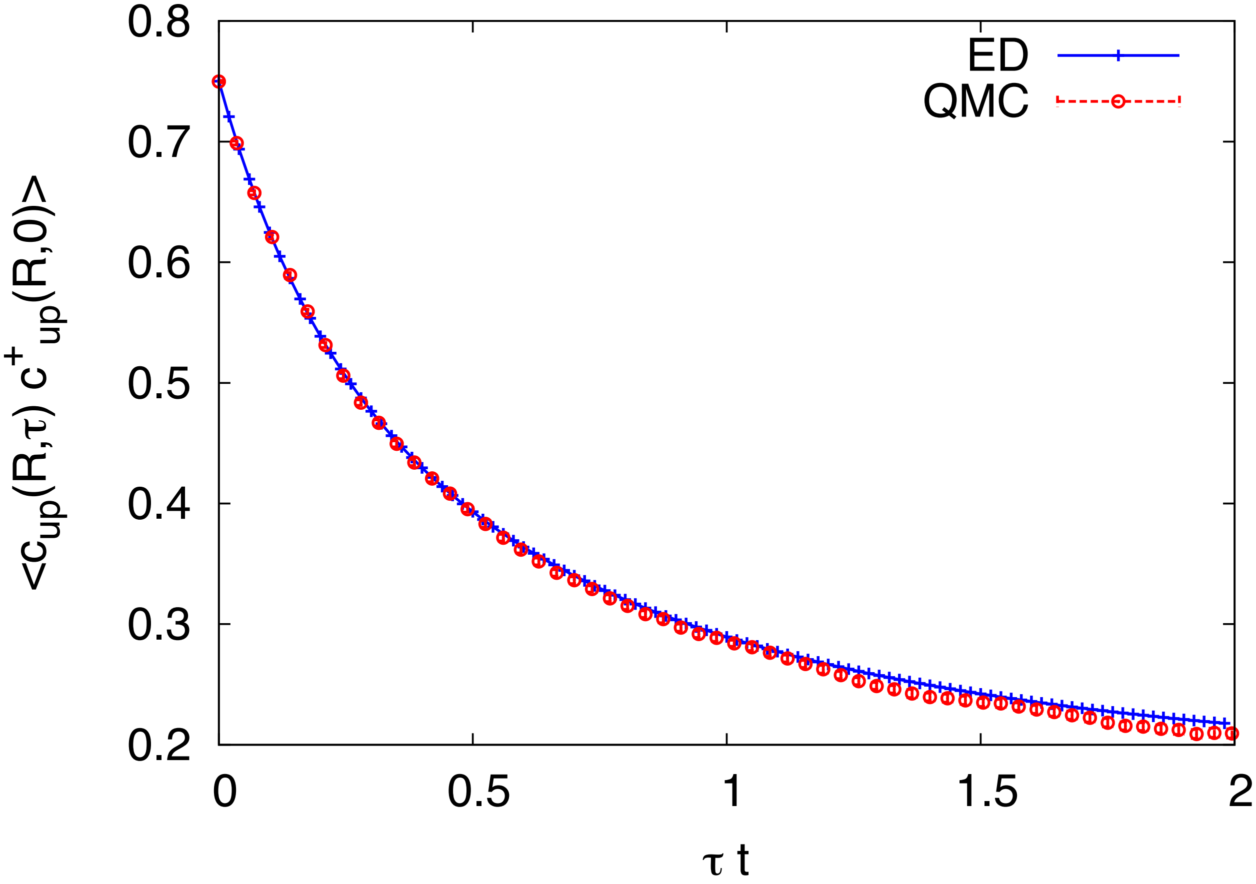

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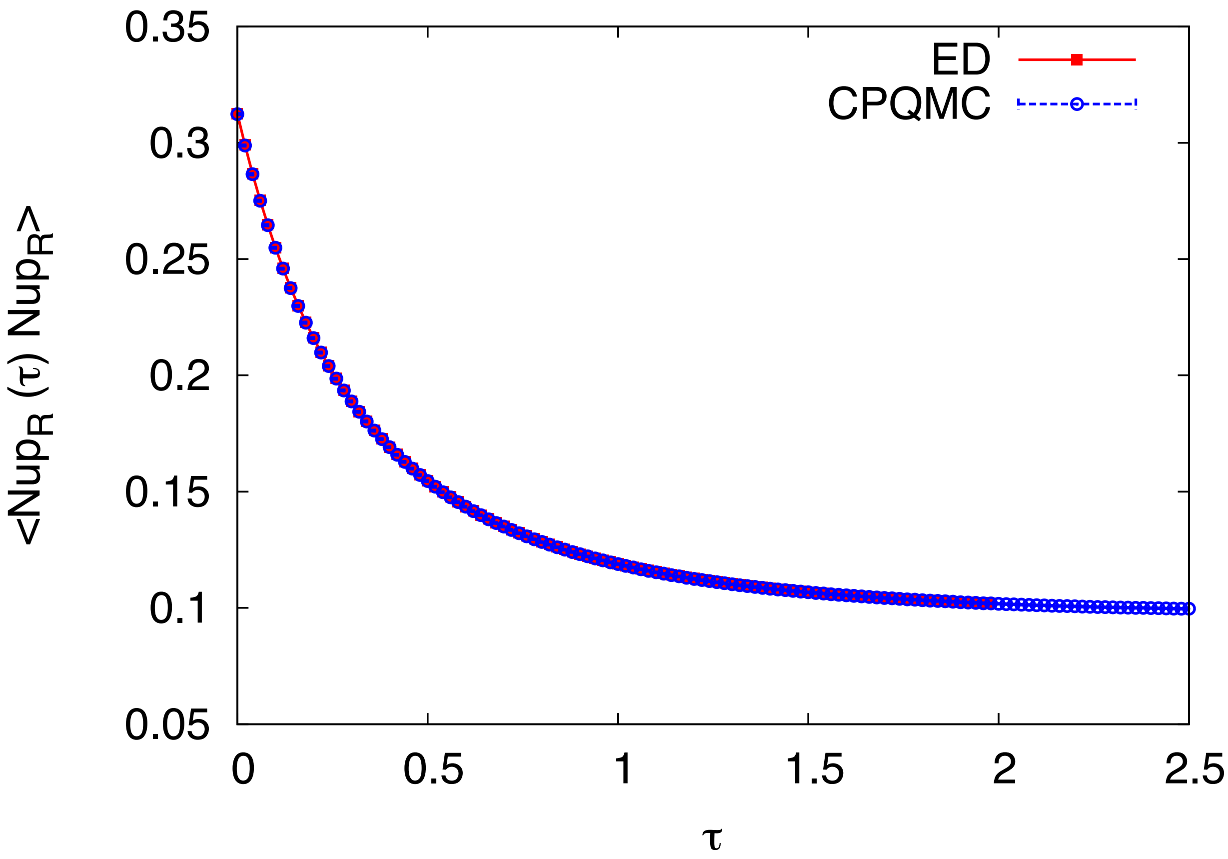

