Auxiliary-field quantum Monte Carlo at zero- and finite-temperatures

Shiwei Zhang

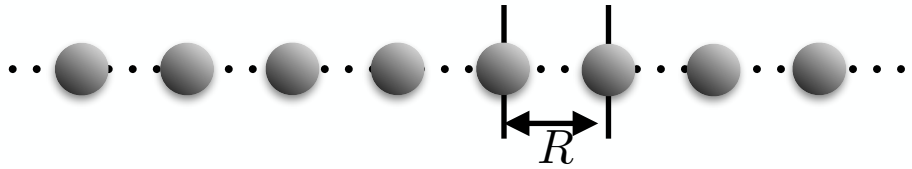
Flatiron Institute, New York

College of William & Mary, Virginia

Homework Assignment

The Hydrogen chain can be a playground that ties together much of what we've learned in this school.

Apply your favorite approach to compute/understand some aspect of the physics of the Hydrogen chain.



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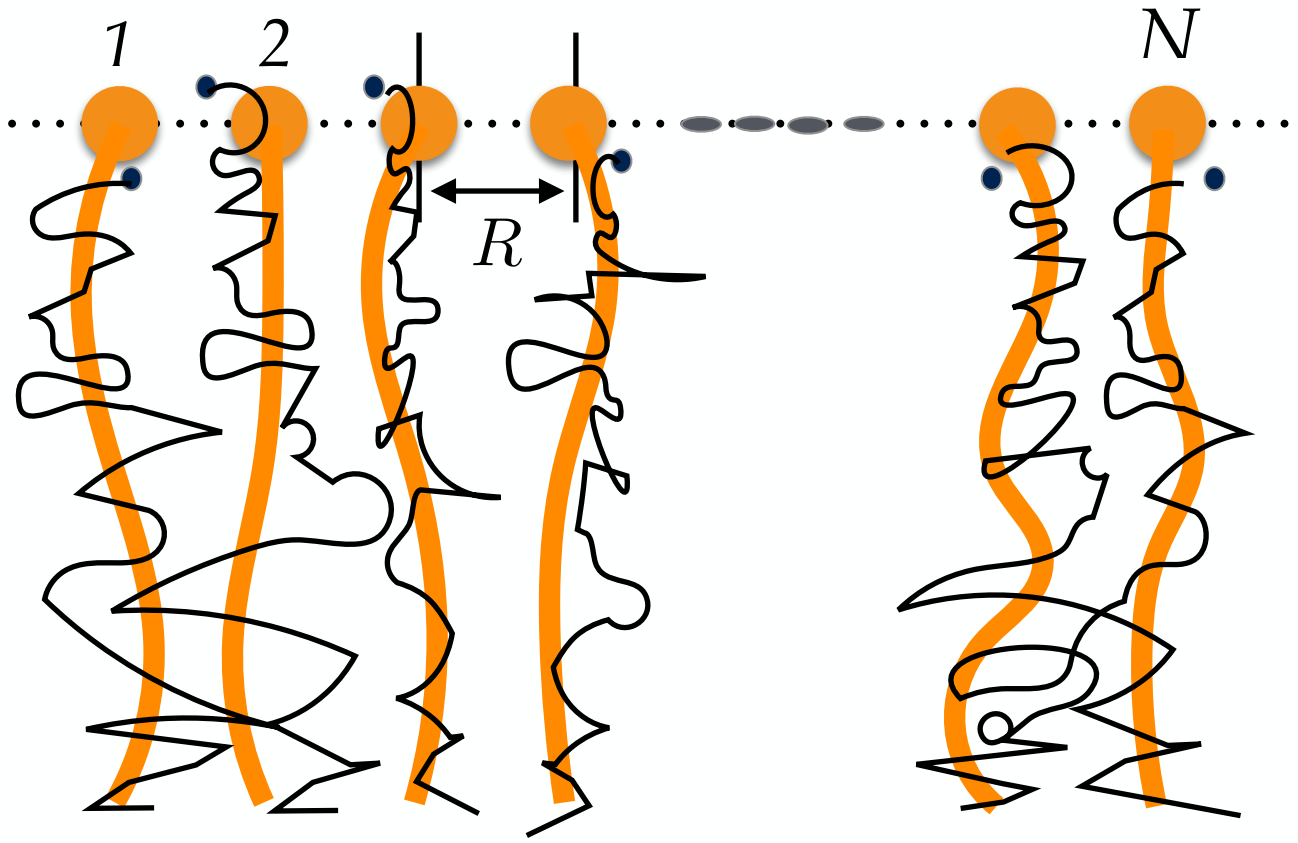
Outline

- Introduction (aka context of HW) - look for overlaps w/ other lects!
- Brief reminder of Monte Carlo
- AFQMC framework, T=0K
  - Many-body ground state as ensembles of entangled DFT solutions
- Finite-T AFQMC - use to introduce sign problem and exact gauge conditions to control it, followed by approximate implementation
- Example of ab initio calculations in solids and quantum chemistry

Inside a materials computation

Hydrogen chain as an illustration:

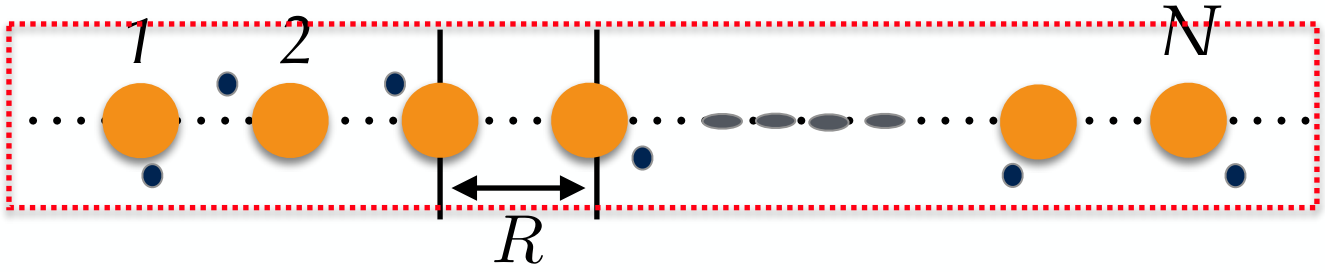
With time:



Electrons respond quickly

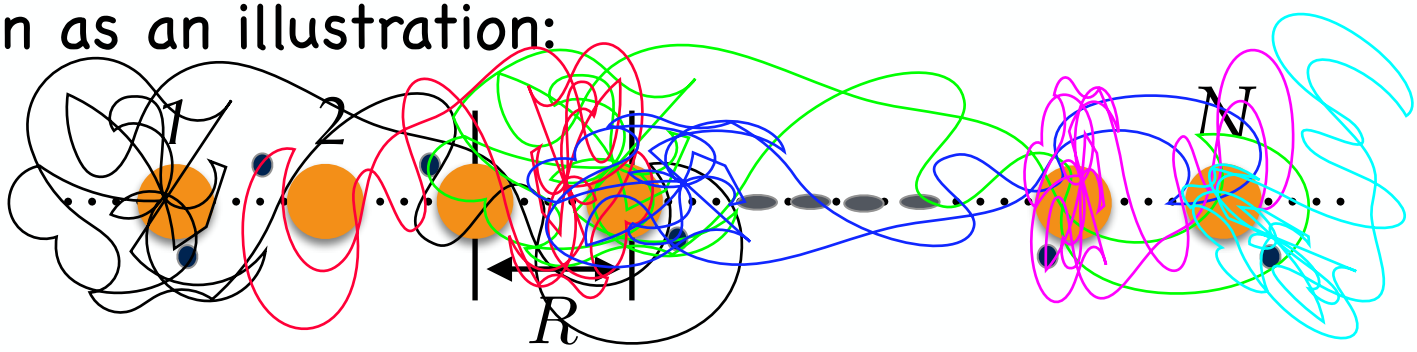
Inside a materials computation

Hydrogen chain as an illustration:



Inside a materials computation

Hydrogen chain as an illustration:



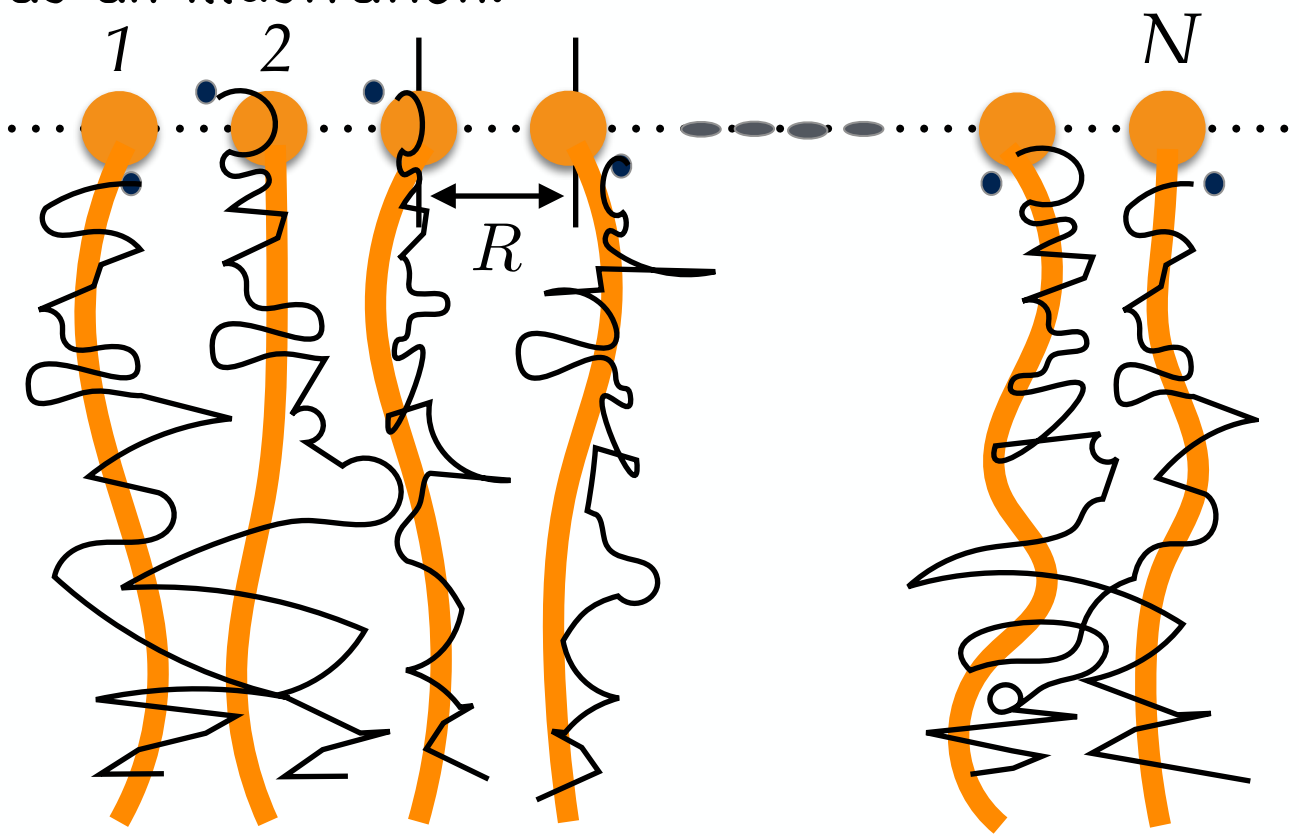
Born-Oppenheimer - for fixed nuclear positions

- Electrons respond instantaneously
- Path integrals - infinite length (imaginary time) for most materials
- Precisely how -> many materials properties
- Electron density distribution -> inter-atomic force for atomic motion

Inside a materials computation

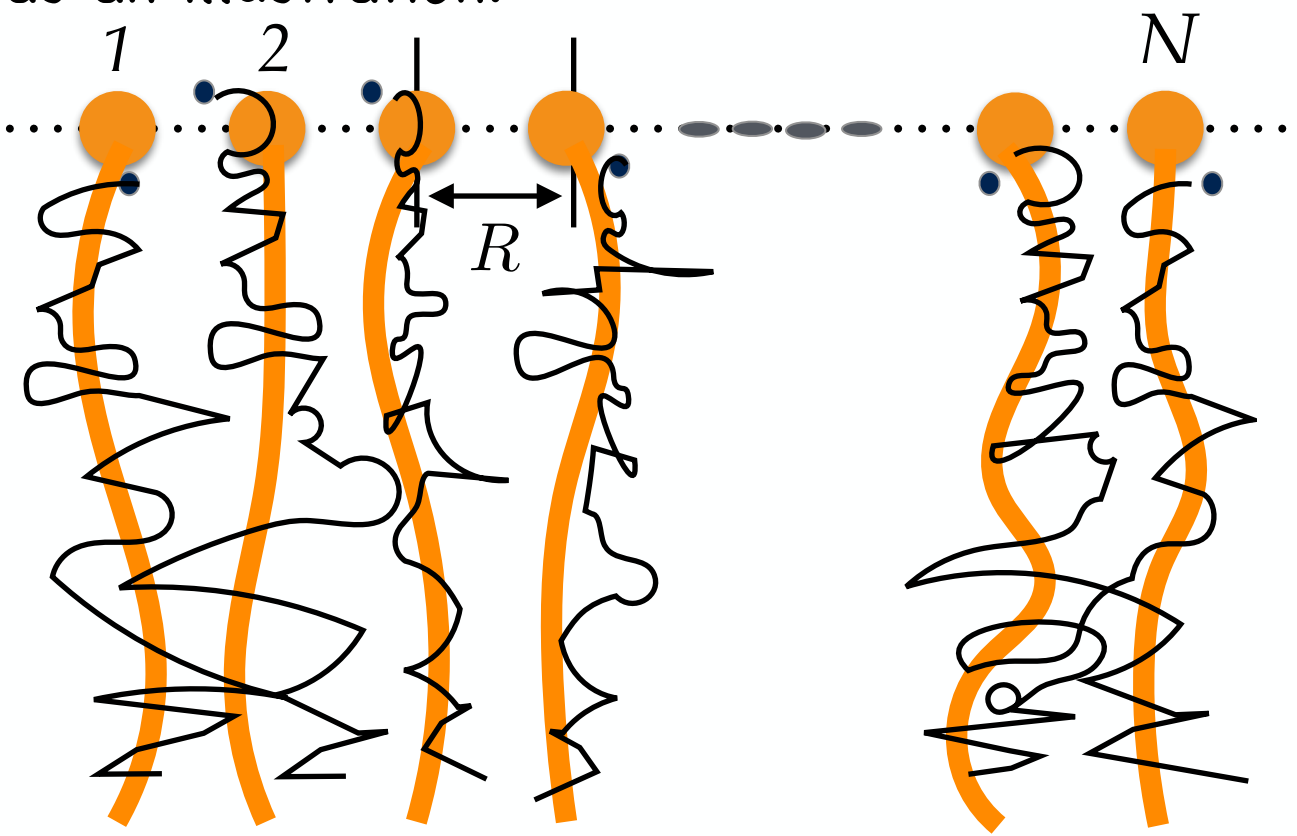
Hydrogen chain as an illustration:

With 'time':



Inside a materials computation

Hydrogen chain as an illustration:



With 'time':

Like stat. mech. ! Formulate as molecular dynamics or MC?

- Path is for wave function, not density
- Pauli – paths have complicated signs from fermion exchange
- Hilbert space exponentially large – natural to use sampling

The Hydrogen benchmark project

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

Mario Motta,[1] David M. Ceperley,[2] Garnet Kin-Lic Chan,[3] John A. Gomez,[4] Emanuel Gull,[5] Sheng Guo,[3] Carlos Jimenez-Hoyos,[3] Tran Nguyen Lan,[6,5,7] Jia Li,[5] Fengjie Ma,[8] Andrew J. Millis,[9] Nikolay V. Prokof'ev,[10,11] Ushnish Ray,[3] Gustavo E. Scuseria,[4,12] Sandro Sorella,[13,14] Edwin M. Stoudenmire,[15] Qiming Sun,[3] Igor S. Tupitsyn,[10,11] Steven R. White,[15] Dominika Zgid,[6] and Shiwei Zhang[1,*]

(The Simons Collaboration on the Many-Electron Problem)

[1] *Department of Physics, College of William and Mary, Williamsburg, VA 23187, USA*
[2] *Department of Physics, University of Illinois at Urbana-Champaign, Champaign, IL 61801, USA*
[3] *Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA 91125, USA*
[4] *Department of Chemistry, Rice University, Houston, TX 77005, USA*
[5] *Department of Physics, University of Michigan, Ann Arbor, MI 48109, USA*
[6] *Department of Chemistry, University of Michigan, Ann Arbor, MI 48109, USA*
[7] *On leave from: Ho Chi Minh City Institute of Physics, VAST, Ho Chi Minh City, Vietnam*
[8] *Department of Physics, Beijing Normal University, Beijing, Beijing 100875, China*
[9] *Department of Physics, Columbia University, New York, NY 10027, USA*
[10] *Department of Physics, University of Massachusetts, Amherst, MA 01003, USA*
[11] *National Research Center "Kurchatov Institute", 123182 Moscow, Russia*
[12] *Department of Physics and Astronomy, Rice University, Houston, TX 77005, USA*
[13] *SISSA – International School for Advanced Studies, Via Bonomea 265, 34136 Trieste, Italy*
[14] *Democritos Simulation Center CNR–IOM Istituto Officina dei Materiali, Via Bonomea 265, 34136 Trieste, Italy*
[15] *Department of Physics and Astronomy, University of California, Irvine, CA 92697-4575 USA*

(Dated: May 1, 2017)

PRX (2017)

The Hydrogen benchmark project

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- 10 groups, 21 authors; > a dozen many-body methods
- Following Hubbard model benchmark (PRX '15), move towards real materials:
  - long-range Coulomb interaction
  - reach complete basis set (continuous space) limit
  - thermodynamic limit

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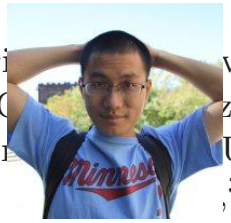
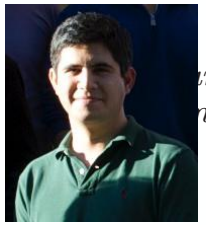








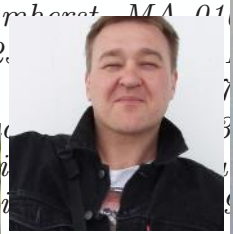








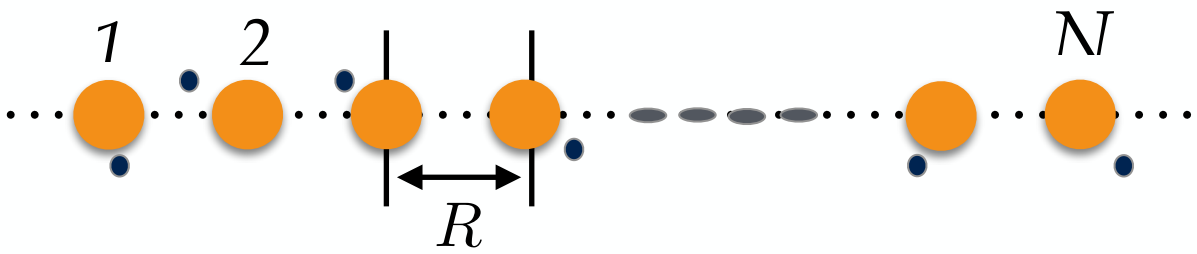





PRX (2017)

