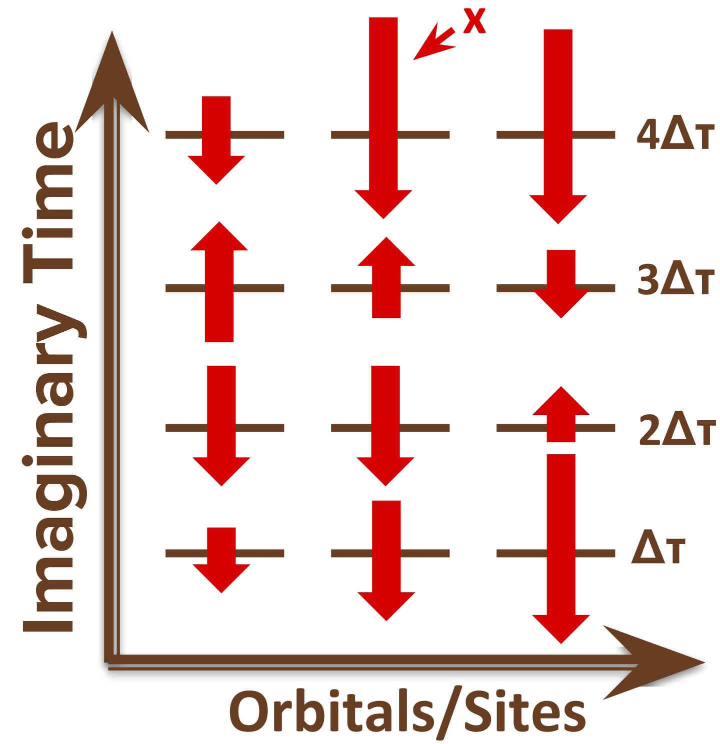
Auxiliary Field Quantum Monte Carlo 101



PROF. BRENDA RUBENSTEIN

Stochastics Methods for Electronic Structure

University of Pittsburgh - July 2019

BROWN

TUTORIAL OUTLINE

1. INTRODUCTION: What Is AFQMC and *Why*?
2. ALGORITHM: How It Actually Works
3. EXERCISES
    - PART ONE: AFQMC Propagation (Non-Interacting); Energy Evaluation
    - PART TWO: Hubbard-Stratonovich Transformation; Weight
4. THE PHASE PROBLEM
5. APPLICATIONS AND OPPORTUNITIES

WHAT IS AND WHY AFQMC?

SOME REFERENCES AND KEY PAPERS

- **USEFUL REVIEW**
  - M. Motta and S. Zhang. *Ab Initio Computations of Molecular Systems by the Auxiliary-Field Quantum Monte Carlo Method*. WIREs Computational Molecular Science (2018). [Molecular Review]
- **(READABLE) ORIGINAL PAPERS**
  - S. Zhang, J. Carlson, and J. Gubernatis. *Constrained Path Monte Carlo for Fermion Ground States*. Physical Review B. **55**, 7464 (1997). [Ground State Constrained Path Monte Carlo Algorithm]
  - S. Zhang and H. Krakauer. *Quantum Monte Carlo Method Using Phase-Free Random Walkers with Slater Determinants. Physical Review Letters*. **90**, 136401 (2003). [Phaseless Algorithm]

THE FIELD THAT MAKES PEOPLE FAMOUS FOR *OTHER THINGS*...

Monte Carlo calculations of coupled boson-fermion systems. I

R. Blankenbecler*
Laboratoire de Physique Théorique et Hautes Energies, University of Paris XI, 91405, Orsay, France

D. J. Scalapino and R. L. Sugar
Institute for Theoretical Physics and Department of Physics, University of California, Santa Barbara, California 93106
(Received 15 June 1981)

Monte Carlo Methods for the Nuclear Shell Model

C. W. Johnson, S. E. Koonin, G. H. Lang, and W. E. Ormand
W. K. Kellogg Radiation Laboratory, California Institute of Technology, Pasadena, California 91125
(Received 31 August 1992)

Quantum Monte Carlo study of the two-impurity Kondo Hamiltonian

R. M. Fye* and J. E. Hirsch
Department of Physics B-019, University of California, San Diego, La Jolla, California 92093
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Doug Scalapino (UCSB)

High-T_c Superconductivity

Steve Koonin

DOE Under-secretary

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Jorge Hirsch (UCSD)

h-Index!