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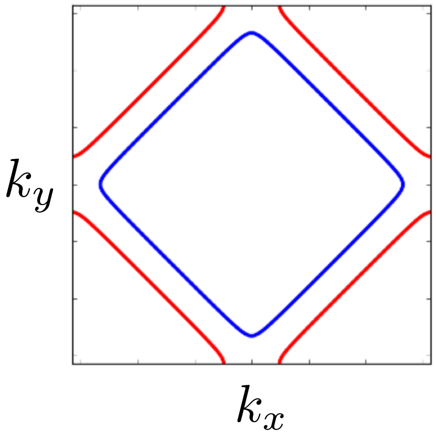
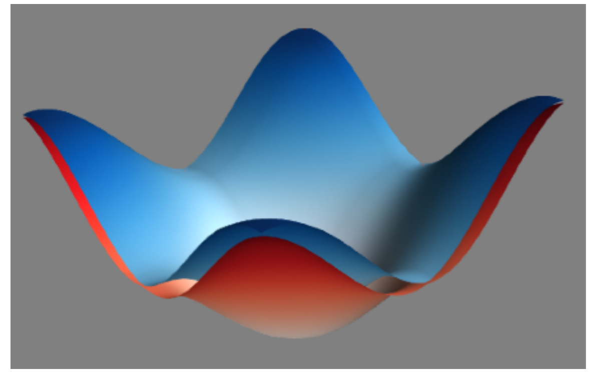
Rashbba SOC in 2D optical lattice