The problem: hydrogen chain

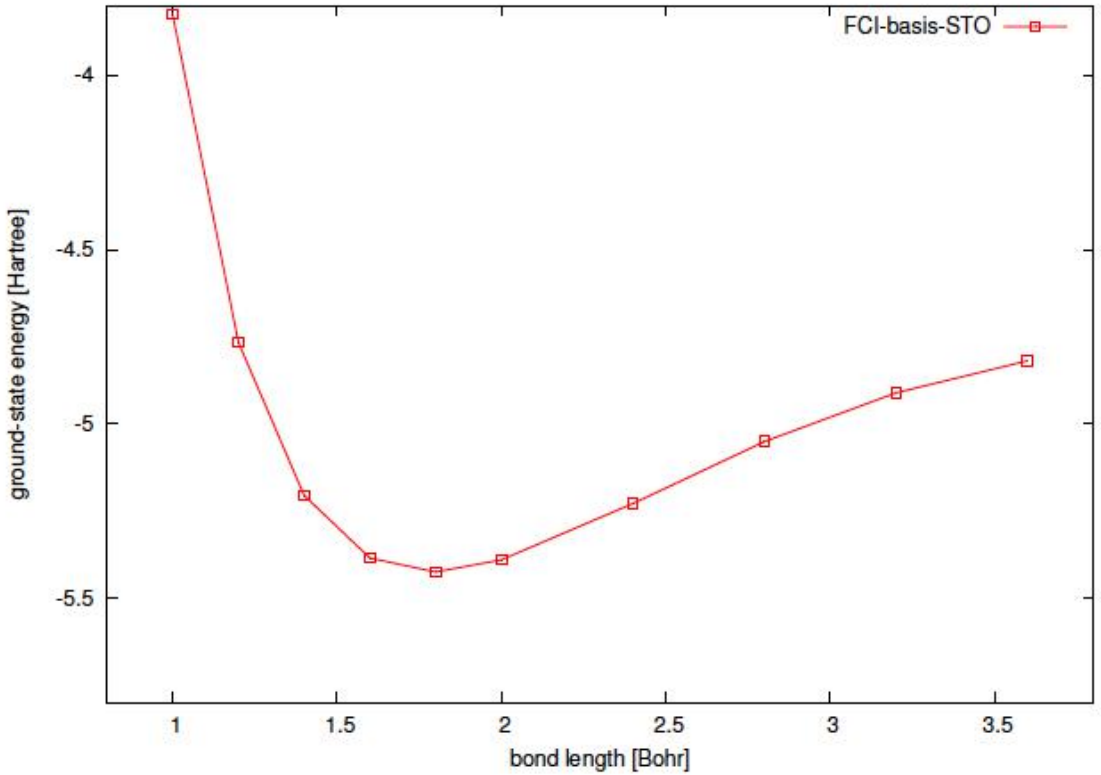
Stretching bonds in H_N:



stretch each bond symmetrically

Born-Oppenheimer

Equation of state (EOS)



The Hamiltonian

- Methods that work in continuous coordinate space
  - DFT (effectively)
  - diffusion Monte Carlo (DMC), VMC

$$H = H_{1-\text{body}} + H_{2-\text{body}} = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2 + \sum_{i=1}^{N} V_{\text{ext}}(\mathbf{r}_i) + \sum_{i<j}^{N} V_{\text{int}}(|\mathbf{r}_i - \mathbf{r}_j|)$$

- Methods that work in a single-particle basis:
  - All QChem methods
  - auxiliary-field QMC (AFQMC)
  - DMRG
  - embedding methods (DMET, SEET)
  - diagrammatic MC; sc-GW

$$\hat{H} = \hat{H}_1 + \hat{H}_2 = \sum_{i,j}^{M} T_{ij}\, c_j^\dagger c_j + \sum_{i,j,k,l}^{M} V_{ijkl} c_i^\dagger c_j^\dagger c_k c_l$$

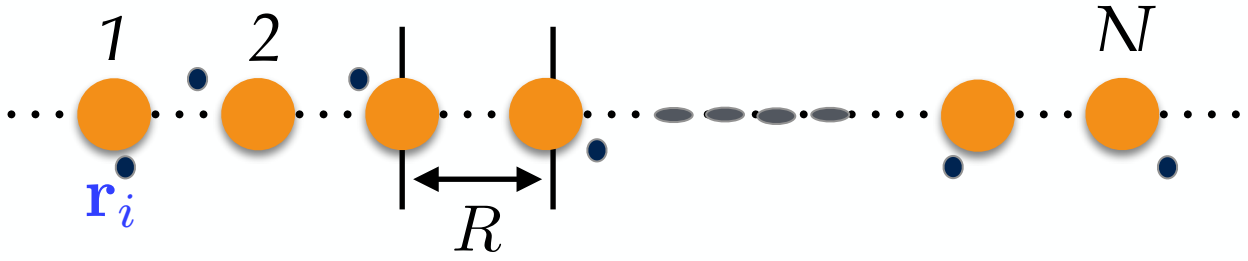
An array of many-body methods

Summary of characteristics

method		deterministic	basis set	self-consistent	variational	scaling
Wave-function	CCSD	yes	b	yes	no	$N^2M^4 + N^3M^3$
	CCSD(T)	yes	b	yes	no	N^3M^4
	DMRG	yes	b	yes	yes	$D^3M^3 + D^2M^4$
	SBDMRG	yes	sb	yes	yes	$NRD^3\left[N_o^3 + D(N_o)\right]$
	HF	yes	b	yes	yes	M^4
	FCI	yes	b	no	yes	$\binom{M}{N}$
	MRCI	yes	b	no	yes	$> \binom{N}{N/2}N^4 + N^2M^4$
	NEVPT2	yes	b	no	no	$\binom{N}{N/2}N^8$
	AFQMC	no	b	no	no	$N^2M^2 + M^2N$
	VMC	no	cs	no	yes	$N^2M + N^3$
	LR-DMC	no	cs	no	yes	$N^2M + N^3$
Embedding	DMET	yes	b	yes	no	$N_f^3D^3 + N_f^2D^4\left[(N_f^3D^3 + N_f^2D^4)M\right]$
	SEET	yes	b	yes	no	$N_{imp}\binom{M_s}{n_e} + M^5n_\tau\left[N_{imp}\binom{M_s}{n_e} + M^4\right]$
Diagrammatic	SC-GW	yes/no	b	yes	no	M^4n_τ
	GF2	yes	b	yes	no	M^5n_τ
	BDMC$_n$	no	b	yes	no	$e^{\alpha n}$

The homework problem

- Physics
  - EOS (benchmark paper) - e.g. implement H_{10} (open or PBC)



MC integration

To evaluate many-dimensional integral $G = \int_\Omega f(x)g(x)dx$

$f(x) > 0; \quad \int_\Omega f(x)dx = 1$

$f(x)$: probability density

- Sampling a PDF $f(x)$ means obtaining a sequence $\{x_1, x_2, \cdots, x_i, \cdots\}$ so that

$$\text{Prob}\{x_i \in (x, x + dx)\} = f(x)dx$$

i.e., the probability distribution of the sequence is $f(x)$

$$f(x) \doteq \frac{1}{M}\sum_{i=1}^{M}\delta(x - x_i)$$

- If $f(x)$ is successfully sampled, then $\quad G_M \equiv \frac{1}{M}\sum_{i=1}^{M} g(x_i) \quad \to G$

Integral eqs by random walk

- An integral equation of the form

$$\Psi'(x) = \int_\Omega G(x,y)w(y)\Psi(y)dy$$

can be viewed as a random walk (transport problem)

- For example,

$$\Psi'(x) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{\pi}} e^{-(x-y)^2} \sqrt{2} e^{-\frac{1}{2}y^2} \Psi(y)dy$$

conditional prob. for particle to jump to x if it is currently at y

"birth/death" at y

prob. for particle to be at y

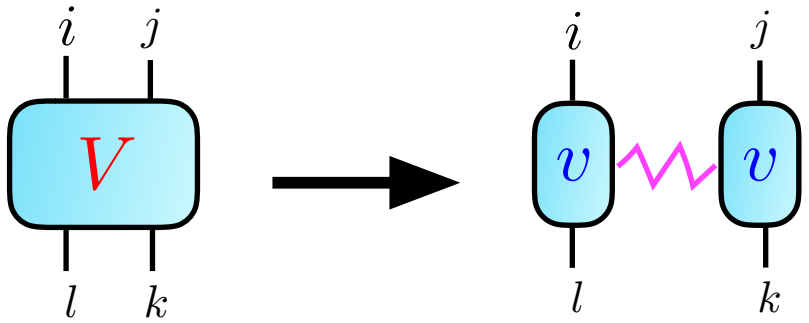
Q: What is the resulting prob. distribution of particles?

An auxiliary-field perspective

General H w/ two-body interaction, in 2nd quantization:

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

Interaction can be decoupled:



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

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

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

An auxiliary-field perspective

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

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

- Independent-electron:

$$\hat{H} = \hat{H}_1 + \hat{H}_2 = \sum_{i,j}^{M} T_{ij} \, c_j^\dagger c_j + \sum_{i,j,k,l}^{M} V_{ijkl} c_i^\dagger c_j^\dagger c_k c_l$$

LDA $\quad \hat{H}_2 \rightarrow \sum_i f_c(n_i) \hat{n}_i$

- Change the Hamiltonian

- Demand a single-determinant solution

An auxiliary-field perspective

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

An auxiliary-field perspective

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- Independent-electron: $e^{-\tau \hat{H}_{\mathrm{LDA}}(n)} \doteq e^{-\tau \hat{H}_1} e^{-\tau \hat{H}_{\mathrm{xc}}(n)}$

An auxiliary-field perspective

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  Thus, LDA calculation:

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$|SD^{(0)}\rangle$

An auxiliary-field perspective

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  Thus, LDA calculation:

$$e^{-\tau \hat{H}_{\mathrm{LDA}}(n^{(0)})} \qquad |SD^{(0)}\rangle$$

An auxiliary-field perspective

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$$e^{-\tau \hat{H}_{\mathrm{LDA}}(n^{(0)})} |SD^{(0)}\rangle$$

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- Independent-electron: $e^{-\tau \hat{H}_{\mathrm{LDA}}(n)} \doteq e^{-\tau \hat{H}_1} e^{-\tau \hat{H}_{\mathrm{xc}}(n)}$

  Thus, LDA calculation:

$$|SD^{(1)}\rangle \leftarrow e^{-\tau \hat{H}_{\mathrm{LDA}}(n^{(0)})} |SD^{(0)}\rangle$$

An auxiliary-field perspective

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

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Thus, LDA calculation:

$e^{-\tau \hat{H}_{\mathrm{LDA}}(n^{(1)})}$

$|SD^{(1)}\rangle \leftarrow e^{-\tau \hat{H}_{\mathrm{LDA}}(n^{(0)})} |SD^{(0)}\rangle$

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$$e^{-\tau \hat{H}_{\mathrm{LDA}}(n^{(1)})} |SD^{(1)}\rangle \leftarrow e^{-\tau \hat{H}_{\mathrm{LDA}}(n^{(0)})} |SD^{(0)}\rangle$$

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$$\cdots \leftarrow e^{-\tau \hat{H}_{\mathrm{LDA}}(n^{(1)})} |SD^{(1)}\rangle \leftarrow e^{-\tau \hat{H}_{\mathrm{LDA}}(n^{(0)})} |SD^{(0)}\rangle$$

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$$|GS\rangle \cdots \leftarrow e^{-\tau \hat{H}_{\mathrm{LDA}}(n^{(1)})} |SD^{(1)}\rangle \leftarrow e^{-\tau \hat{H}_{\mathrm{LDA}}(n^{(0)})} |SD^{(0)}\rangle$$

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Single-determinant solution

An auxiliary-field perspective

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  Thus, LDA calculation:

  $$|GS\rangle \cdots \leftarrow e^{-\tau \hat{H}_{\mathrm{LDA}}(n^{(1)})} |SD^{(1)}\rangle \leftarrow e^{-\tau \hat{H}_{\mathrm{LDA}}(n^{(0)})} |SD^{(0)}\rangle$$

  Single-determinant solution

- Many-body: $\hat{H}_2 = -\sum_\gamma \hat{v}_\gamma^2$

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

  Propagation leads to multi-determinants

  Importance sampling to make practical (Lect. notes; web - Matlab)

An auxiliary-field perspective

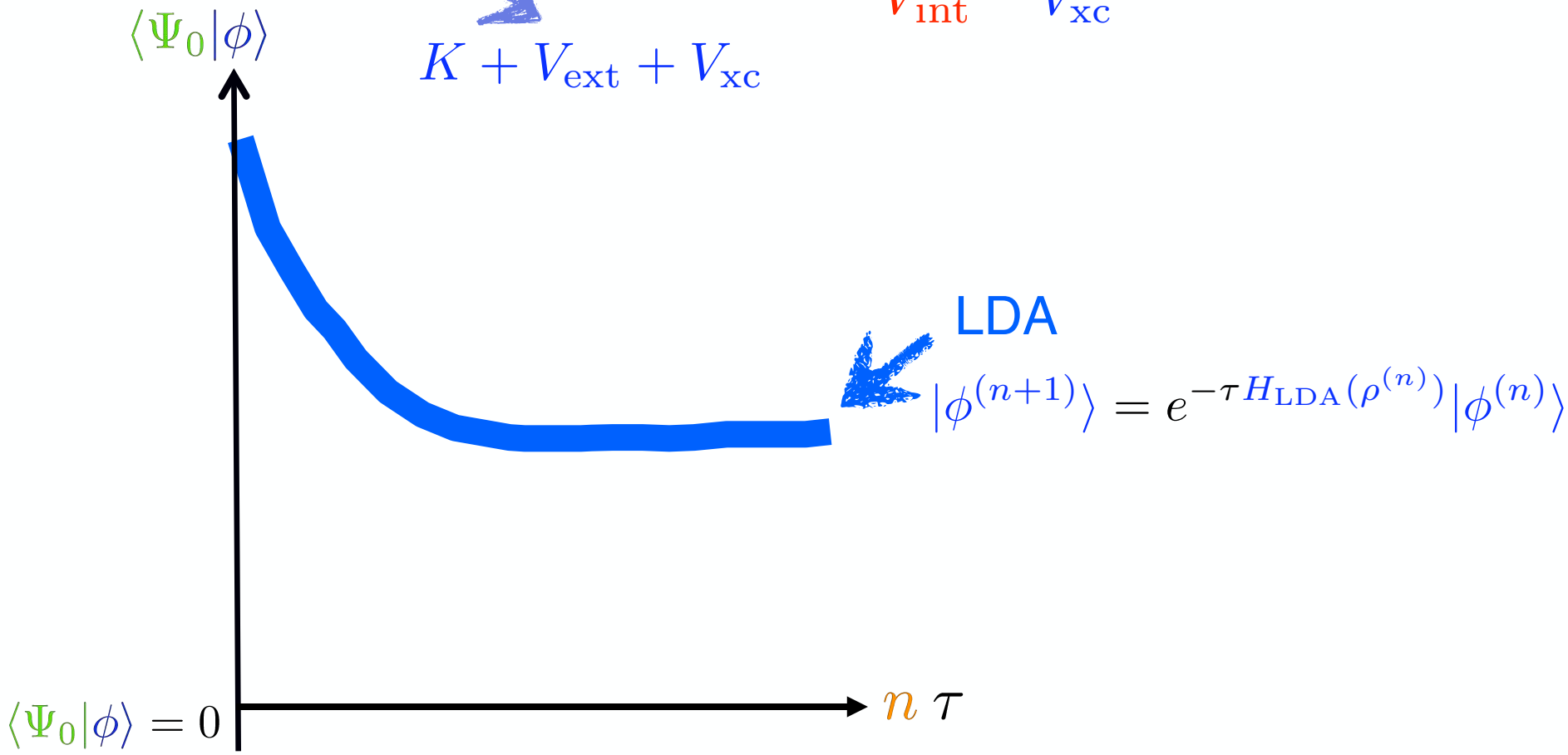
Reformulating field theory:

many-body effects as fluctuations around 'DFT soln':

$$H_{\mathrm{MB}} = H_{\mathrm{LDA}} + \Delta V$$

$H_{\mathrm{LDA}} \rightarrow K + V_{\mathrm{ext}} + V_{\mathrm{xc}}$

$\Delta V \rightarrow V_{\mathrm{int}} - V_{\mathrm{xc}}$



next →

An auxiliary-field perspective

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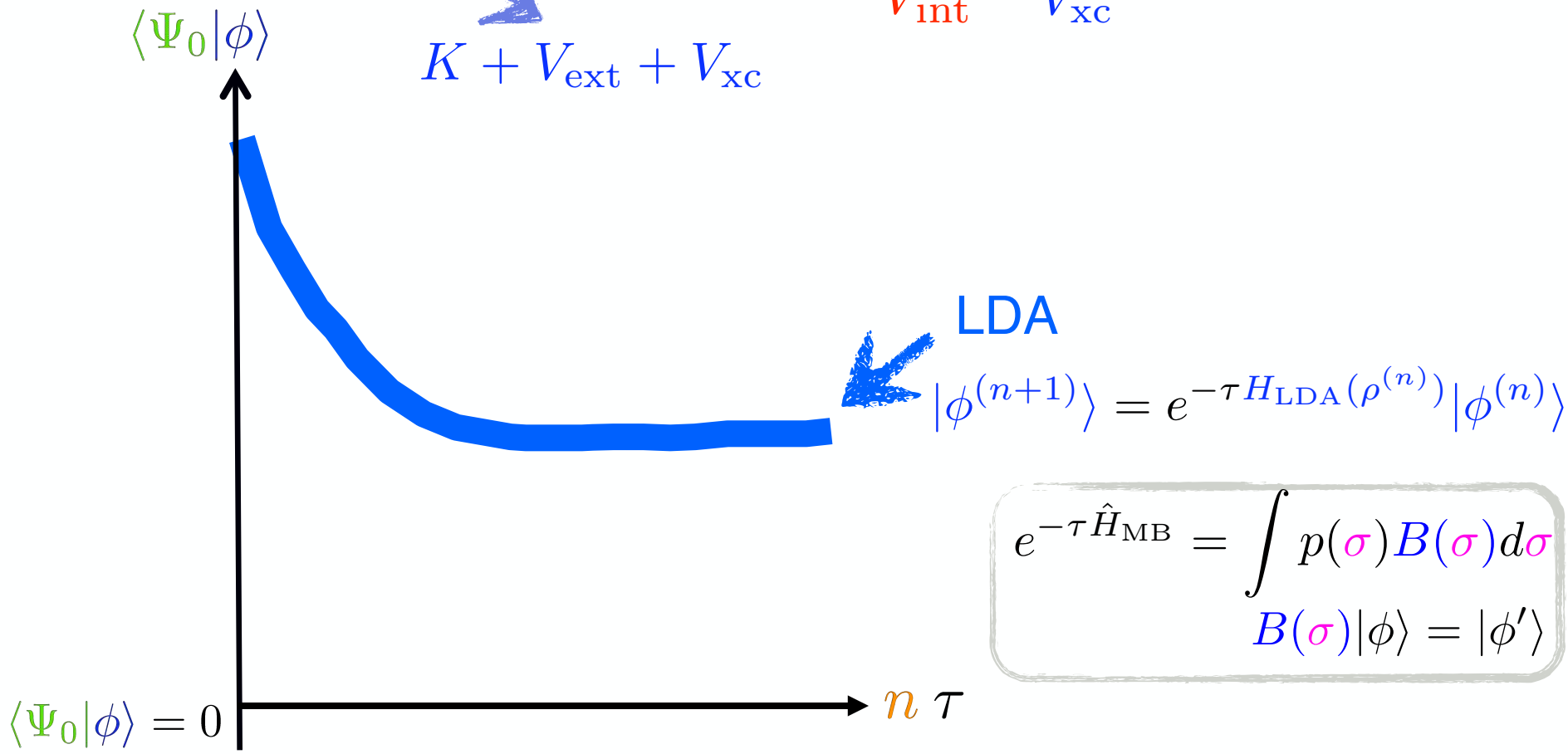

$$e^{-\tau \hat{H}_{\mathrm{MB}}} = \int p(\sigma) B(\sigma) d\sigma$$

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

next →

An auxiliary-field perspective

Reformulating field theory:

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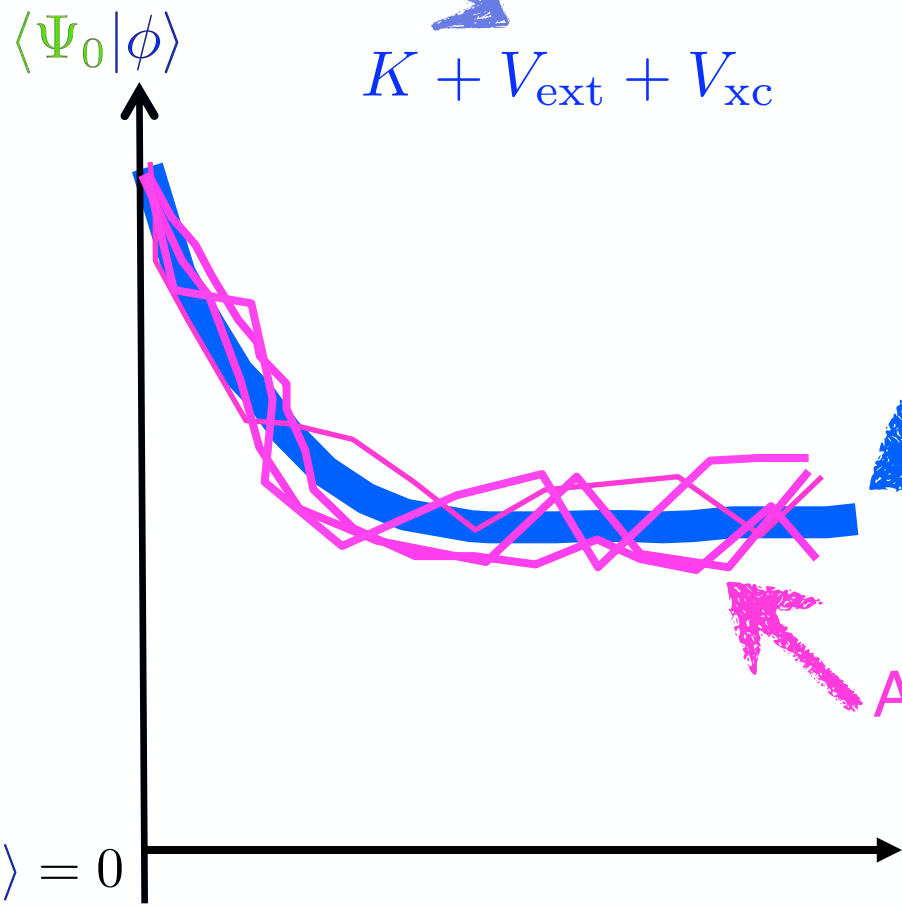

$$|\phi^{(n+1)}\rangle = e^{-\tau H_{\mathrm{LDA}}(\rho^{(n)})} |\phi^{(n)}\rangle$$

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

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

next →

Path integral over AFs

Imaginary-time projection --> random walk:

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

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

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

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

Path integral over AFs

Imaginary-time projection --> random walk:

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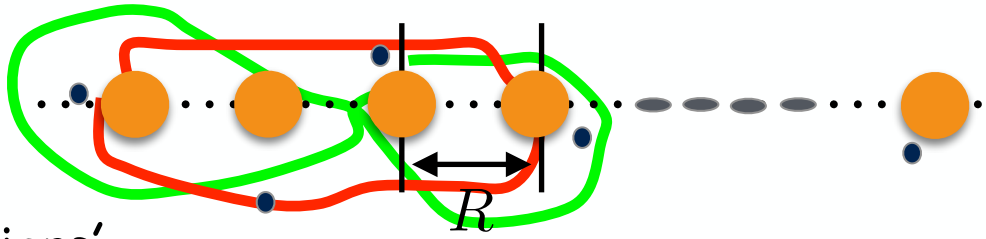

A step advances the SD by 'rotations'

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

Path integral over AFs

Imaginary-time projection --> random walk:

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

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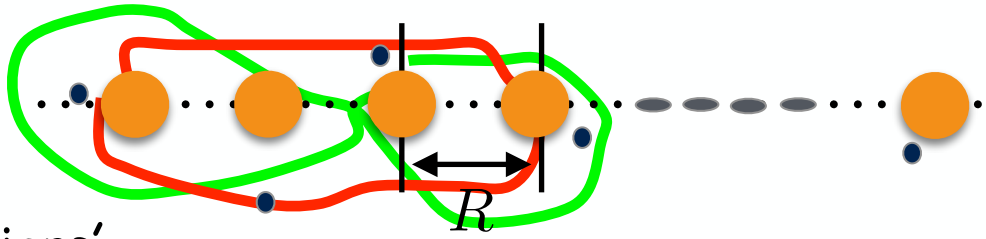

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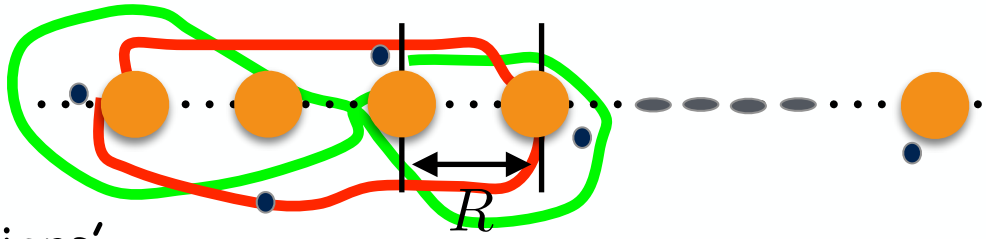

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1-body op

AF variable -- sample

Path integral over AFs

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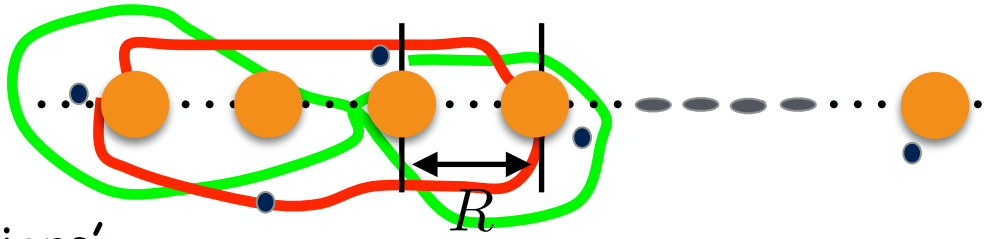

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NxN matrix

N is size of 'basis'

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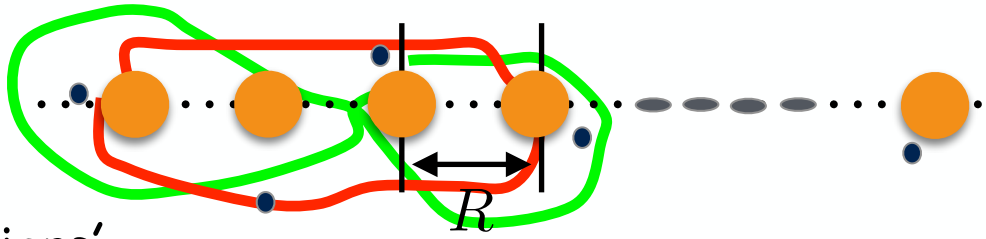

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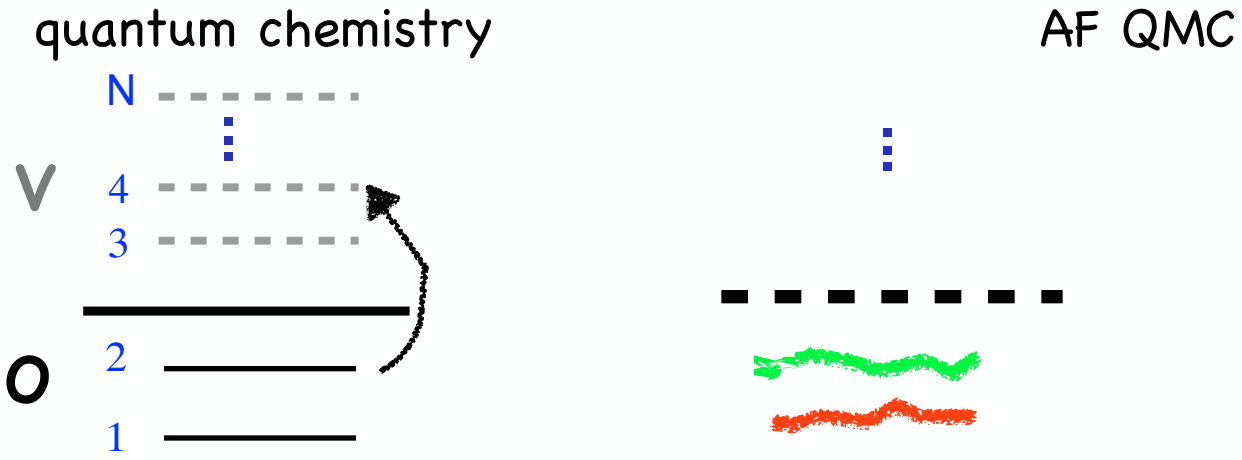
$$e^{\sigma \hat{v}} \begin{pmatrix} \psi_1 & \psi_1 \\ \psi_2 & \psi_2 \\ . & . \\ . & . \\ \psi_N & \psi_N \end{pmatrix} \rightarrow \begin{pmatrix} \psi'_1 & \psi'_1 \\ \psi'_2 & \psi'_2 \\ . & . \\ . & . \\ \psi'_N & \psi'_N \end{pmatrix}$$

Relation & differences with QC methods

Sampling Slater determinant space:



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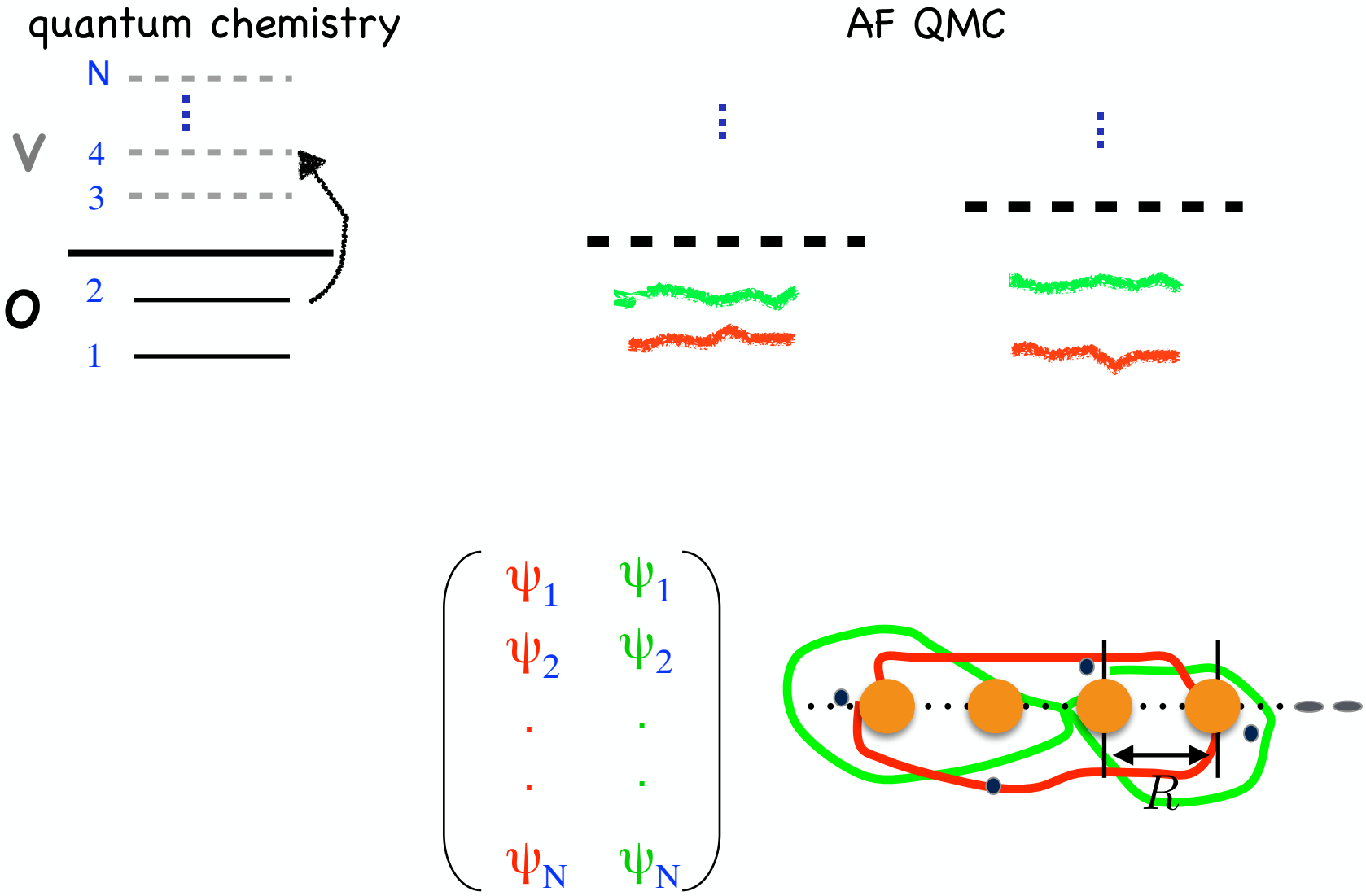

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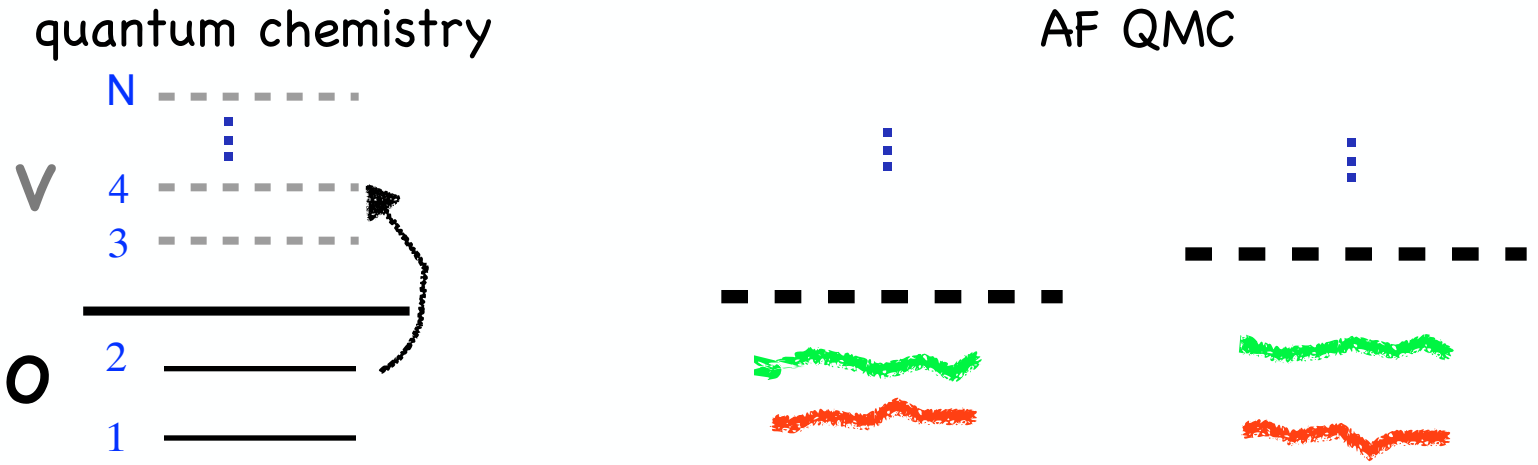
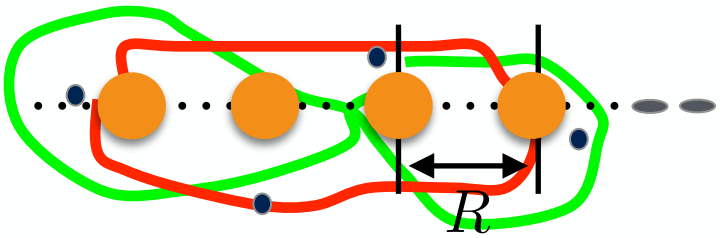


$$|\Psi_0\rangle = \sum_{\phi} c\,|\phi\rangle$$

AF QMC:

- non-orthogonal $|\phi\rangle$
- more compact rep
- weaker sign problem (FCIQMC or DMC)
- constraint - O(N^3)

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



Introduction - T>0 method

Standard finite-T method *Blankenbecler, Scalapino, and Sugar, '81*

Partition function for Hamiltonian H is: $(\beta = 1/k\,T)$

$$\mathrm{Tr}(e^{-\beta H}) = \mathrm{Tr}(\, e^{-\tau H}\, e^{-\tau H}\, \cdots\, e^{-\tau H}\,)$$

Need:

$$\langle O \rangle = \frac{\mathrm{Tr}(O\, e^{-\beta H})}{\mathrm{Tr}(e^{-\beta H})}$$

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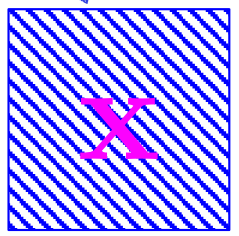

$N_s \times N_s$ matrix

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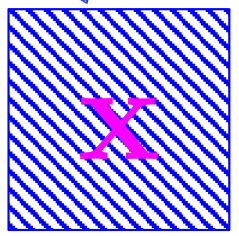
Sample fields $\{\mathbf{x}_l\}$ by Metropolis Monte Carlo to compute sum.



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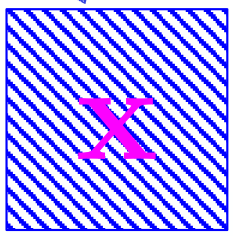
Sign Problem in standard finite-T AF QMC:

- As T lowers, average sign of $\det[\ ] \to 0$ exponentially.