WHAT IS AFQMC?

An **exponential** projector QMC technique that samples the space of **non-orthogonal Slater determinants**.

Taxonomy of Projector QMC Methods

Method	Projector	Single-Particle Basis	Quantization
Diffusion Monte Carlo (DMC)			
Full Configuration Interaction QMC (FCIQMC)			
Auxiliary Field QMC (AFQMC)			

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Full Configuration Interaction QMC (FCIQMC)	$-\tau(\hat{H}-E_T)$	ϕ_i^{orthog}	Second
Auxiliary Field QMC (AFQMC)			

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Auxiliary Field QMC (AFQMC)	$e^{-\tau(\hat{H}-E_T)}$	$\phi_i^{non-orthog}$	Second

WHAT DOES THIS MEAN?

An **exponential** projector QMC technique that samples the space of **non-orthogonal Slater determinants**.

Second-Quantized Hamiltonians

$$\hat{H} = \sum_{\sigma}\sum_{ij}^{N} T_{i\sigma,j\sigma}\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + \frac{1}{2}\sum_{\sigma\nu}\sum_{ijkl}^{N} V^{\sigma\nu\sigma\nu}_{ijkl}\hat{c}^{\dagger}_{i\sigma}\hat{c}^{\dagger}_{j\nu}\hat{c}_{l\nu}\hat{c}_{k\sigma}$$

Can use all of the standard tools of quantum chemistry - same bases, same contractions!

Remember Second Quantization...*from Yesterday?*

$$\{\hat{c}_{\alpha}, \hat{c}_{\beta}\} = 0$$

$$\{\hat{c}^{\dagger}_{\alpha}, \hat{c}^{\dagger}_{\beta}\} = 0$$

$$\{\hat{c}_{\alpha}, \hat{c}^{\dagger}_{\beta}\} = \delta_{\alpha,\beta}$$

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$$\{\hat{c}_{\alpha}, \hat{c}_{\beta}^{\dagger}\} = \delta_{\alpha,\beta}$$

$$T_{i\sigma,j\sigma} = \int d\vec{r}\phi_{p,\sigma}(\vec{r})\left(-\frac{1}{2}\frac{\partial^2}{\partial\vec{r}^2} - \sum_{a=1}^{N_n}\frac{Z_a}{|\vec{r}-\vec{R}_a|}\right)\phi_{q,\sigma}(\vec{r})$$

$$V_{ijkl}^{\sigma\nu\sigma\nu} = \int d\vec{r}d\vec{r}'\phi_{i,\sigma}(\vec{r})\phi_{j,\nu}(\vec{r}')\frac{1}{|\vec{r}-\vec{r}'|}\phi_{k,\sigma}(\vec{r})\phi_{l,\nu}(\vec{r}')$$

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Exponential Projection Operator

$$|\Psi_0\rangle = \lim_{n\to\infty} \boxed{\left(e^{-\Delta\tau\hat{H}}\right)}^{n} |\Phi_T\rangle$$

Like DMC...But in second-quantization, must be evaluated in a different way...(more later!)

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Non-Orthogonal Slater Determinants

Non-Orthogonal Orbitals

$$|\Psi\rangle = \prod_{i=1}^{N_\uparrow}\hat{c}_{u_{i,\uparrow}}^{\dagger}\prod_{i=1}^{N_\downarrow}\hat{c}_{v_{i,\downarrow}}^{\dagger}|\Phi\rangle$$

$$|u_i\rangle = \sum_{p}(U_\uparrow)_{pi}|\phi_p\rangle$$

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$$|u_i\rangle = \sum_p (U_\uparrow)_{pi} |\phi_p\rangle$$

Non-Zero Overlap!

$$\langle\Phi|\Psi\rangle = \prod_{\sigma} det(V_\sigma^\dagger U_\sigma) \neq 0$$

WHY DO WE NEED ANOTHER QMC?