Hubbard dispersion, half-filling





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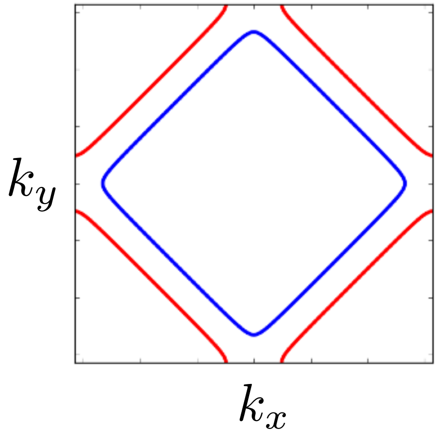

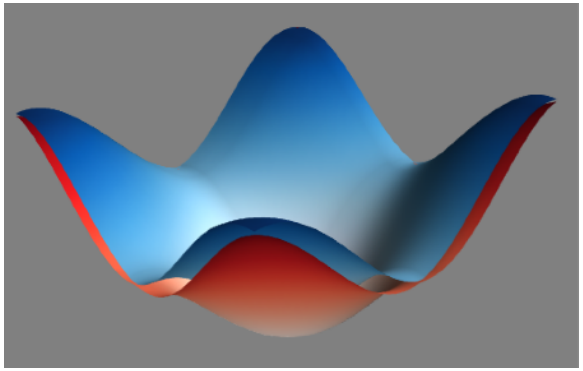

Attractive interaction, U<0

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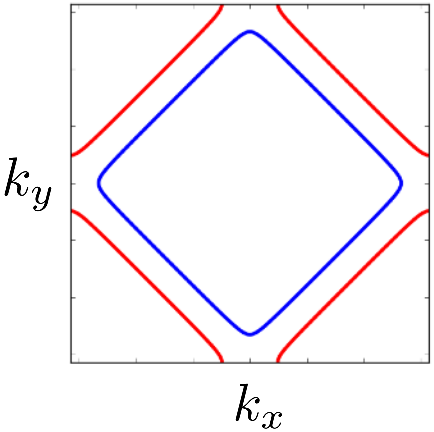

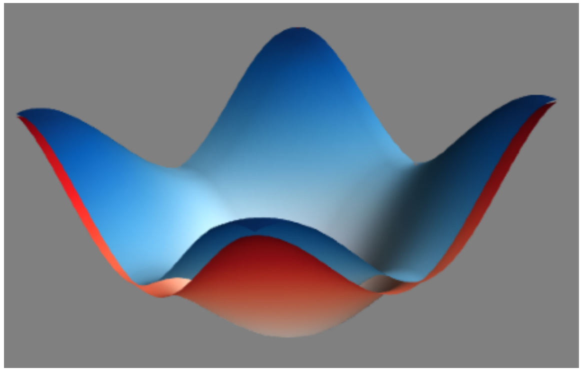

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Supersolid phase:

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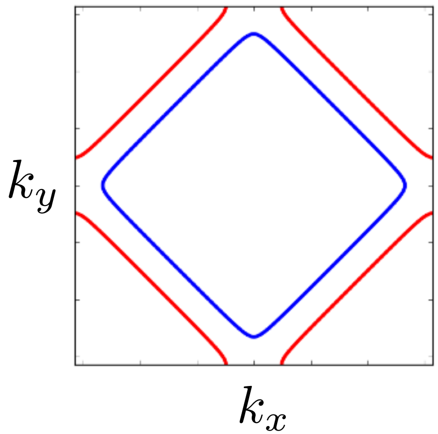