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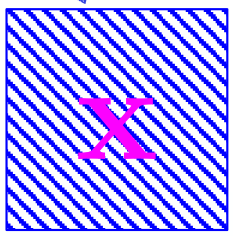
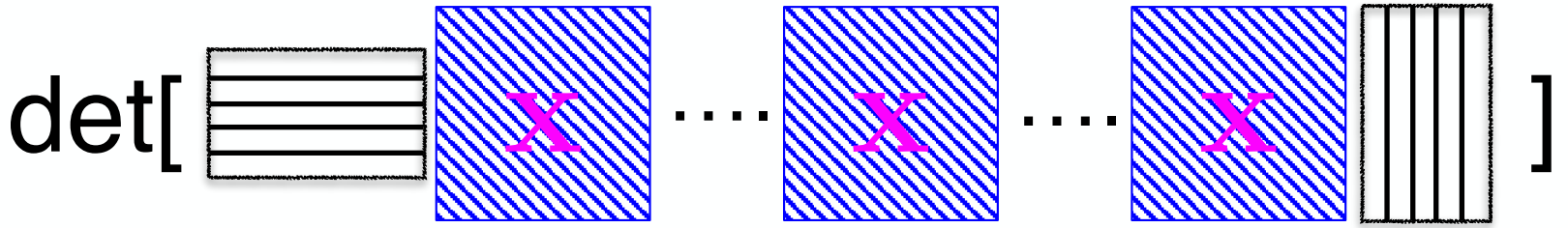


$N_s \times N_s$ matrix

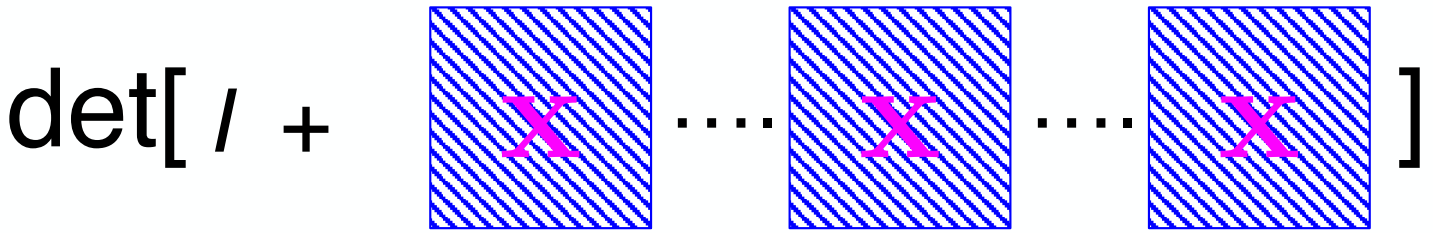
Referred to as DQMC

Path integral over AFs

T=0K:



finite-T:



The sign problem

Imaginary-time projection for GS. —> random walk:

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

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

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

The sign problem

* happens whenever $B \ldots B|\phi\rangle \rightarrow -|\phi\rangle$ exists
  symmetry can prevent this:
  - attractive interaction (det[ ])^2
  - repulsive half-filling bipartite (particle-hole)
  - a more general formulation PRL 116, 250601 (2016)

An exact gauge condition on the paths

Imagine introducing path integrals one time slice at a time: *Zhang, '99*

$$Z = \mathrm{Tr}(e^{-\tau H} e^{-\tau H} \cdots e^{-\tau H} e^{-\tau H}) \qquad P_0$$

$$e^{-\tau H} = \sum_{\mathbf{x}} B(\mathbf{x})$$

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&= \cdots \\
&= \sum_{\{\mathbf{x}_l\}} \det[\, I + B(\mathbf{x}_L)\, B(\mathbf{x}_{L-1}) \cdots B(\mathbf{x}_1)\,] && P_L(\{\mathbf{x}_1,\mathbf{x}_2,\cdots,\mathbf{x}_L\})
\end{aligned}$$

An exact gauge condition on the paths

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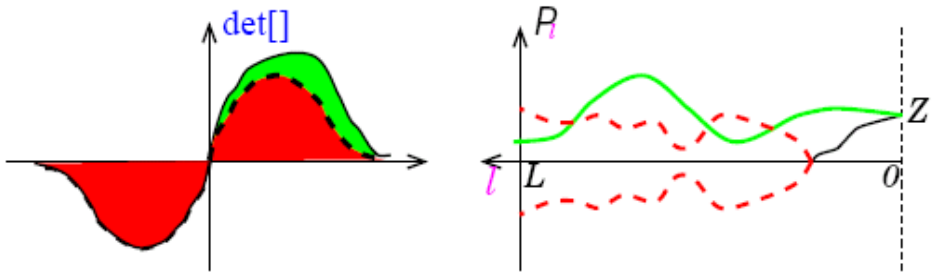
\end{aligned}$$

Suppose we know $e^{-\tau H}$. Consider P_l:



- If $P_l = 0$, all future paths $\{\mathbf{x}_{l+1}, \mathbf{x}_{l+2}, \cdots, \mathbf{x}_L\}$ collectively contribute 0 in Z.
- A complete path $\{\mathbf{x}_l\}$ contributes to Z **iff** $P_l > 0$ for all l.

An exact gauge condition on the paths

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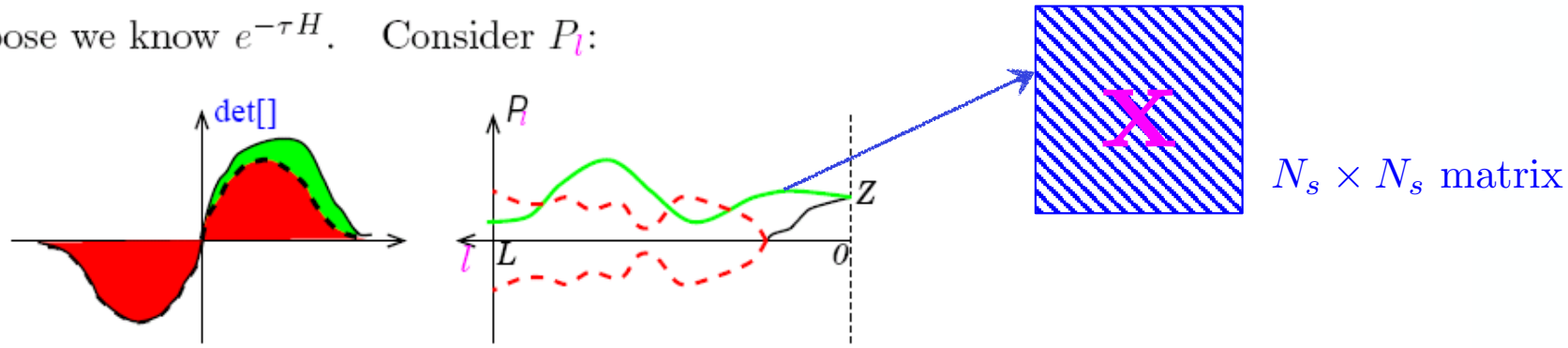

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Impose gauge condition approximately

Constraint to control the sign problem

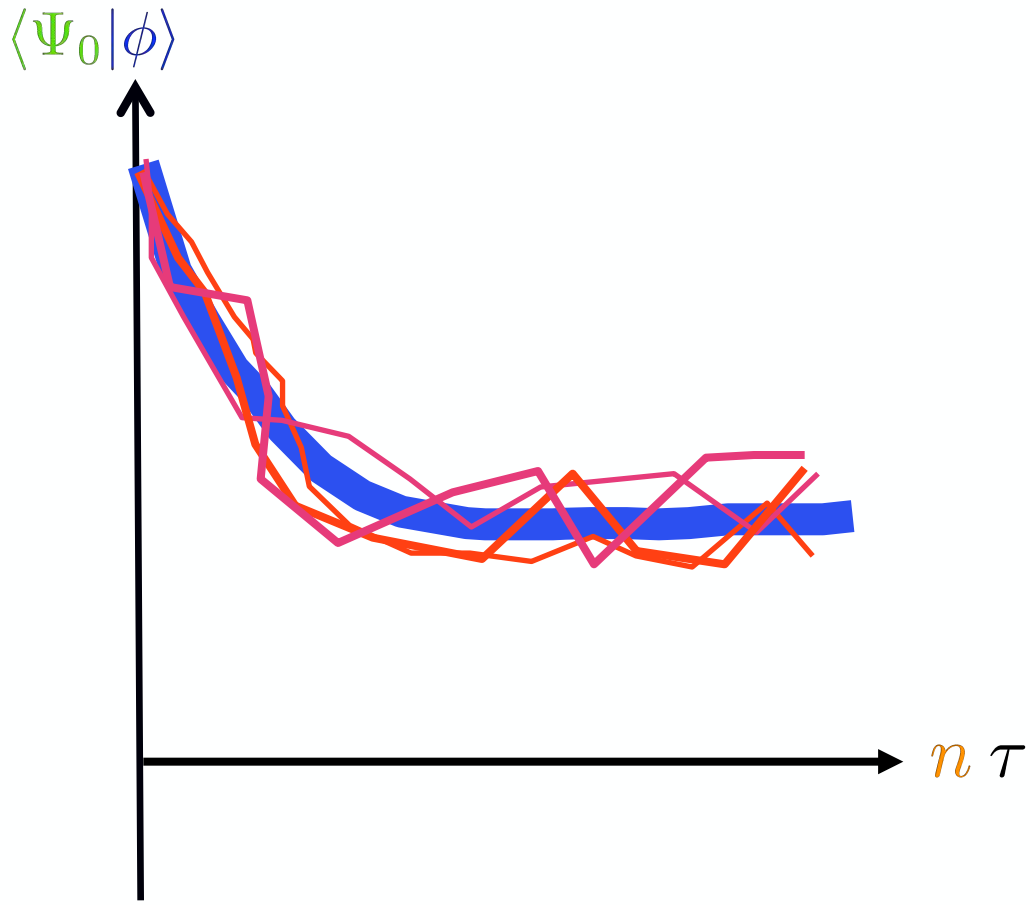
Require: $P_1(\{\mathbf{x}_1\}) > 0$; $P_2(\{\mathbf{x}_1, \mathbf{x}_2\}) > 0$; ....; $P_L(\{\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_L\}) > 0$.

- Constraint eliminates all noise paths ('dashed lines').
- In practice, we use trial B_T for $e^{-\tau H}$ — approximate.

Impose gauge condition approximately

T=0K: many-body effects as fluctuations around "LDA soln"

$$H = H_{\mathrm{LDA}} + \Delta V$$



$$e^{-\tau H} = e^{-\tau H_{\mathrm{LDA}}}\, e^{-\tau \Delta V}$$

next →

Impose gauge condition approximately

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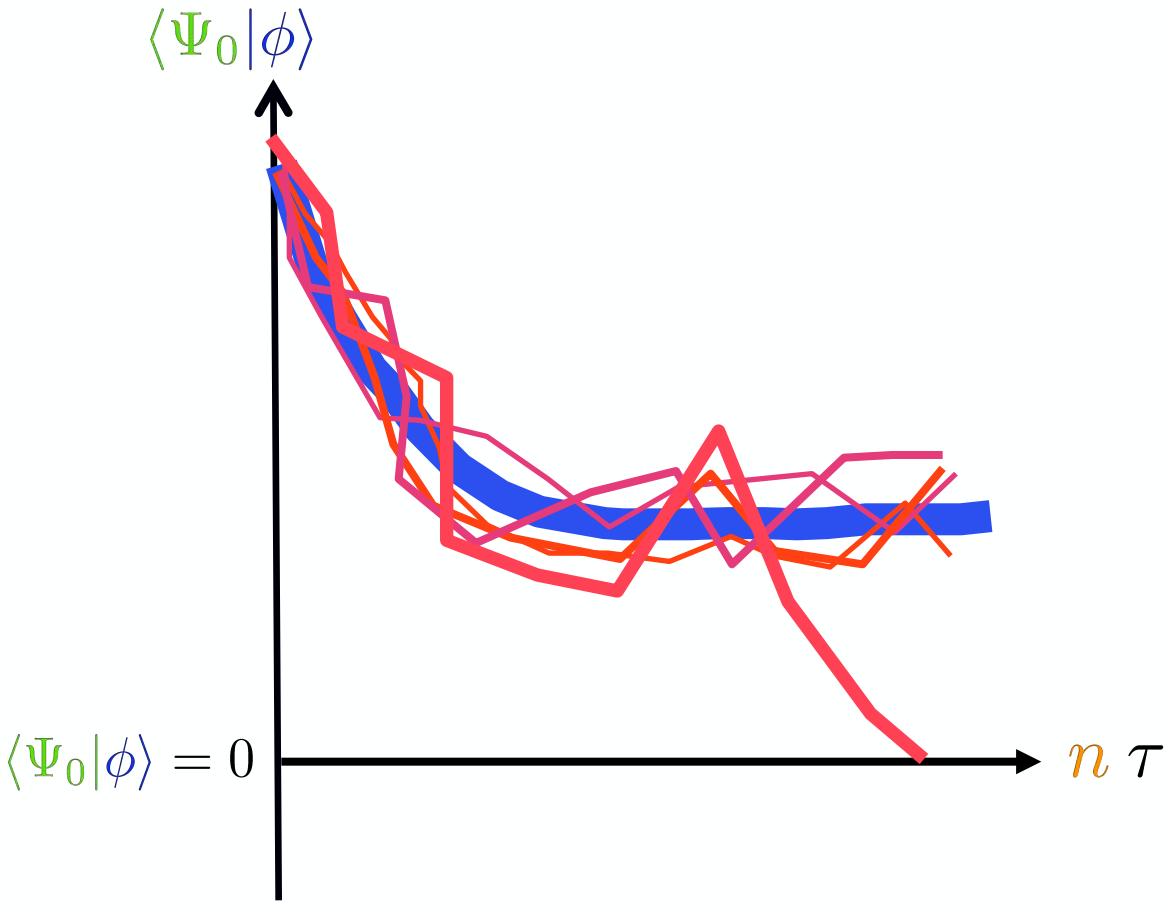

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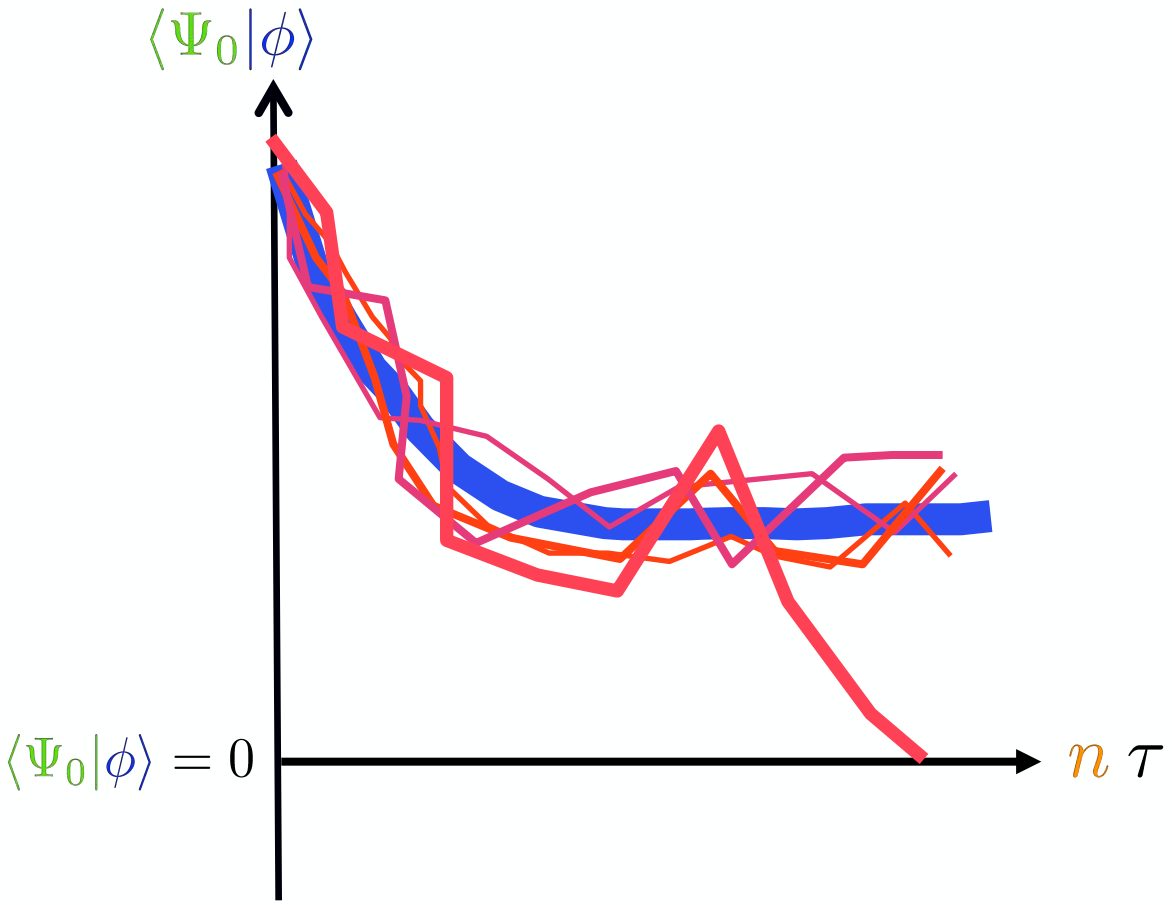

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Degeneracy between

$+|\phi\rangle$ and $-|\phi\rangle$

next →

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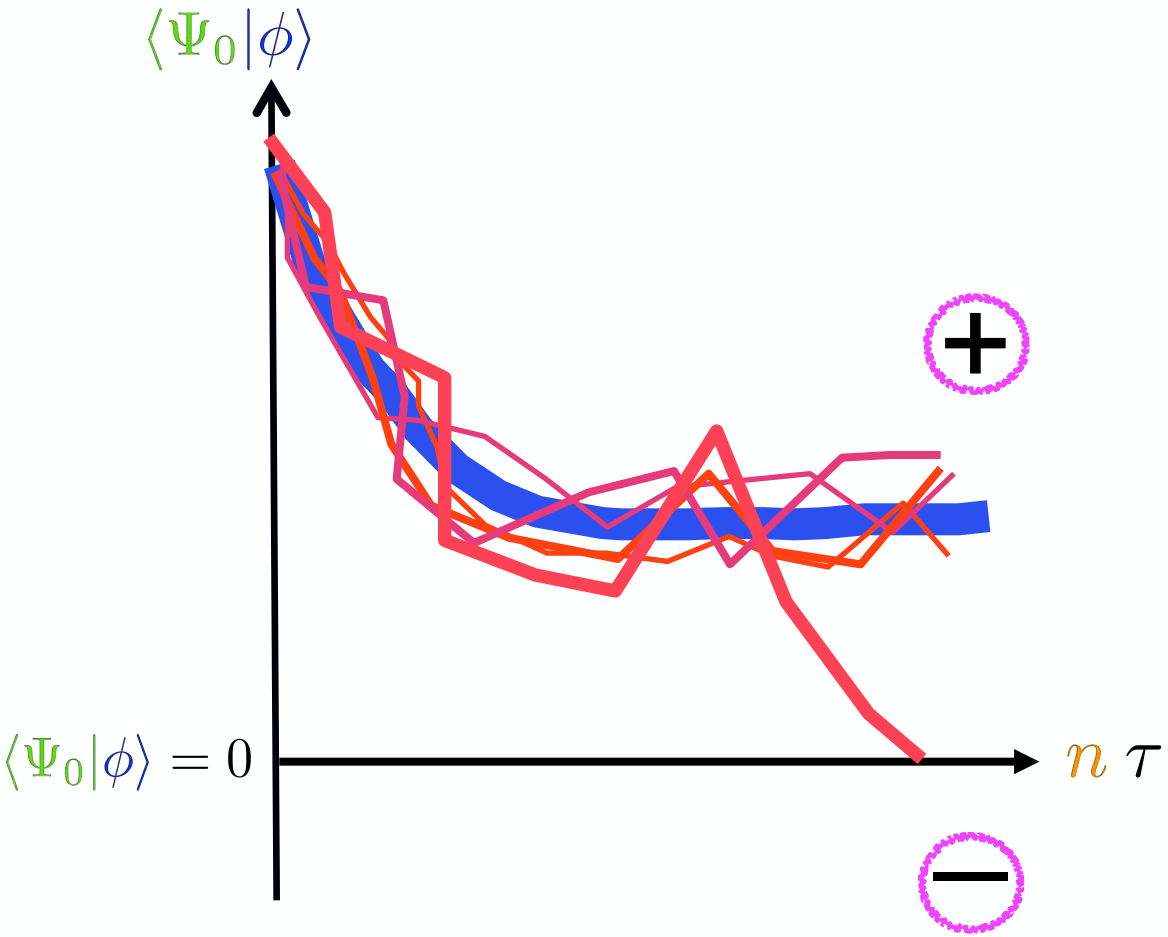