- **Being able to exploit conventional quantum chemical techniques is a HUGE advantage**
    - Can directly import trial wave functions (HF, CASSCF, etc.) from other codes
    - Can directly import one- and two-body integrals, same PPs
    - Can potentially mix techniques

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  - Can potentially mix techniques

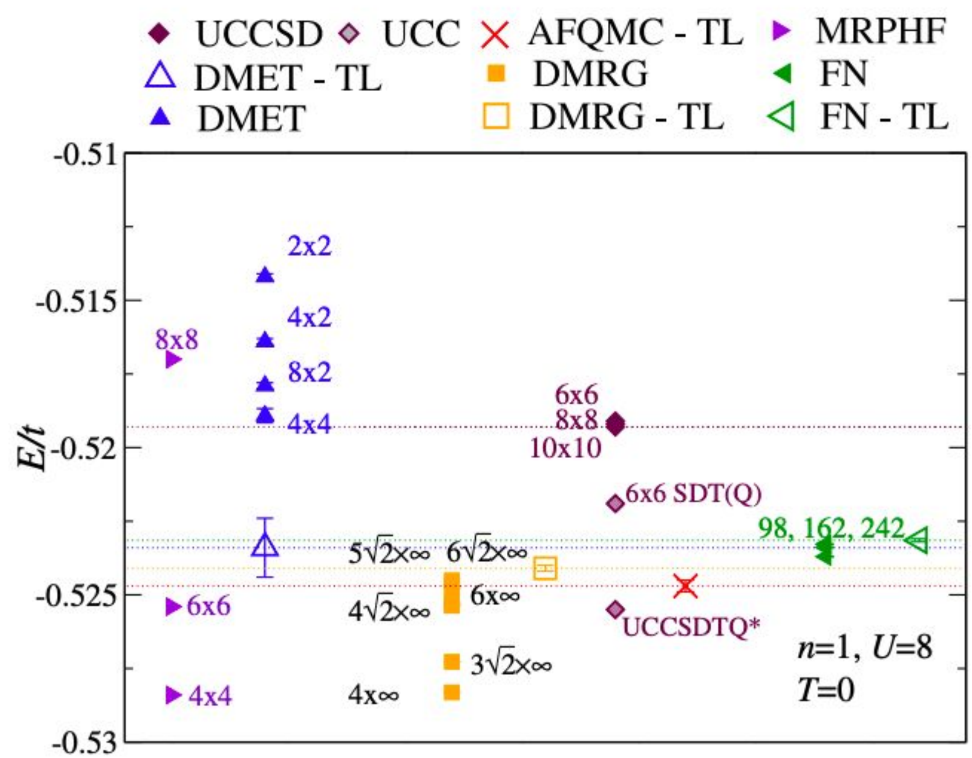
- **The sign problem varies in different representations**
  - For several key cases (1D lattices, half-filling), no sign problem!
  - Sign constraints *thought* to be more accurate, mild

AFQMC: THE GOLD STANDARD IN PHYSICS

Half-Filled Hubbard Model in Thermodynamic Limit

AFQMC Is THE BENCHMARK Against Which All Other Methods Are Compared

One could imagine perturbing off of half-filling to get other non-trivial results



J.P.F. Le Blanc et al., *PRX* (2015).