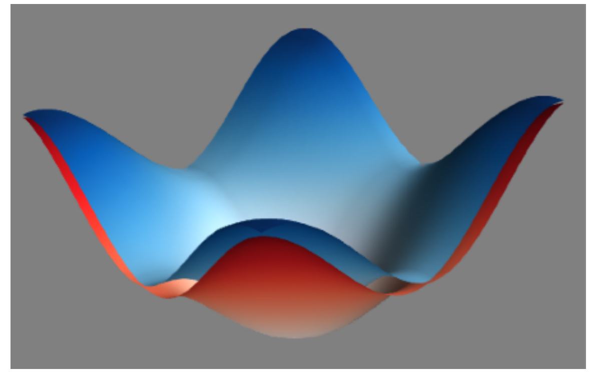

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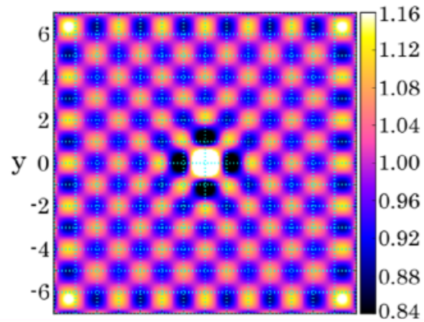
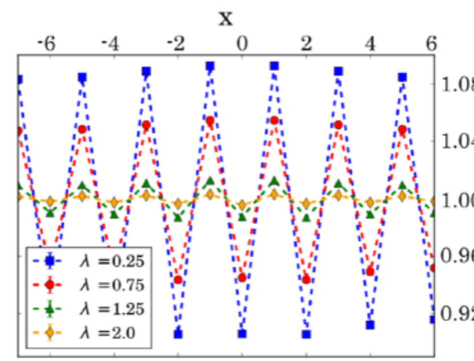
Supersolid phase:

- charge density wave





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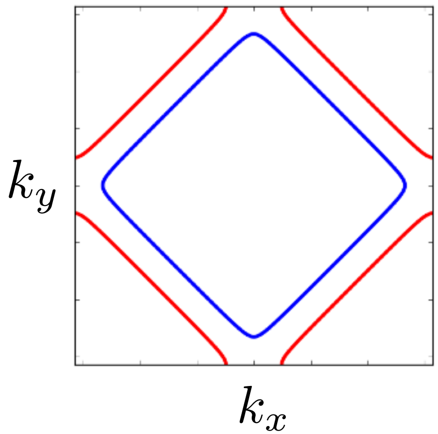

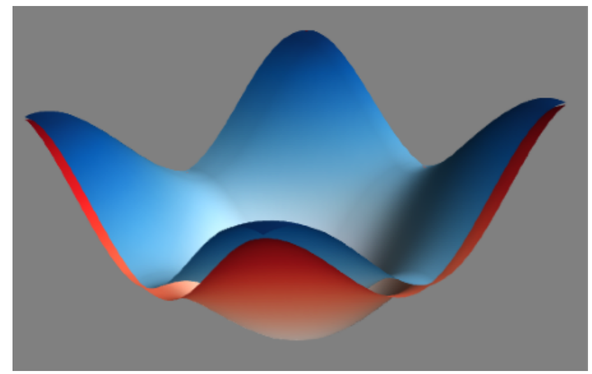

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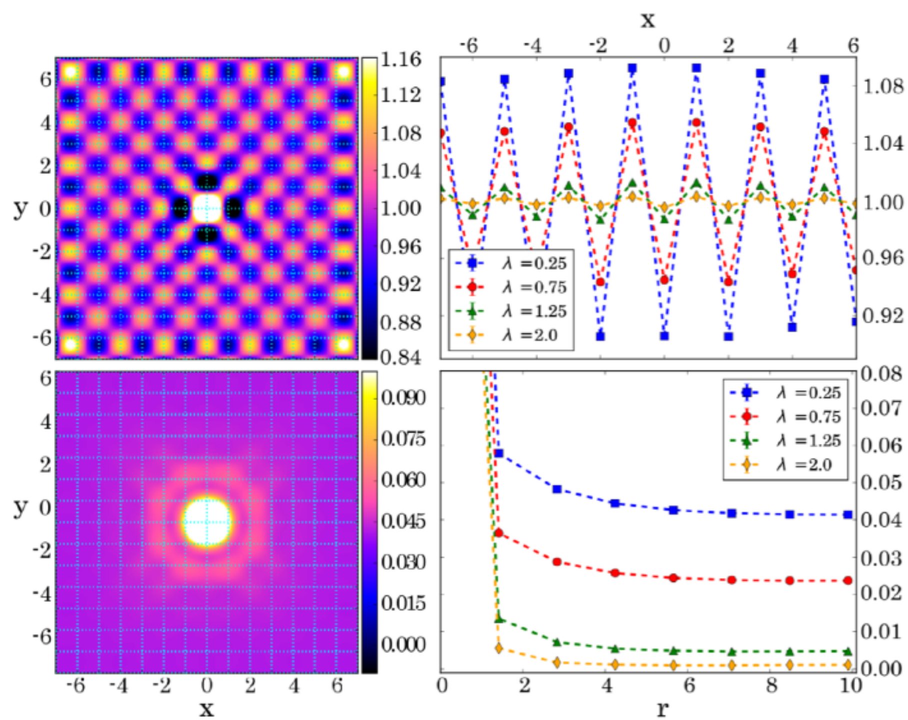
Supersolid phase:

- charge density wave
- superfluid order



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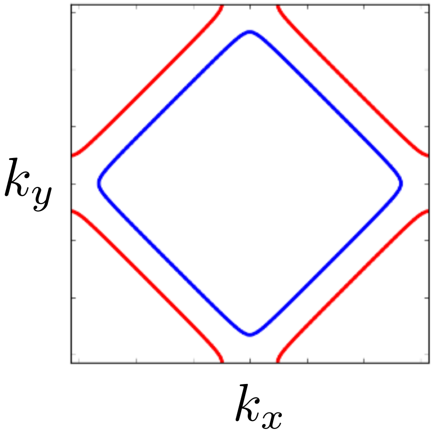

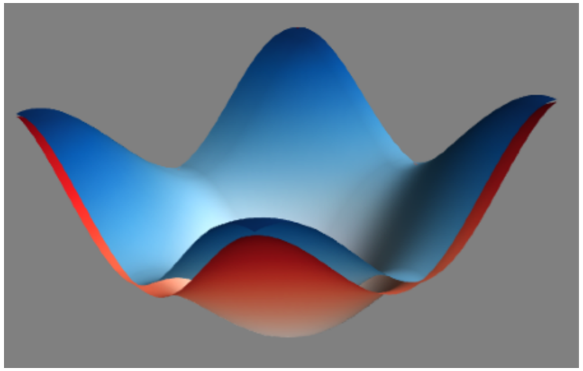

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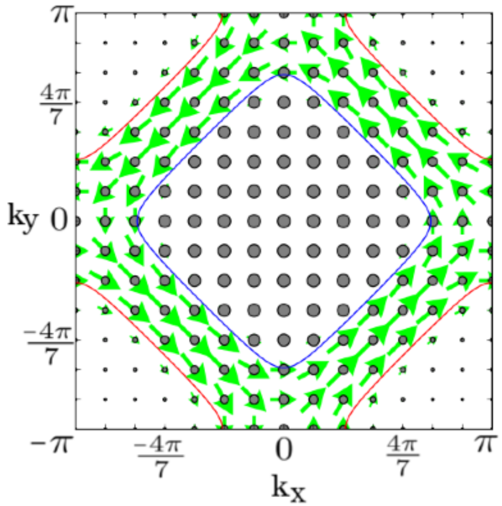

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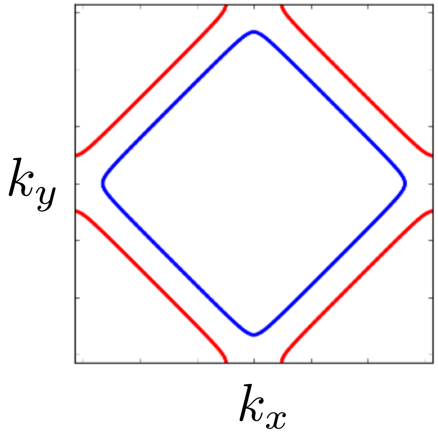

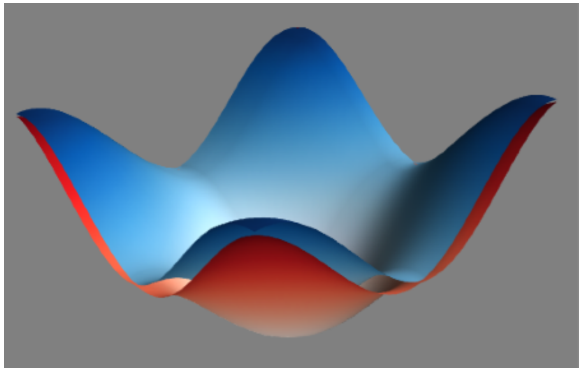

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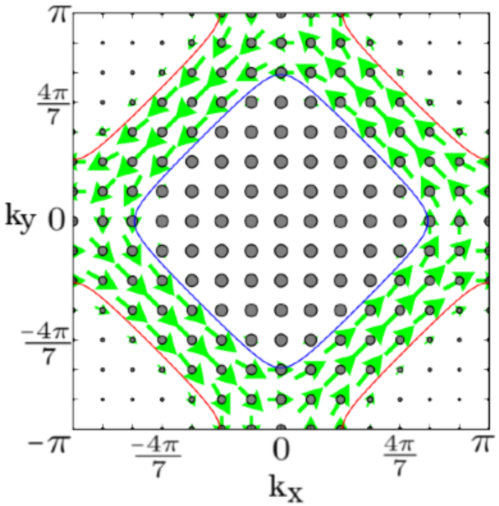
- n(k) - spin