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Degeneracy between

$+|\phi\rangle$ and $-|\phi\rangle$

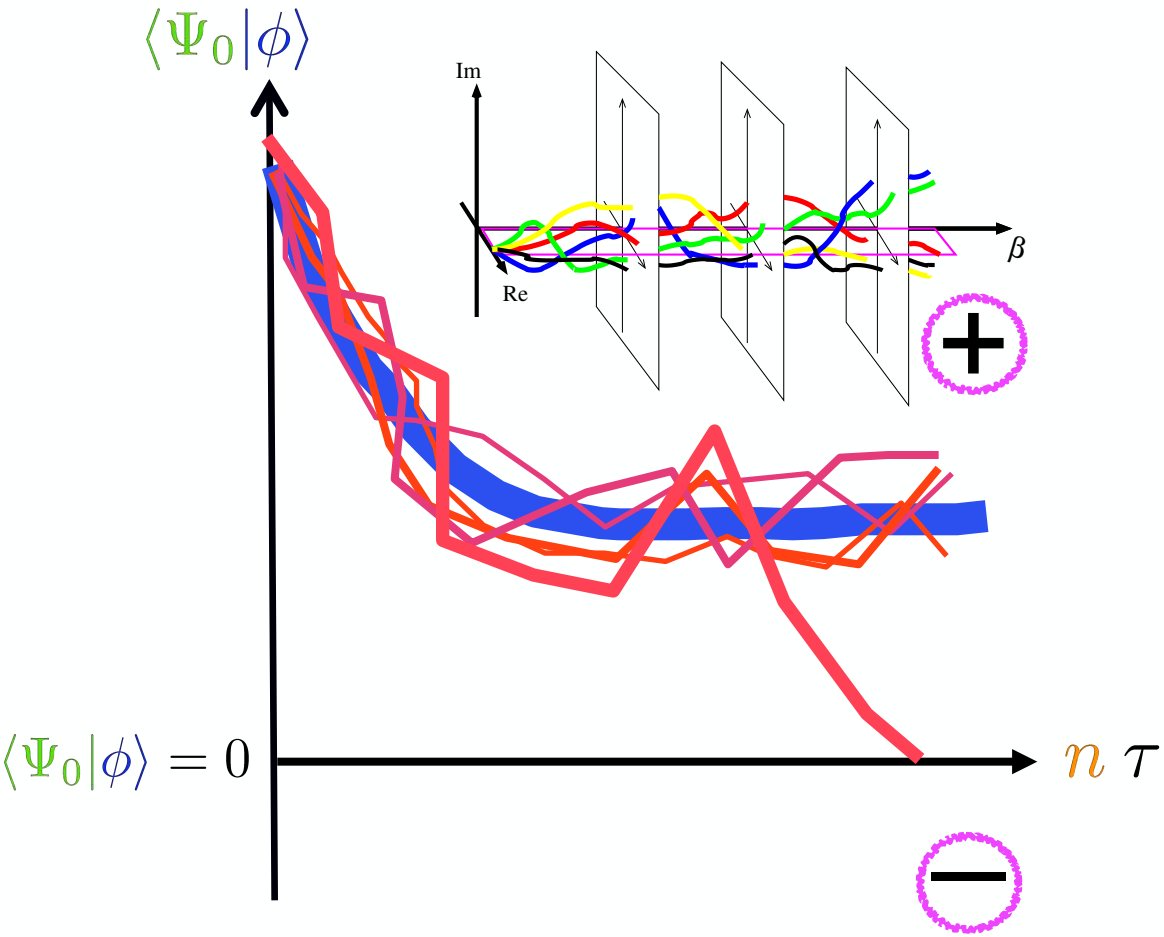
Coulomb +/- $\longrightarrow e^{i\theta}$

next →

Impose gauge condition approximately

T=0K: many-body effects as fluctuations around "LDA soln"

$$H = H_{\mathrm{LDA}} + \Delta V$$



$$e^{-\tau H} = e^{-\tau H_{\mathrm{LDA}}}\, e^{-\tau \Delta V}$$

Degeneracy between

$+|\phi\rangle$ and $-|\phi\rangle$

Coulomb +/- $\longrightarrow e^{i\theta}$

next →

Impose gauge condition approximately

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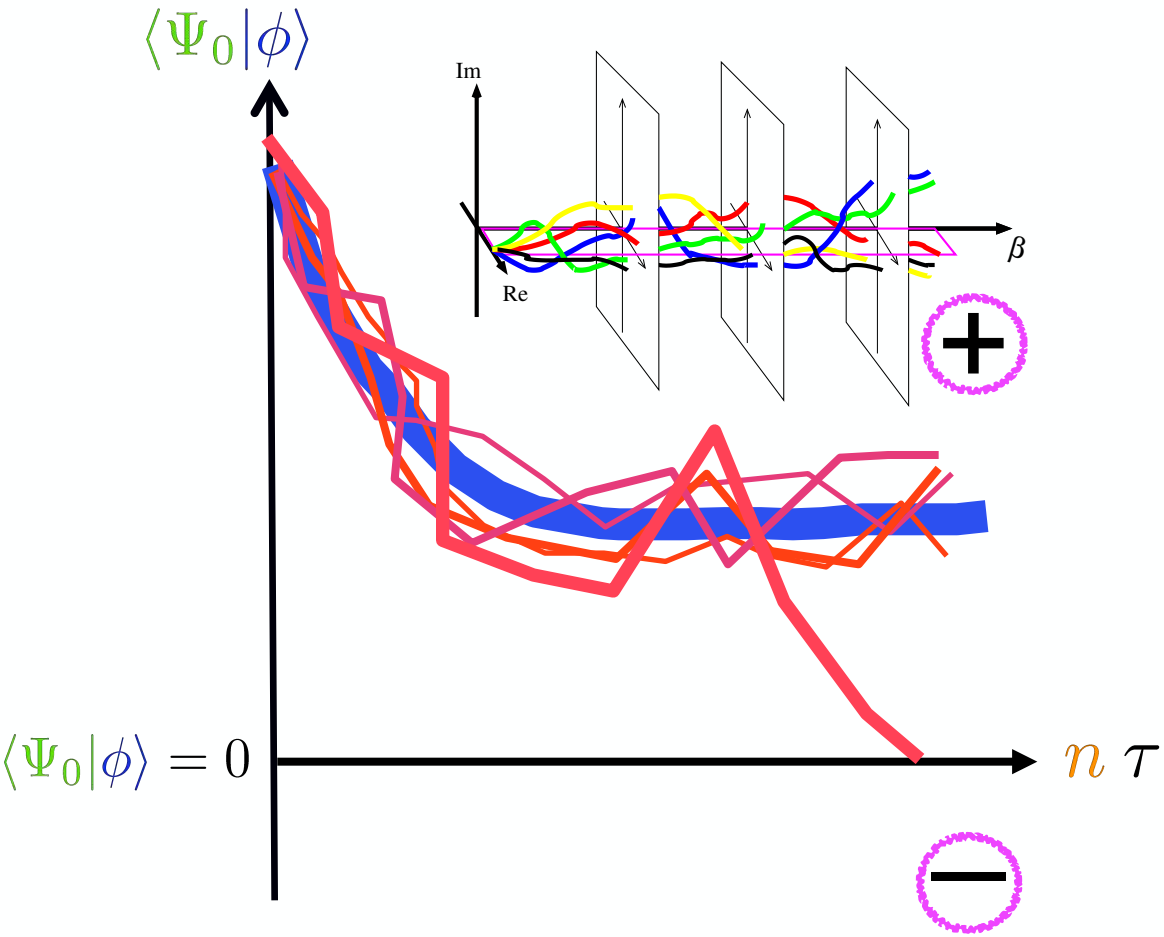


Gauge cond. w/ $|\Psi_T\rangle$
-> approximation

$$e^{-\tau H} = e^{-\tau H_{\mathrm{LDA}}}\, e^{-\tau \Delta V}$$

Degeneracy between

$+|\phi\rangle$ and $-|\phi\rangle$

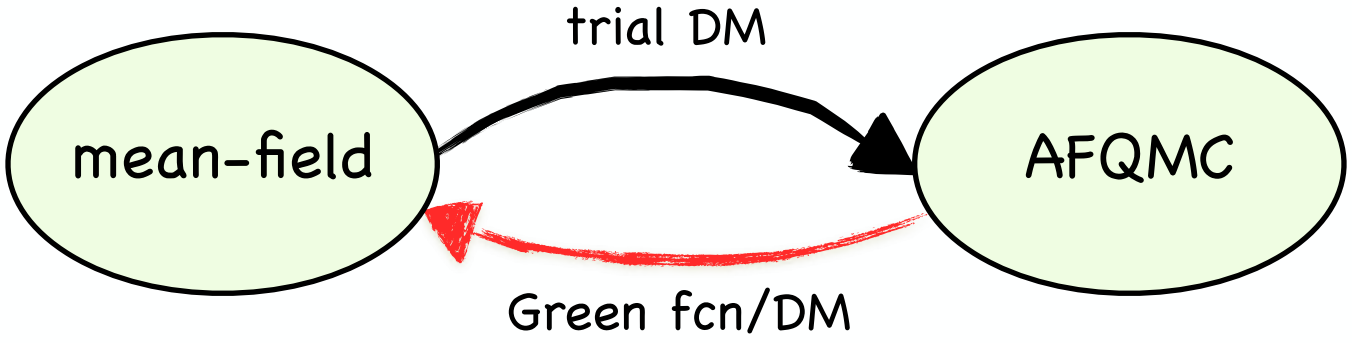
Coulomb +/- $\longrightarrow e^{i\theta}$

next →

Impose gauge condition approximately

Self consistent algorithm

1. Hartree-Fock ("DFT") solution -> AFQMC trial density matrix (DM)
2. Carry out AFQMC calculation with trial DM as constraint
3. Solve mean-field H, tune interaction strength (or form!), e.g U_eff, to match (minimize difference) DM with QMC from prev. iteration
4. Take new mean-field solution as trial DM
5. Repeat 2-4 until convergence: final QMC answer; optimal mean-field



He et al, PRB 99, 045108 (2019)

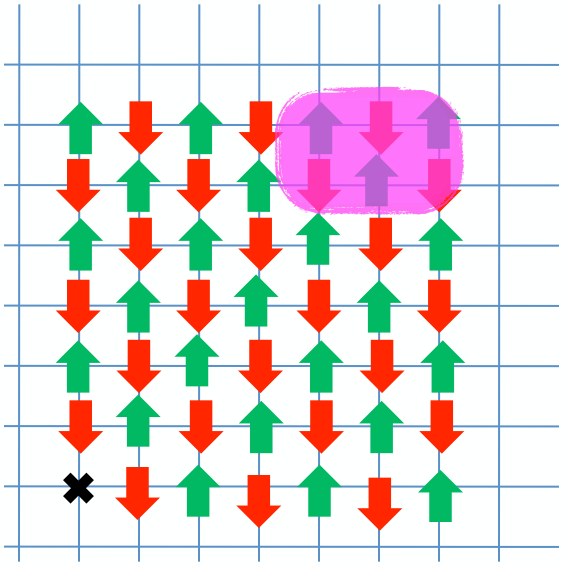
Magnetic properties in the Hubbard model

- Model for CuO plane in cuprates ? doping of a Mott insulator
- Half-filling: antiferromagnetic (AF) order at T=0K

(Furukawa & Imada 1991; Tang & Hirsch 1983; White et al, 1989; ....)

AF correlation:

$$C(\mathbf{r}) = \frac{1}{L \times L} \sum_{\mathbf{r}'} \langle \mathbf{S}_{\mathbf{r}} \cdot \mathbf{S}_{\mathbf{r}+\mathbf{r}'} \rangle$$



What happens to the AF order upon doping?

next →

Illustration in Hubbard ladders

Add pinning field to break translational invariance:

Cylindrical systems:

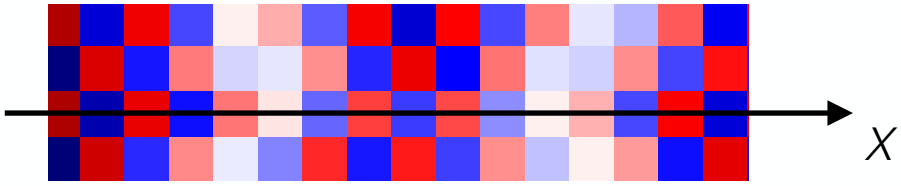
- Allows direct comparison with DMRG, which can treat narrow cylinders very accurately
- Calculations made easier! :
  correlation function ==> spin density

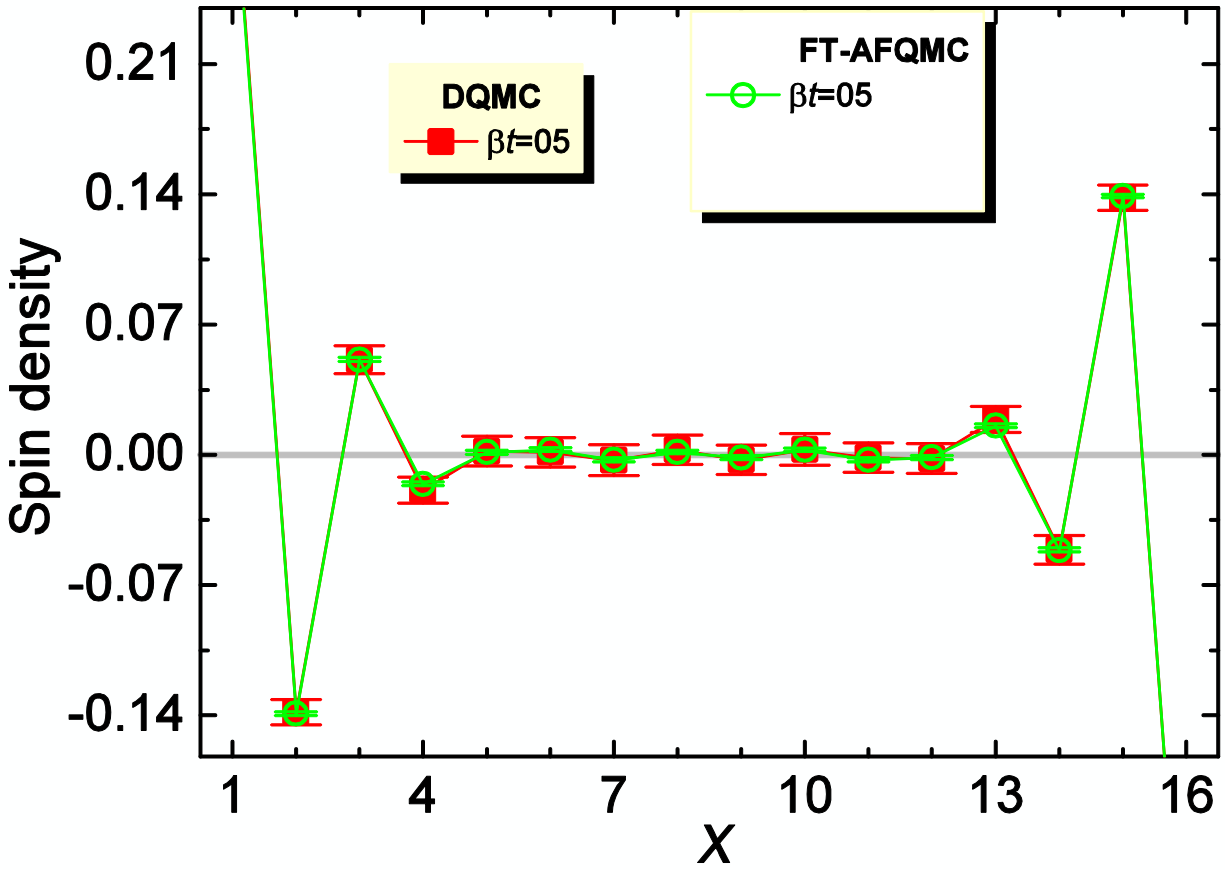
He et al, PRB 99, 045108 (2019)

Stripe order in 2D Hubbard model

4x16 cylinder, U=6t, doping h=1/8, pinning field at x=1, 16

- High T
  - No order
  - Agree with DQMC to beta=5 (when DQMC breaks down)





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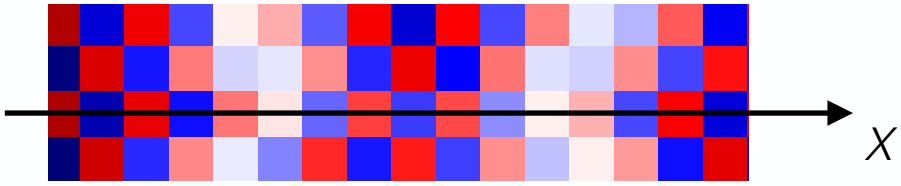

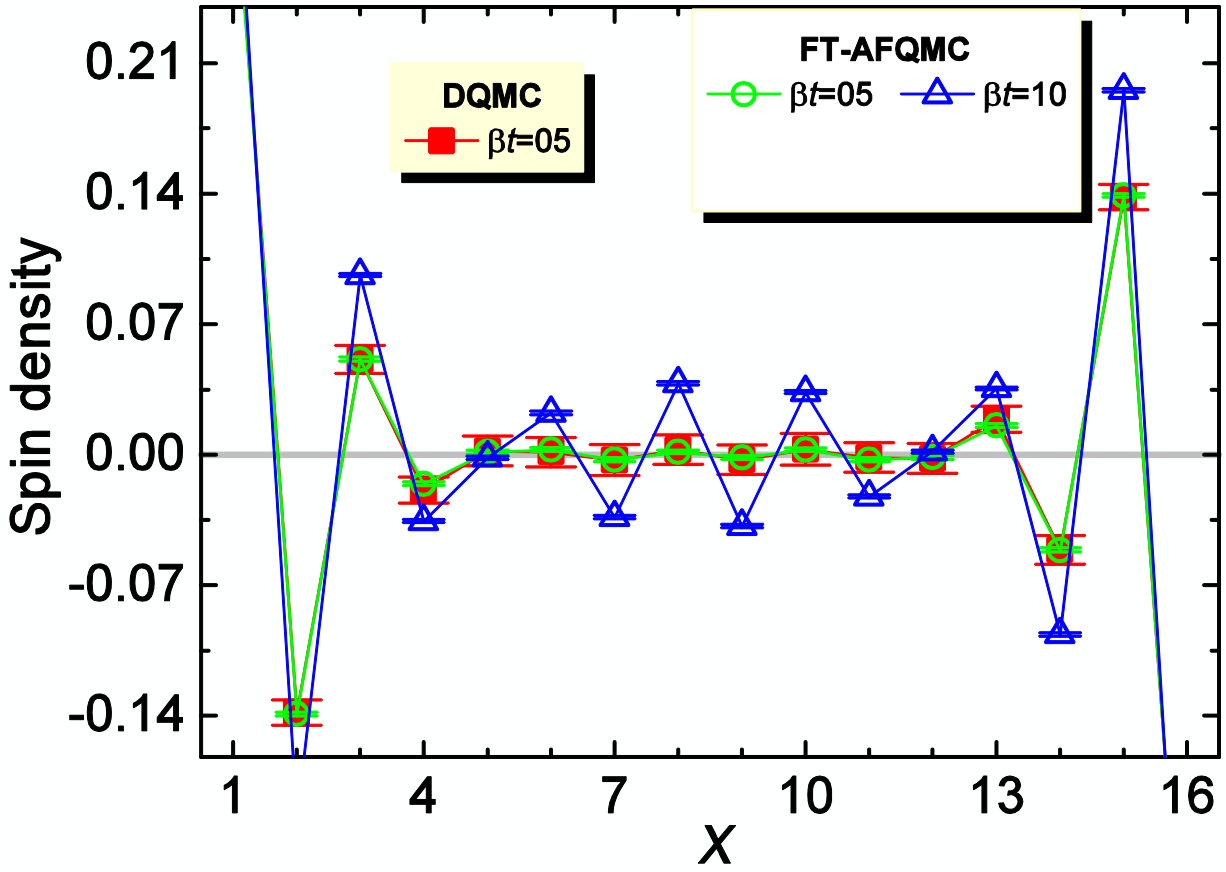

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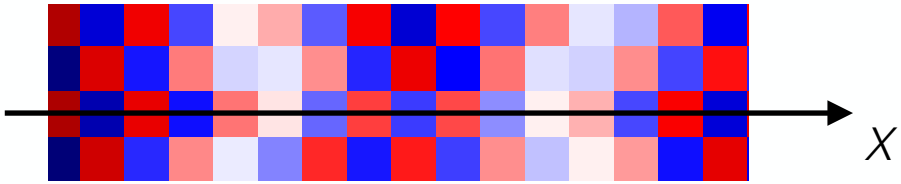