THE LEAP TO CHEMISTRY

Method for Performing Monte Carlo Calculations for Systems with Fermions

D. J. Scalapino and R. L. Sugar
Phys. Rev. Lett. **46**, 519 – Published 23 February 1981

Article | References | Citing Articles (132) | PDF | Export Citation

Monte Carlo calculations of coupled boson-fermion systems. II

D. J. Scalapino and R. L. Sugar
Phys. Rev. B **24**, 4295 – Published 15 October 1981

Article | References | Citing Articles (64) | PDF | Export Citation

1981

THE LEAP TO CHEMISTRY

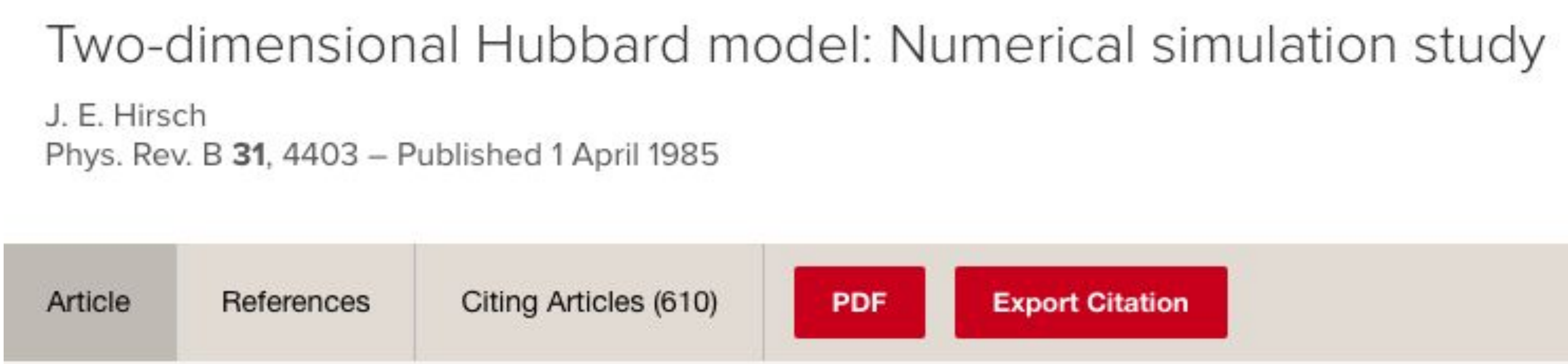
Discrete Hubbard-Stratonovich transformation for fermion lattice models

J. E. Hirsch

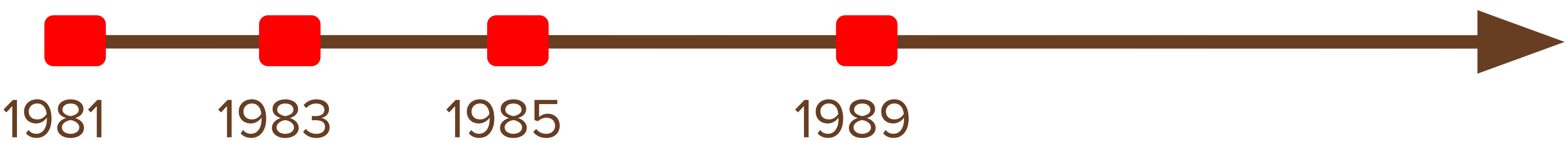
Phys. Rev. B **28**, 4059(R) – Published 1 October 1983; Erratum Phys. Rev. B **29**, 4159 (1984)

Article | References | Citing Articles (236) | PDF | Export Citation

THE LEAP TO CHEMISTRY



THE LEAP TO CHEMISTRY

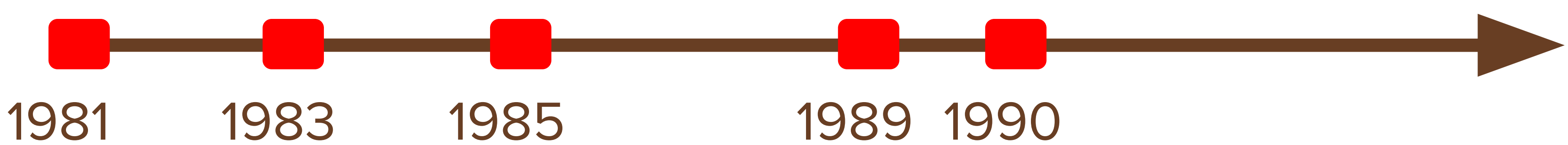


THE LEAP TO CHEMISTRY

Sign problem in the numerical simulation of many-electron systems

E. Y. Loh, Jr., J. E. Gubernatis, R. T. Scalettar, S. R. White, D. J. Scalapino, and R. L. Sugar
Phys. Rev. B **41**, 9301 – Published 1 May 1990