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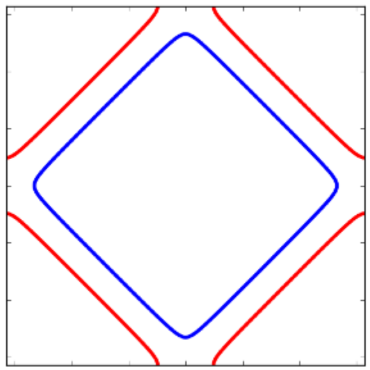

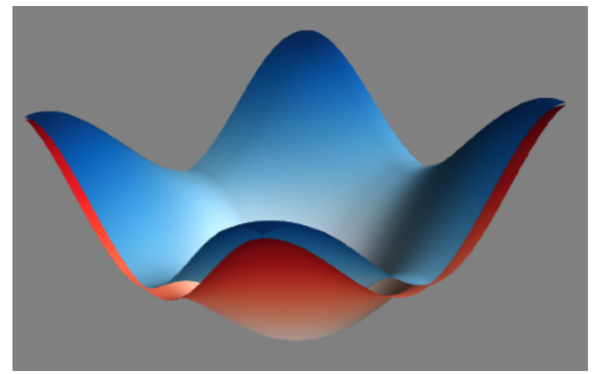

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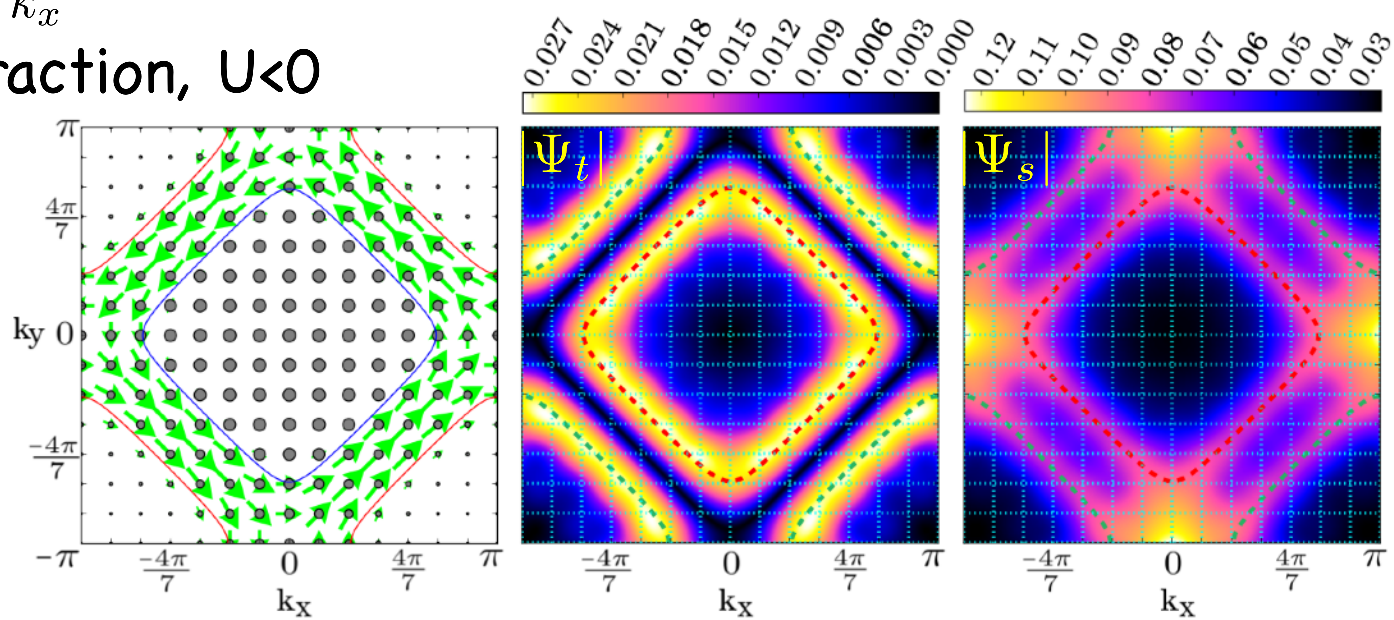
- n(k) - spin
- pairing wfs