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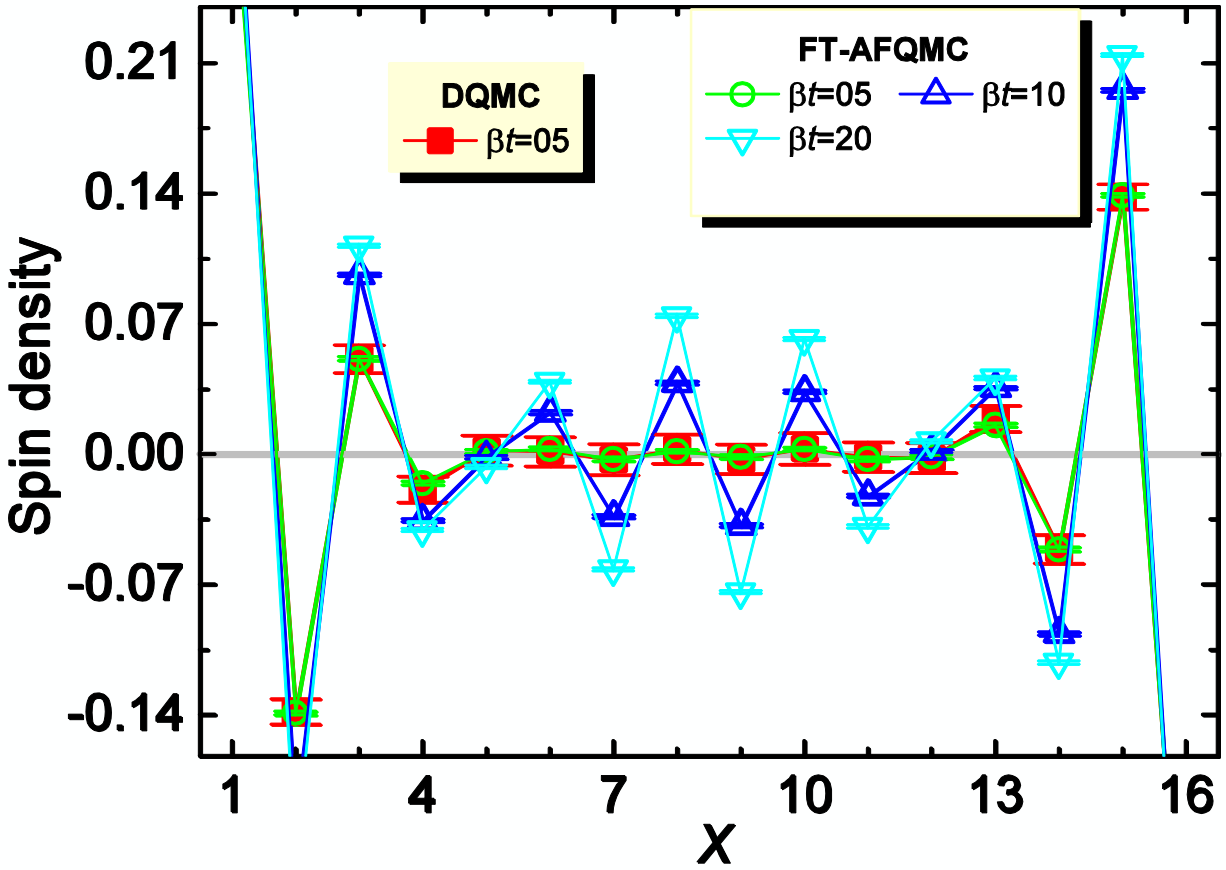

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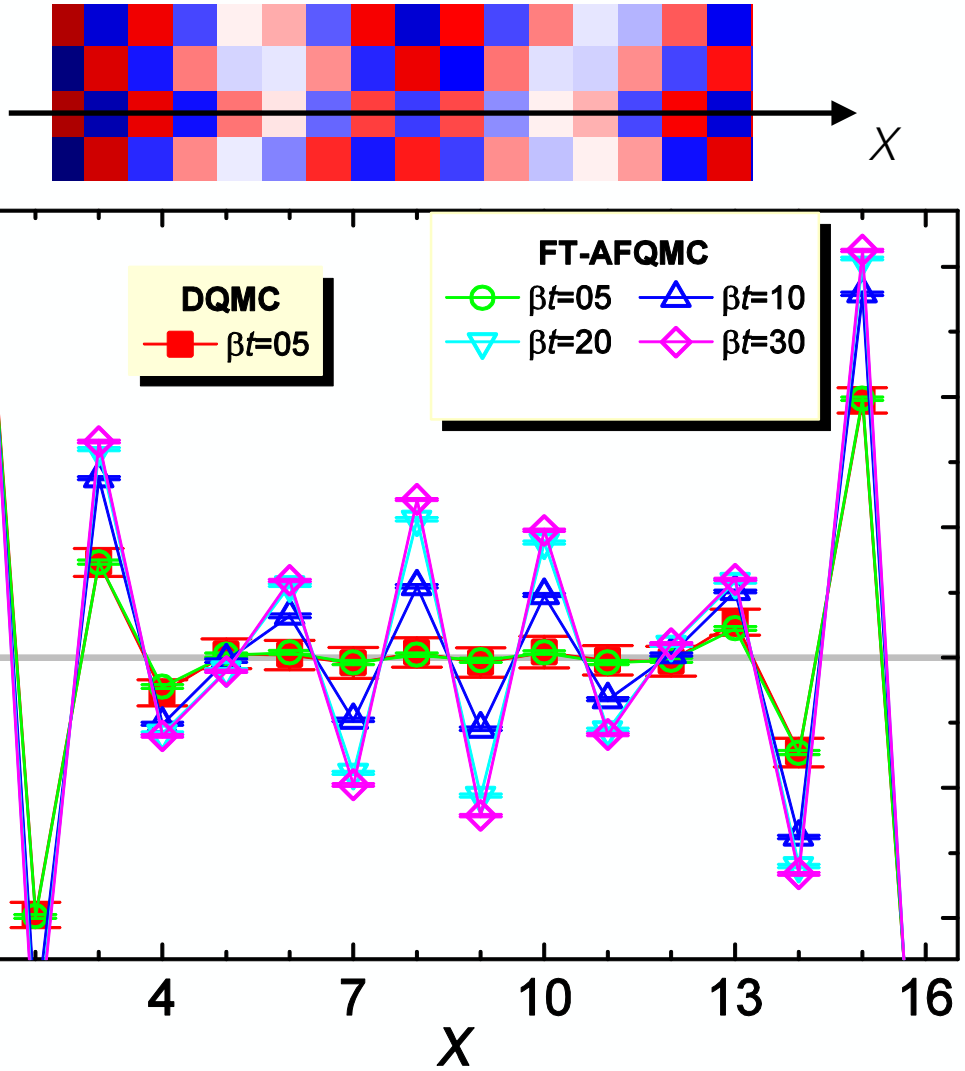

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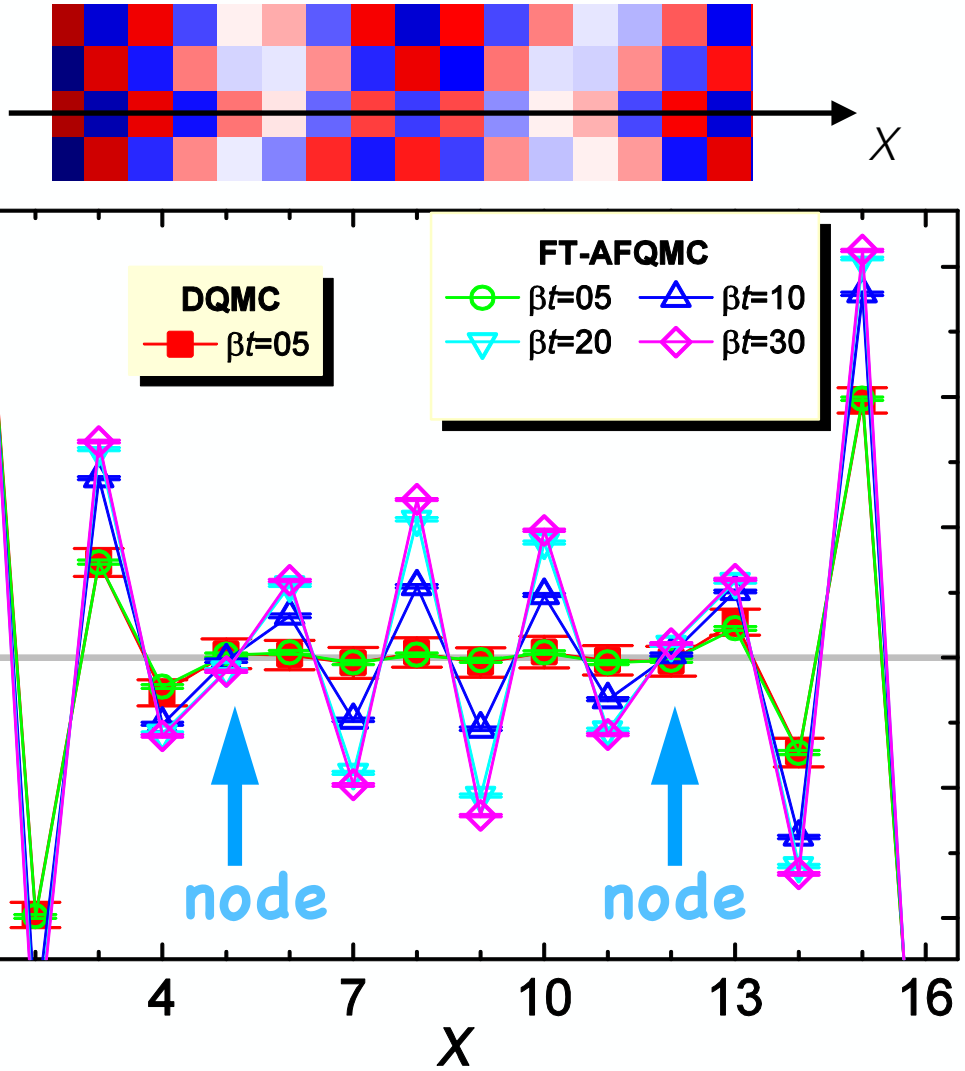

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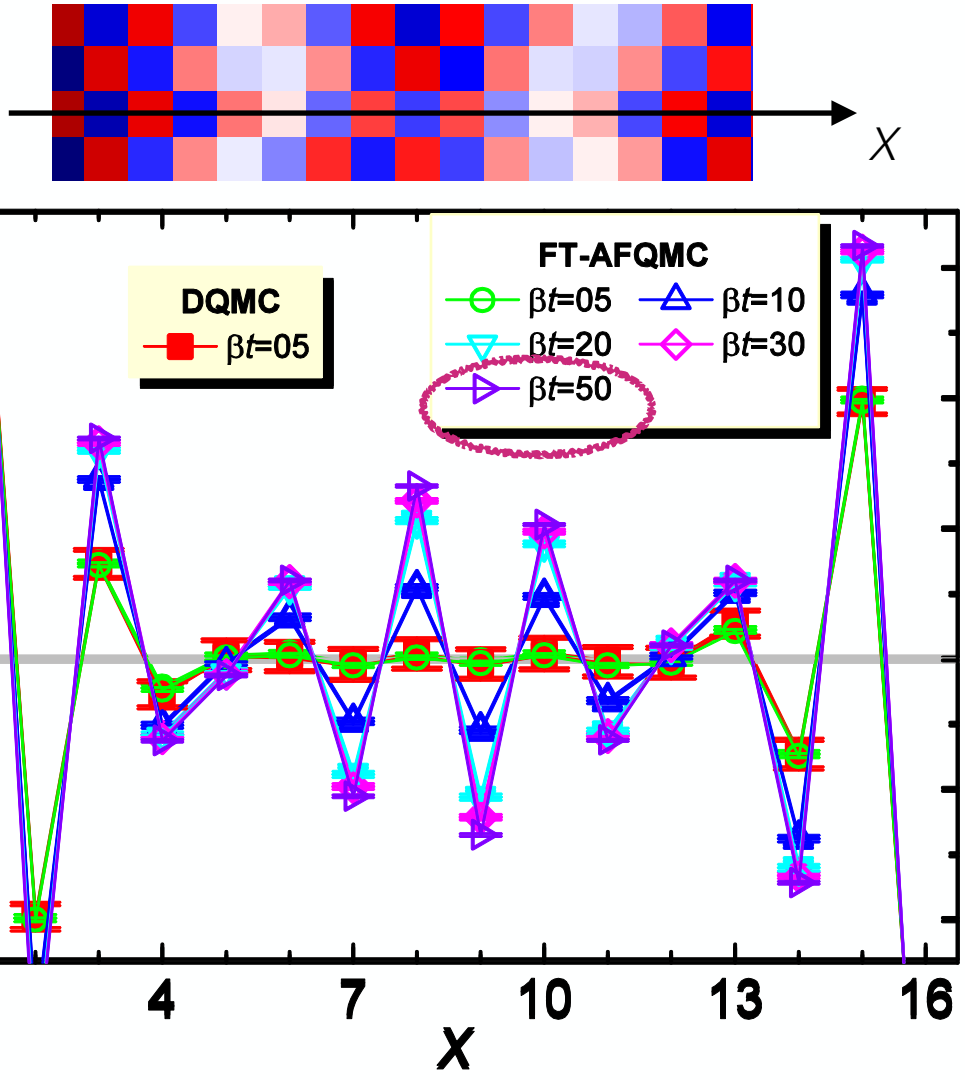

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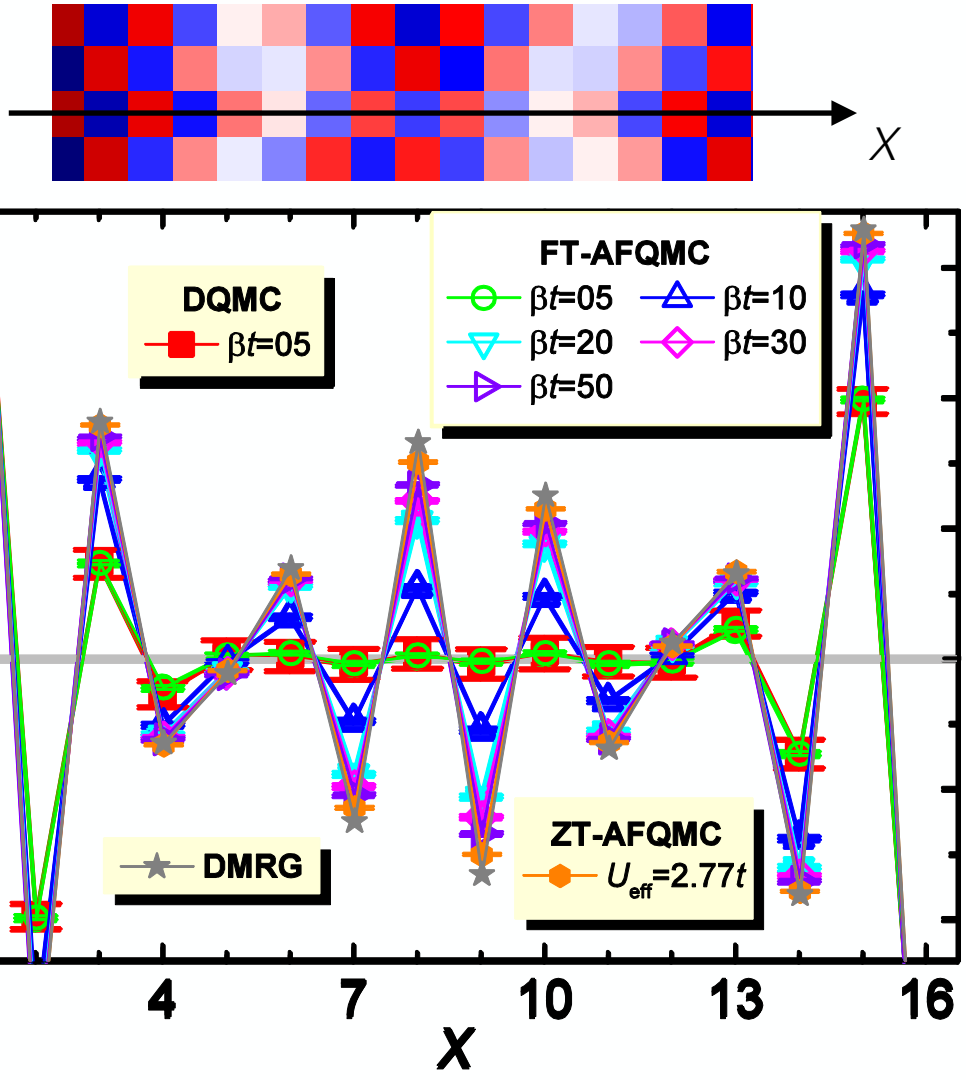
- As T lowers, order develops
- Approaches zero-T AFQMC, and DMRG



Hubbard model ground-state order

Collaboration determines 'stripe phase': (1/8 doping, U=8)

- Combines best methods
  - complement (size)
  - cross-check
- Careful approach to TDL
  - resolves 0.005t scale

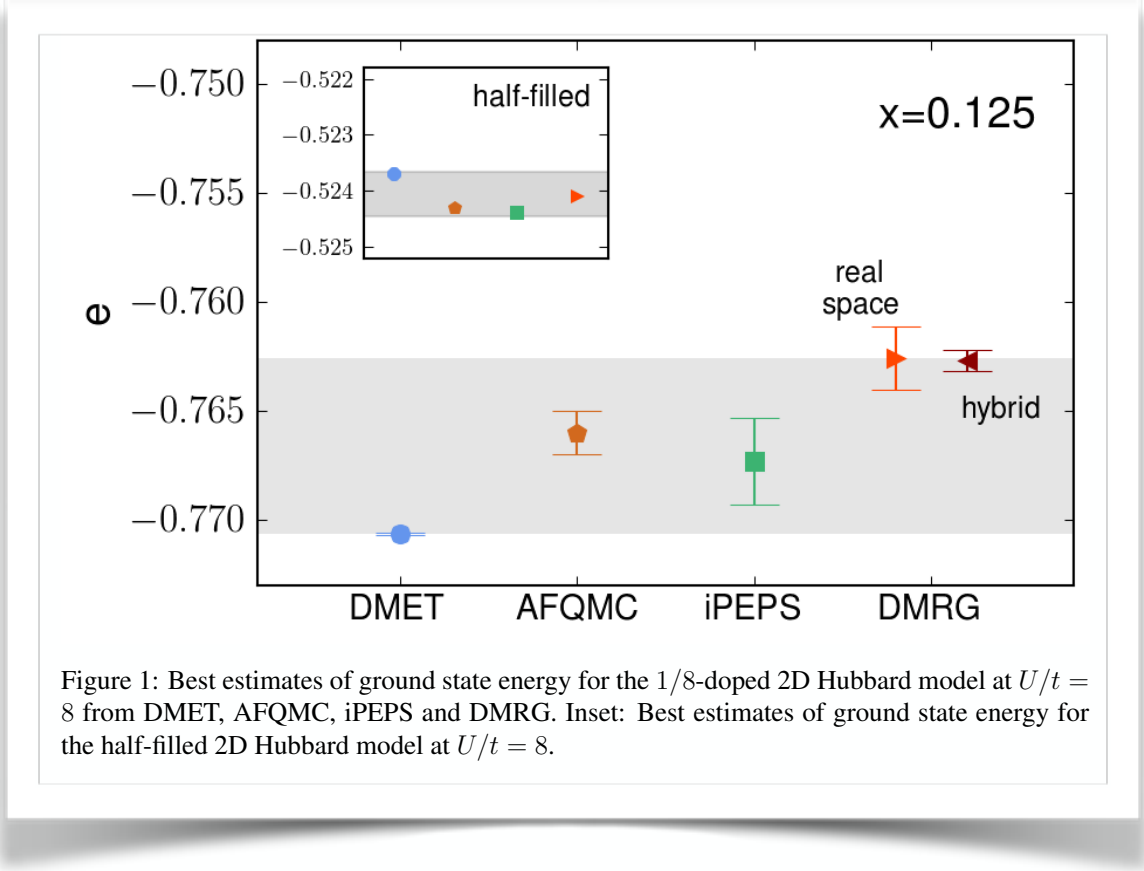


Figure 1: Best estimates of ground state energy for the $1/8$-doped 2D Hubbard model at $U/t = 8$ from DMET, AFQMC, iPEPS and DMRG. Inset: Best estimates of ground state energy for the half-filled 2D Hubbard model at $U/t = 8$.