Article | References | Citing Articles (260) | PDF | Export Citation

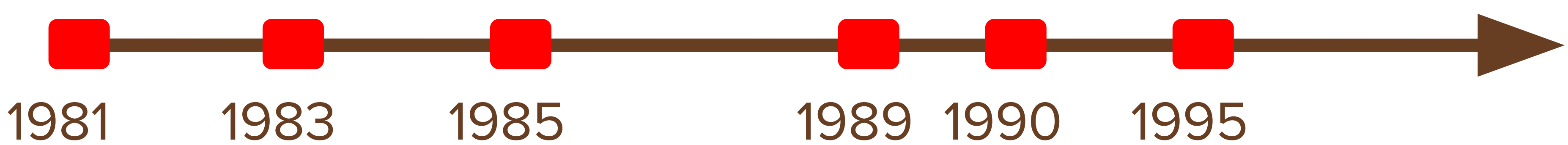


THE LEAP TO CHEMISTRY

Constrained Path Quantum Monte Carlo Method for Fermion Ground States

Shiwei Zhang, J. Carlson, and J. E. Gubernatis
Phys. Rev. Lett. **74**, 3652 – Published 1 May 1995

Article | References | Citing Articles (85) | PDF | Export Citation



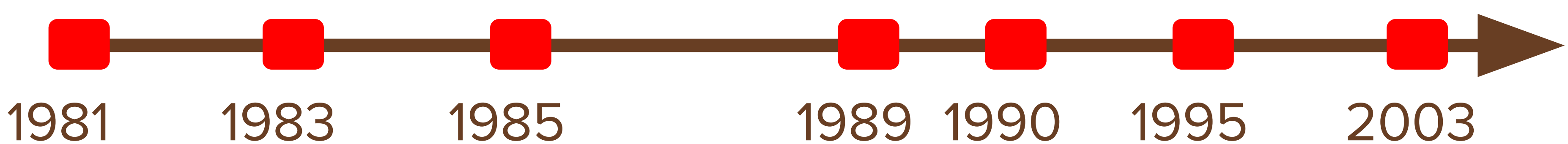
THE LEAP TO CHEMISTRY

Finally Chemistry (Sort Of)!

Quantum Monte Carlo Method using Phase-Free Random Walks with Slater Determinants

Shiwei Zhang and Henry Krakauer
Phys. Rev. Lett. **90**, 136401 – Published 4 April 2003

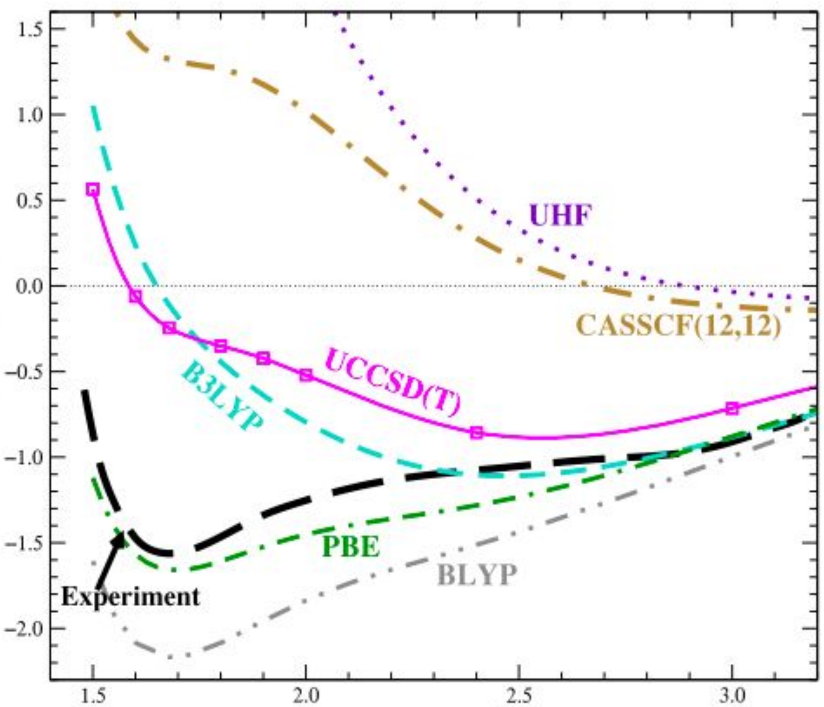
Article | References | Citing Articles (124) | PDF | HTML | Export Citation