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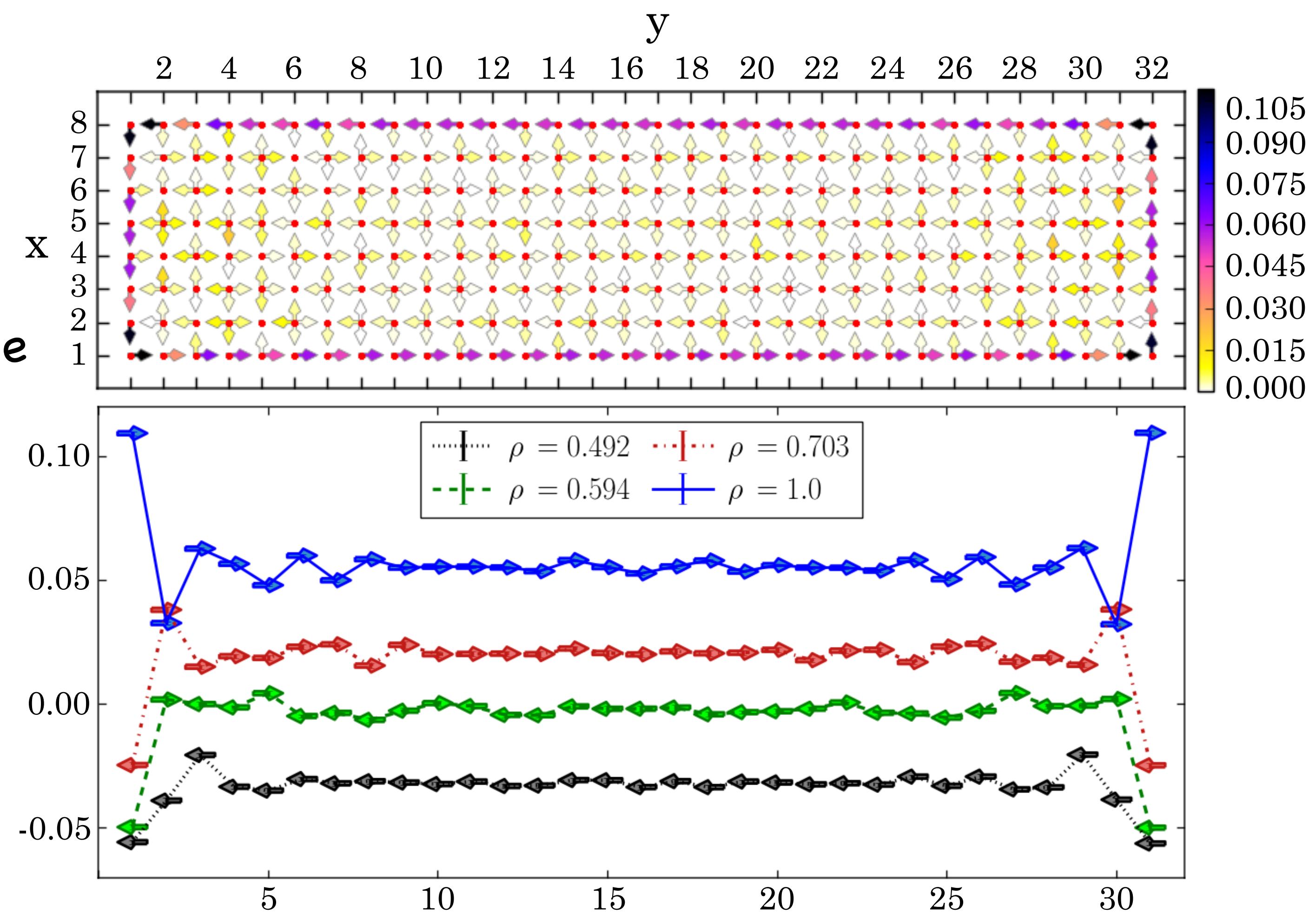
Rashbba SOC in 2D optical lattice