Chan, Corboz, White, Zhang groups: Science (2017)

Hubbard model ground-state order

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- Combines best methods
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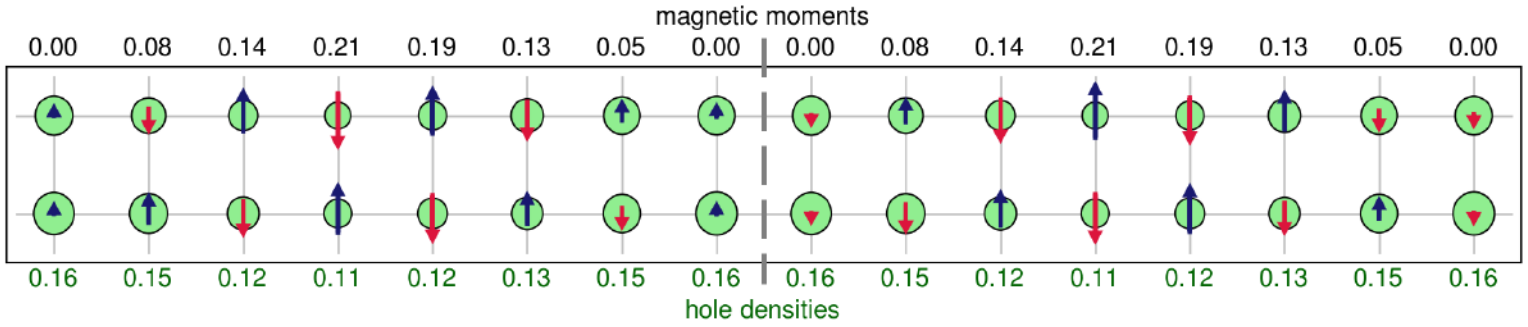
  - wavelength = 1/h



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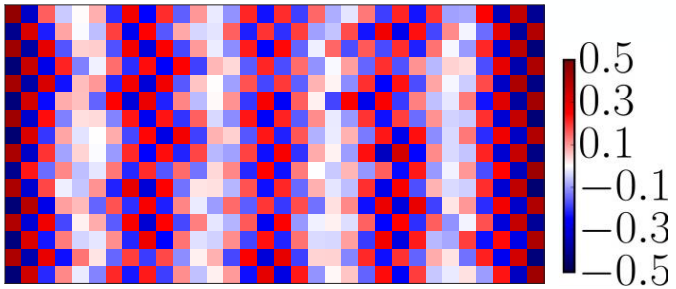
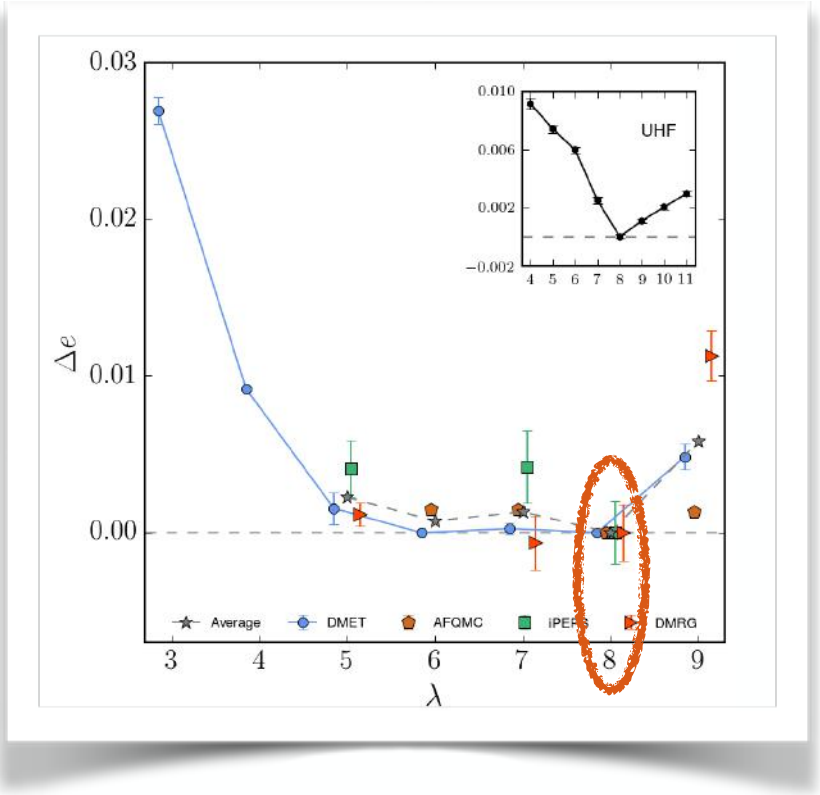
- Careful approach to TDL
  - resolves 0.005t scale
- Properties
  - wavelength = 1/h
  - fluctuating stripes (sloppy)





16x32 lattice: AFQMC

Chan, Corboz, White, Zhang groups: Science (2017)

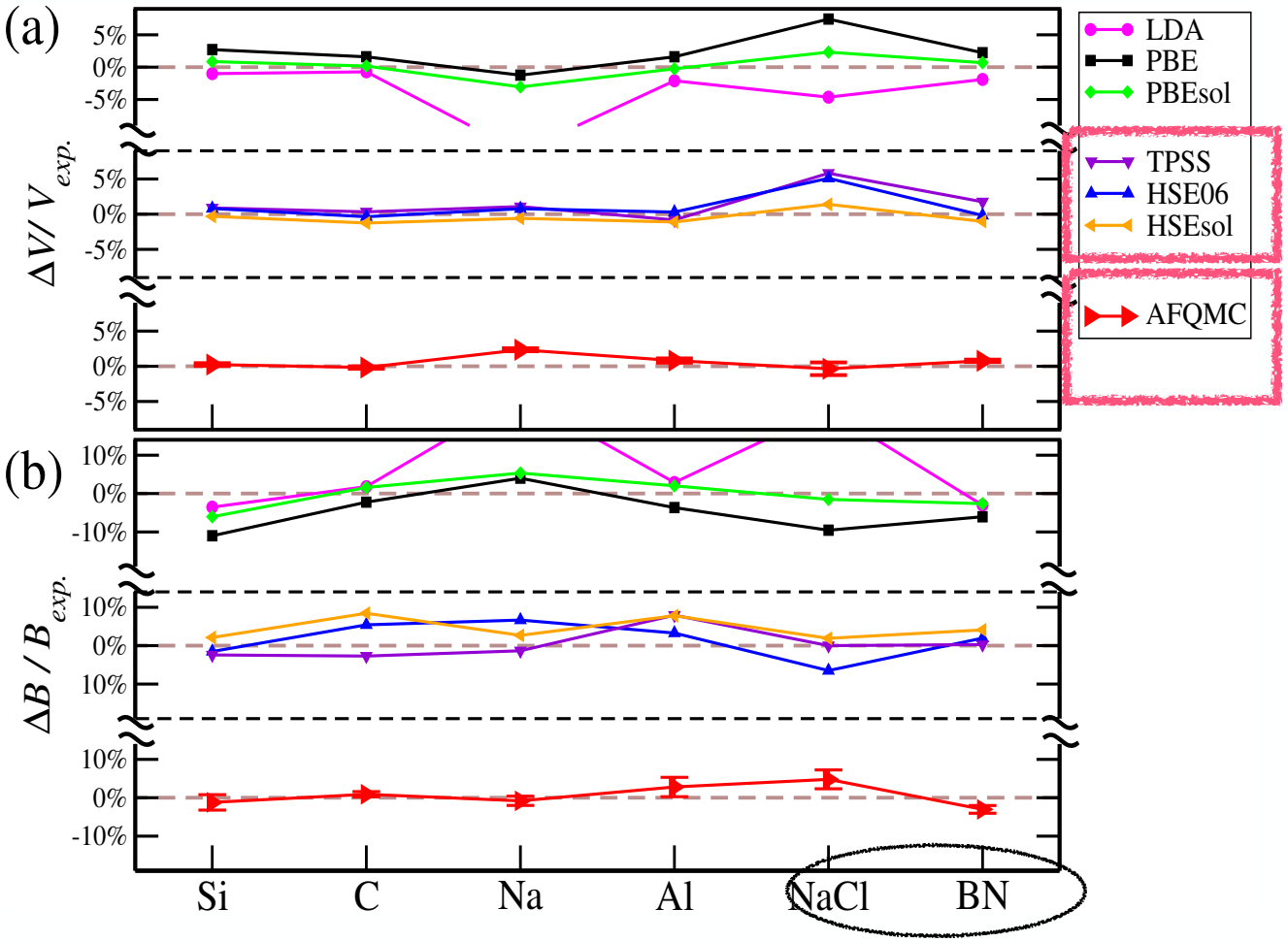
Total energy calculations in solids

- Basis from downfolding (Kohn-Sham orbitals: occupied and virtual)

Relative error vs. expt

Eq volume

Bulk mod



Ma, et al, PRL 114, 226401 (2015)

Quantum chemistry

JCTC Journal of Chemical Theory and Computation

Article

Cite This: J. Chem. Theory Comput. XXXX, XXX, XXX–XXX

pubs.acs.org/JCTC

On Achieving High Accuracy in Quantum Chemical Calculations of 3*d* Transition Metal-Containing Systems: A Comparison of Auxiliary-Field Quantum Monte Carlo with Coupled Cluster, Density Functional Theory, and Experiment for Diatomic Molecules

James Shee,[*,†] Benjamin Rudshteyn,[†] Evan J. Arthur,[‡] Shiwei Zhang,[¶,§] David R. Reichman,[†] and Richard A. Friesner[†]

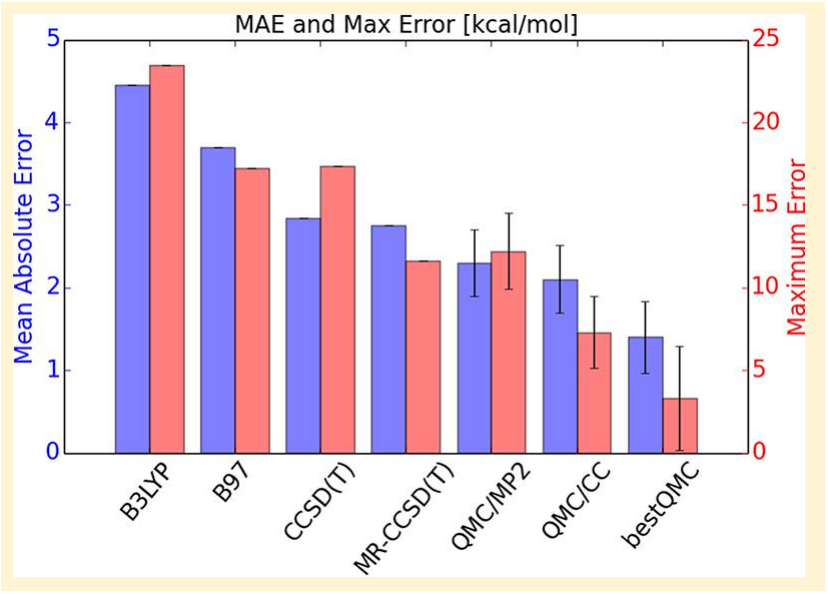
[†]Department of Chemistry, Columbia University, 3000 Broadway, New York, New York 10027, United States

[‡]Schrodinger Inc., 120 West 45th Street, New York, New York 10036, United States

[¶]Center for Computational Quantum Physics, Flatiron Institute, 162 5th Avenue, New York, New York 10010, United States

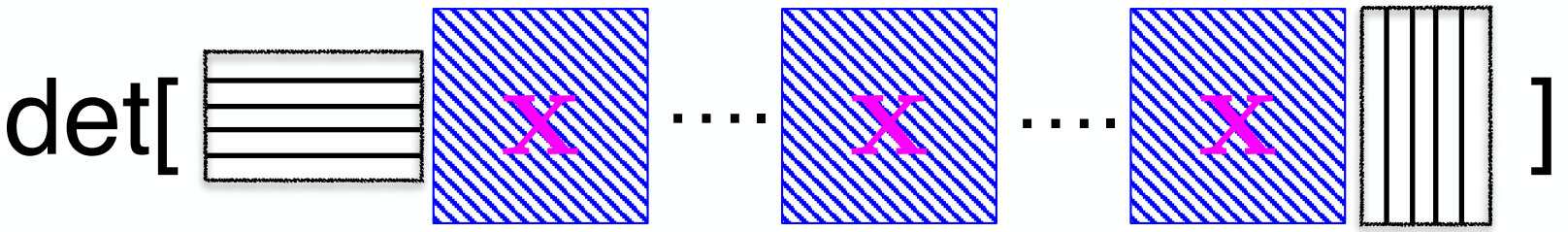
[§]Department of Physics, College of William and Mary, Williamsburg, Virginia 23187, United States

- Bond dissociation energy of 44 3d transition metal diatomics
- 10 DFT functionals; CCSD(T); multi-reference CCSD(T)
- Questioned 3 expt values
- AFQMC systematically reaches chemical accuracy



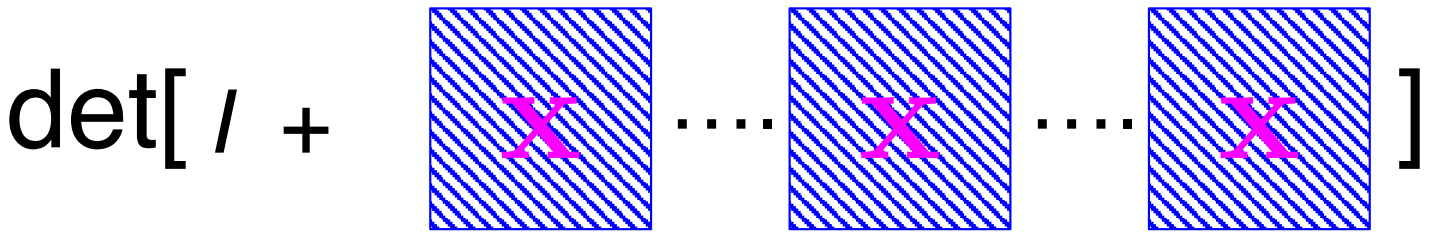
A major obstacle in finite-T method

T=0K:



$\mathcal{O}(N_s N_e^2)$

finite-T:



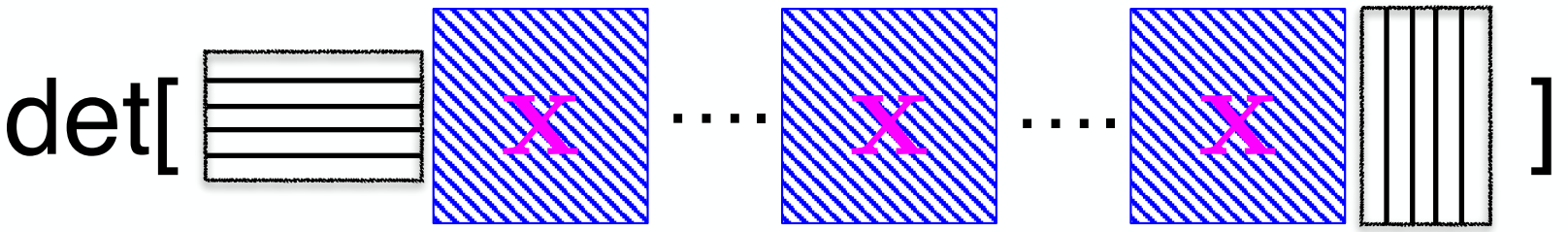
$\mathcal{O}(N_s^3)$

Continuum limit is required in ab initio computations in molecules and solids (basis set, or grid/planewaves) $N_s/N_e \to \infty$

Major obstacle for finite-T calculations

A major obstacle in finite-T method

T=0K:



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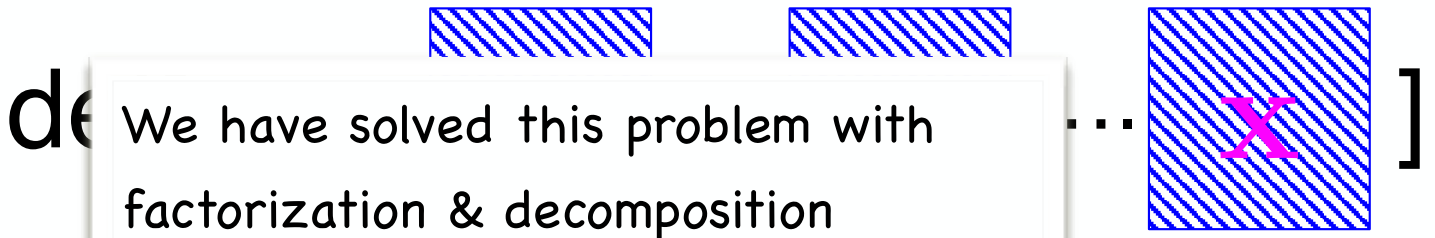