Edge currents:

$$\mathbf{j}_{nm\sigma} = -it(c^\dagger_{m\sigma}c_{n\sigma} - c^\dagger_{n\sigma}c_{m\sigma})$$

- Open BC here
- equal magnitude in opposite dir. for spins



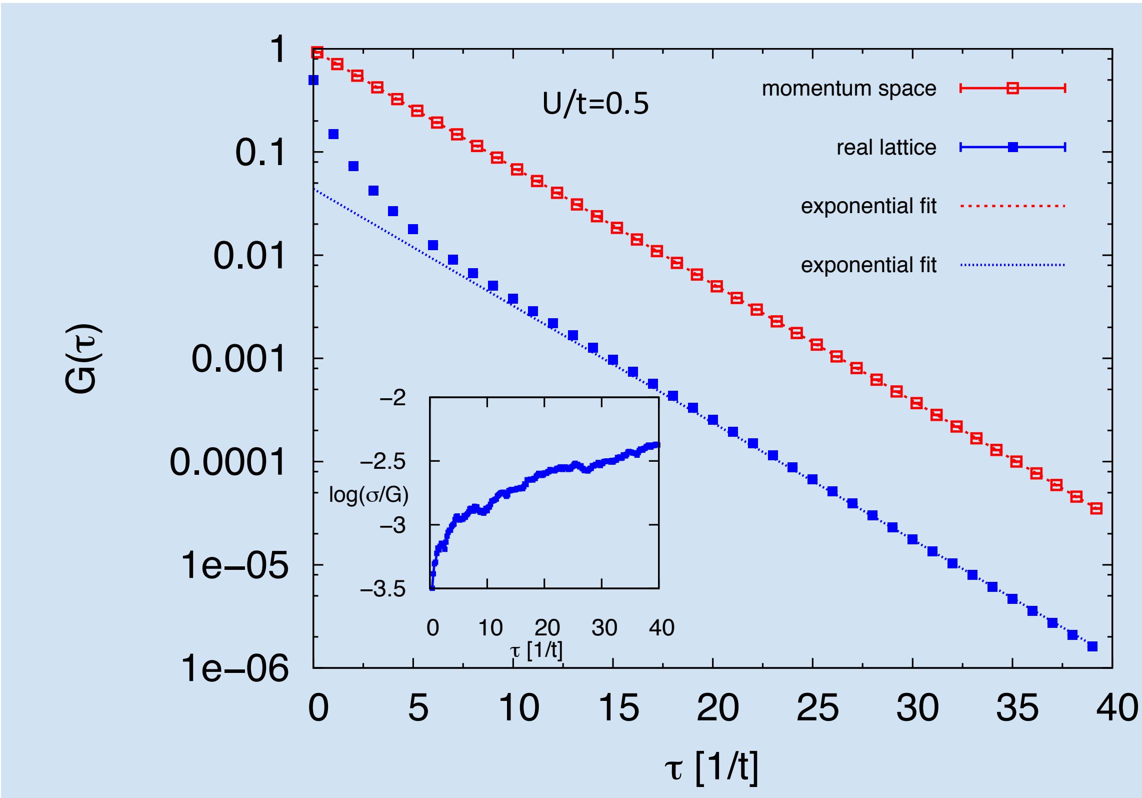
Rosenberg, Shi, SZ, PRL '17

Summary

- 2D Fermi gas
  - Clean & tunable; exciting new possibilities, especially useful to CM
- We use auxiliary-field QMC to carry out exact simulations in large systems (>120 particles, > 3000 sites, large beta)
  - Metropolis with force bias to accelerate sampling and improve acceptance ratio (Note standard deteminantal MC has infinite variance)
  - Method to compute gaps and imaginary-time correlations
- 2D: equation of state; n(k); pairing wf; cond frac. ..
- Pairing gaps, spectral info, and response (analytic cont)
- Rashba spin-orbit coupling in 2D optical lattice: super solid phase, singlet vs triplet pairing, topological signatures

Example: gaps from imaginary-time GFs

Example - charge gap in the Hubbard model at half-filling



- Gap is slope at large tau
- Can work with real-space or k-space GF
- k-space (k near FS) works better at low U

$$G(k,\tau) = \langle \Psi_0 | c_k e^{-\tau \hat{H}} c_k^\dagger | \Psi_0 \rangle$$

Vitali et al, PRB, '16