$\mathcal{O}(N_s^3)$

We have solved this problem with factorization & decomposition

– PRL (in press) arXiv:1906.02247

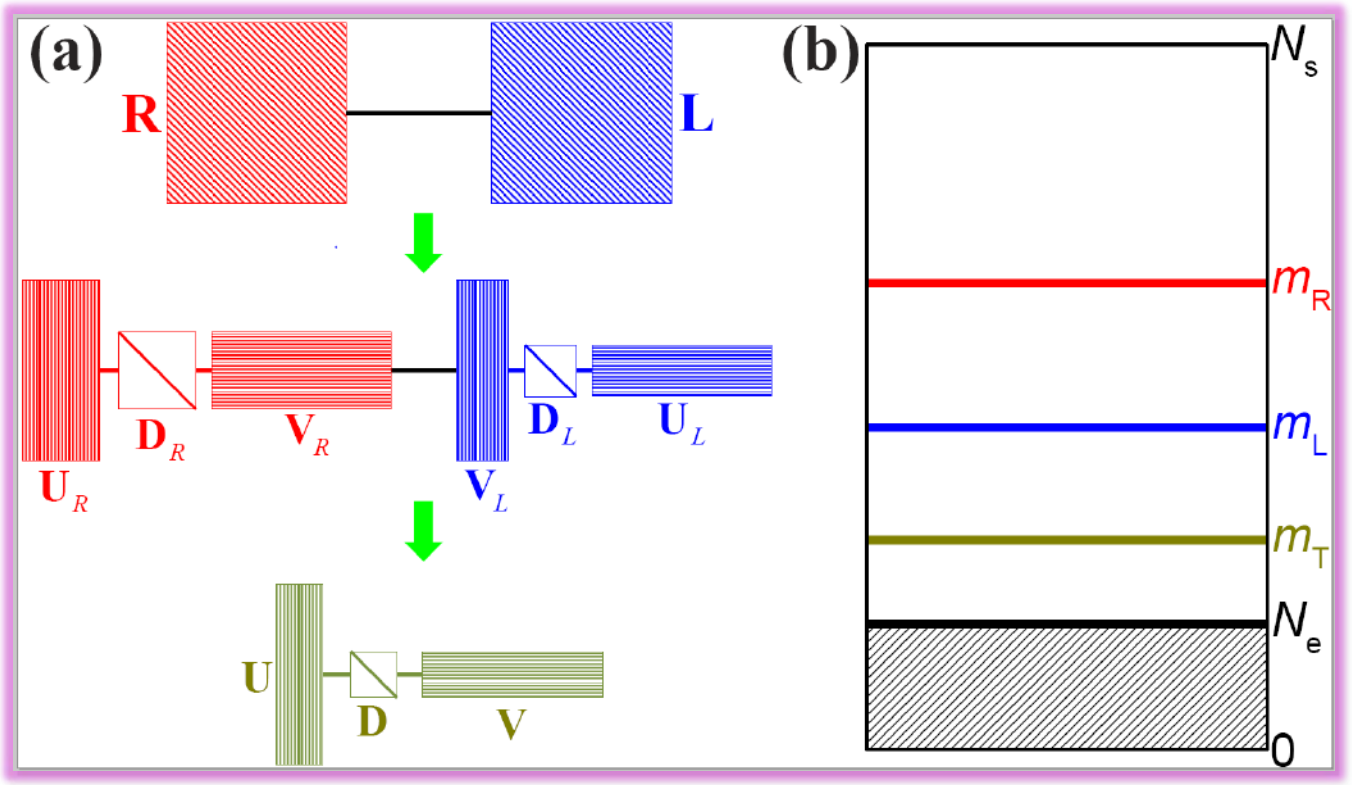
Continuum limit is required in ab initio computations in molecules and solids (basis set, or grid/planewaves) $N_s/N_e \to \infty$

Major obstacle for finite-T calculations

Approaching the continuum limit

Solution — low-rank decomposition:

$$\mathbf{R} = \mathbf{B}_\ell \mathbf{B}_{\ell-1} \cdots \mathbf{B}_2 \mathbf{B}_1 = \mathbf{U}_R \mathbf{D}_R \mathbf{V}_R \qquad \mathbf{L} = \mathbf{B}_M \mathbf{B}_{M-1} \cdots \mathbf{B}_{\ell+1} = \mathbf{V}_L \mathbf{D}_L \mathbf{U}_L$$

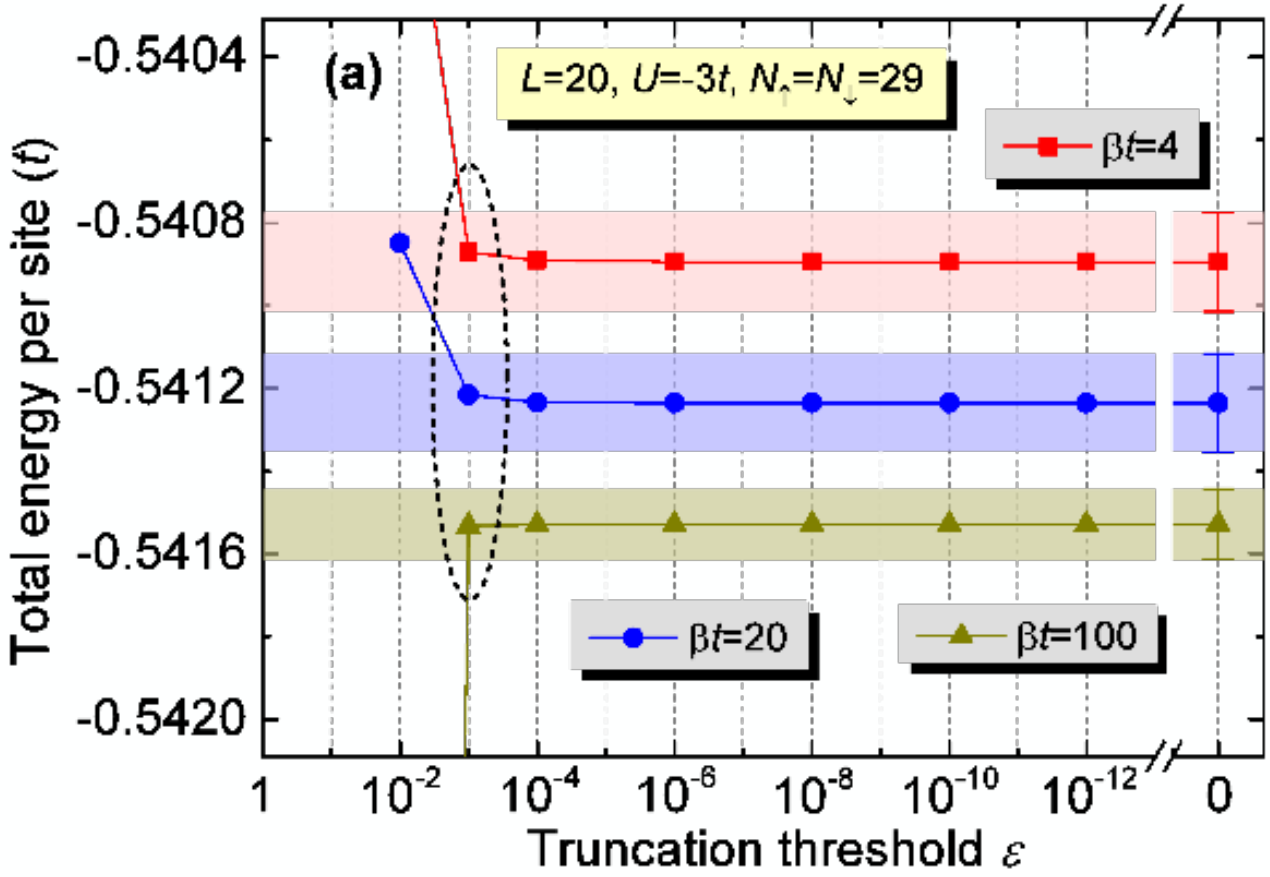


Note that in T=0: $m = N_e$!

He et al, PRL (in press)

Approaching the continuum limit

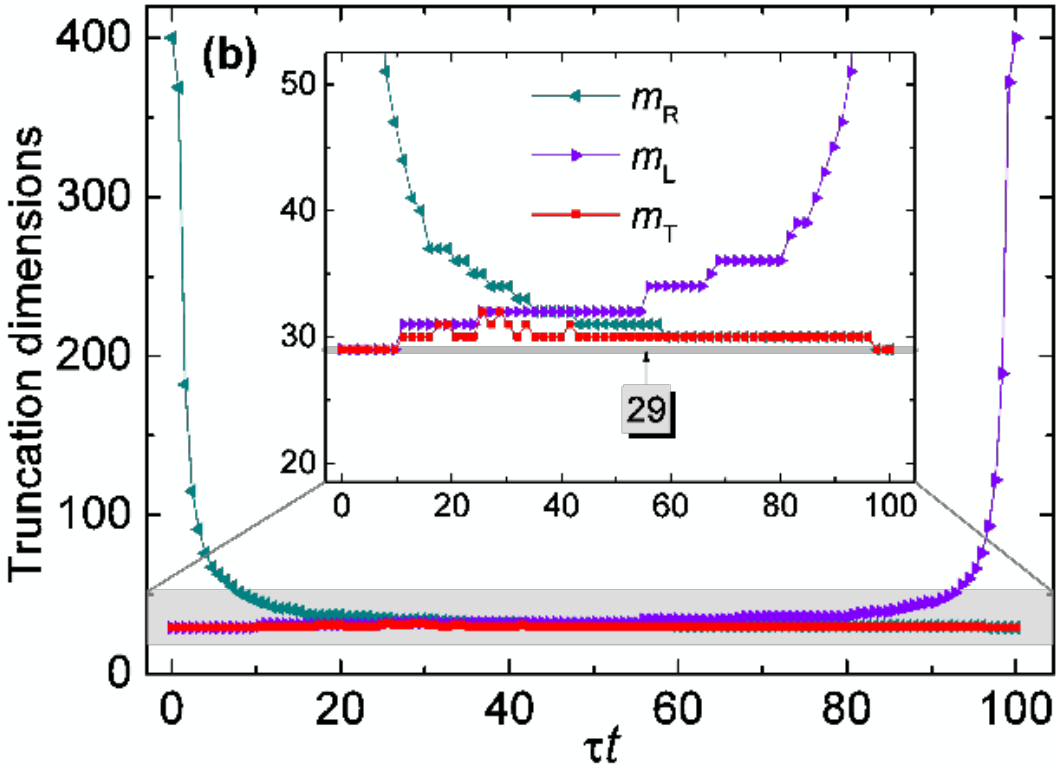
Can tune truncation threshold: (negligible error w/ 0.001t (aggressive))



He et al, PRL (in press)

Approaching the continuum limit

Dynamic truncation along the path; large speedups



He et al, PRL (in press)

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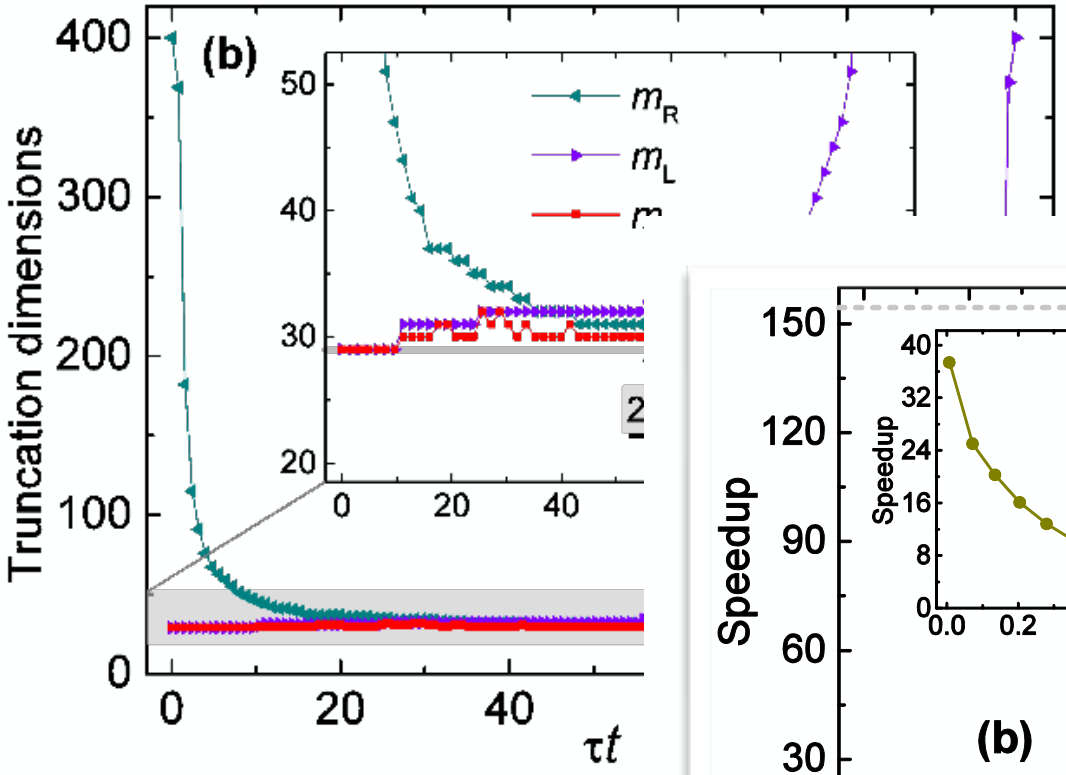
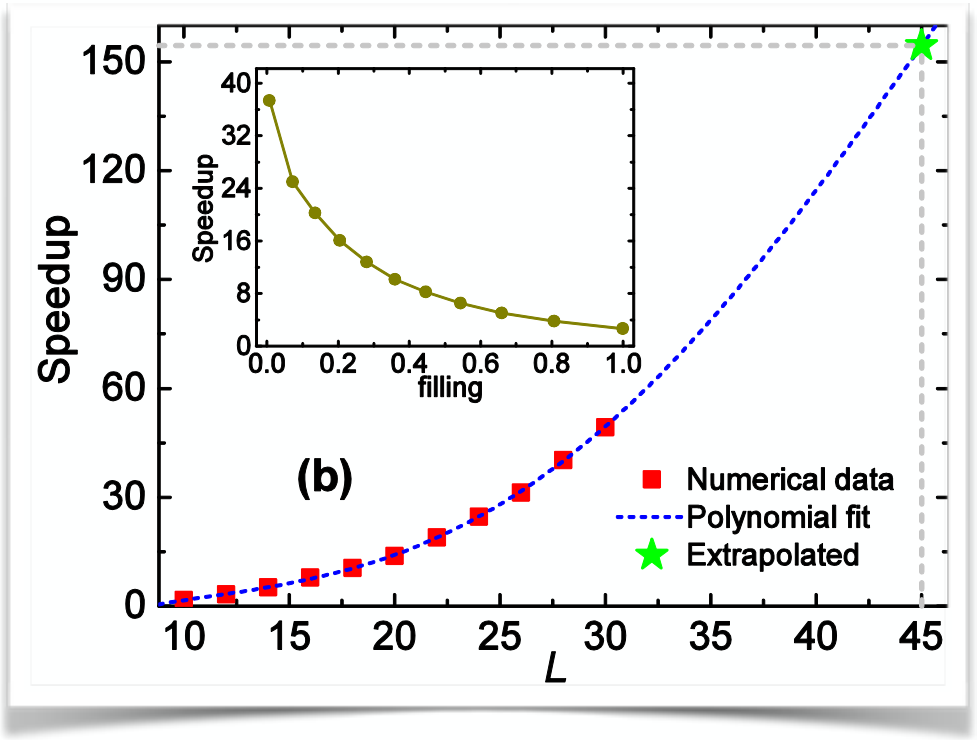


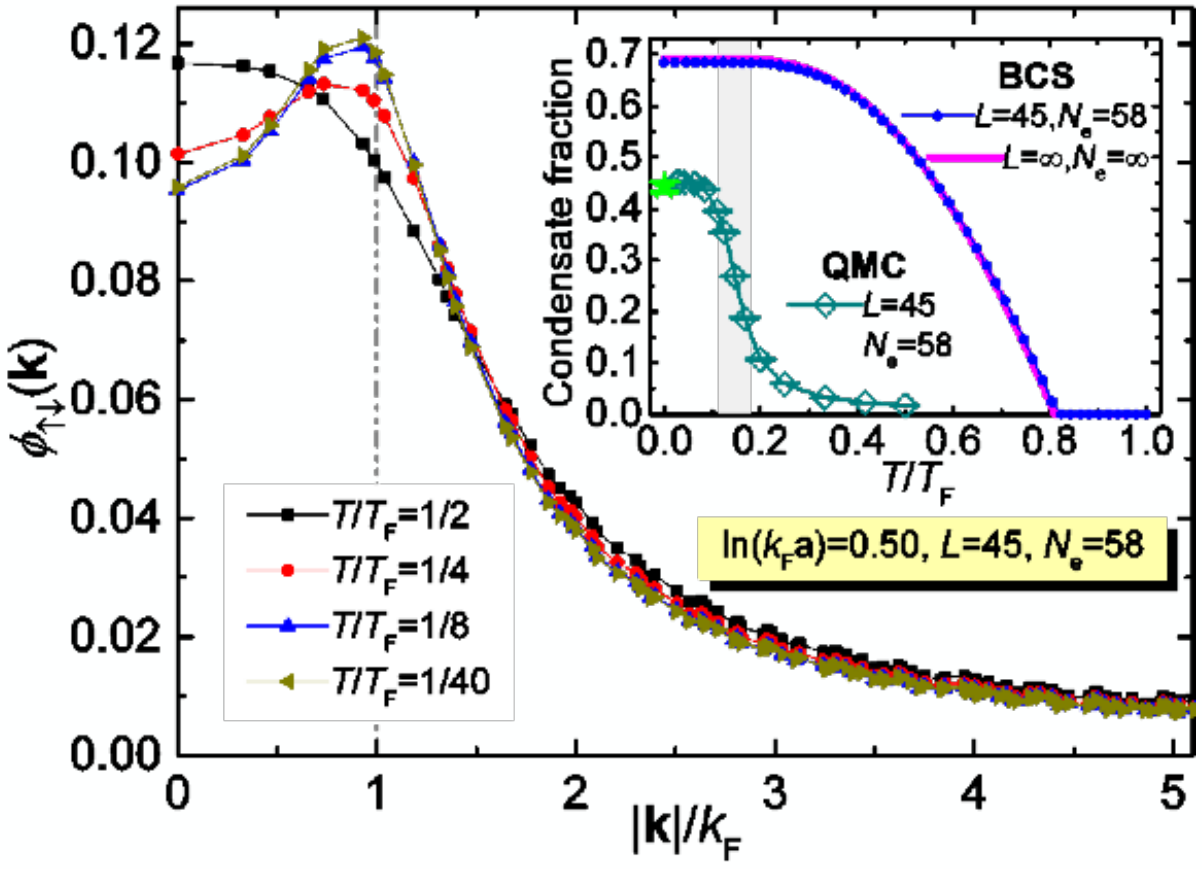


He et al, PRL (in press)

Application to Fermi gas - *on-going*

Allows access to very low T, large systems sizes

- computing exact properties in both normal and superfluid states
- examine BKT transition in 2D Fermi gas



Pairing wf

Condensate frac

He et al, PRL (in press)

Summary

- Advances in computation —> new opportunities for synergy
  - progress in auxiliary-field QMC
  - sign problem $\neq$ can't do very accurate computation
- Ab initio calculations in quantum many-body systems:
  - Reformulate field theory for post-DFT calculation which utilizes much of the DFT machinery
  - Many-body wave function or density matrix expressed as a linear combination of DFT solutions in stochastic auxiliary fields
  - Controls sign/phase problem with gauge condition
- Many opportunities for further algorithmic and coding development
- Exceptional potential for parallelism -- petascale computing makes a wide range of problems accessible with this framework