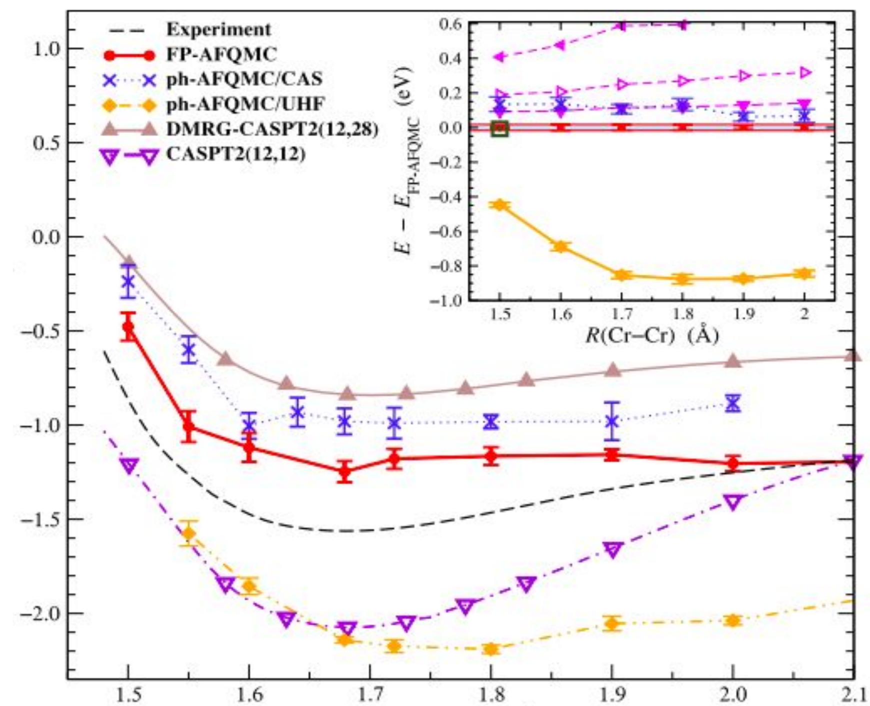
BUT, ALSO USEFUL IN CHEMISTRY…

The Binding Energy of the Chromium Dimer (Historically Difficult!)

Binding Energy (eV)



R(Cr-Cr) (Å)



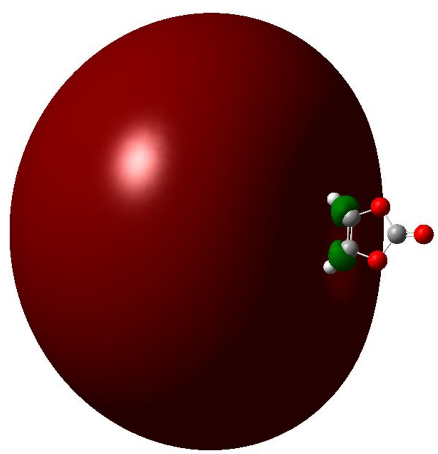
R(Cr-Cr) (Å)

W. Purwanto and S. Zhang, JCP (2015).

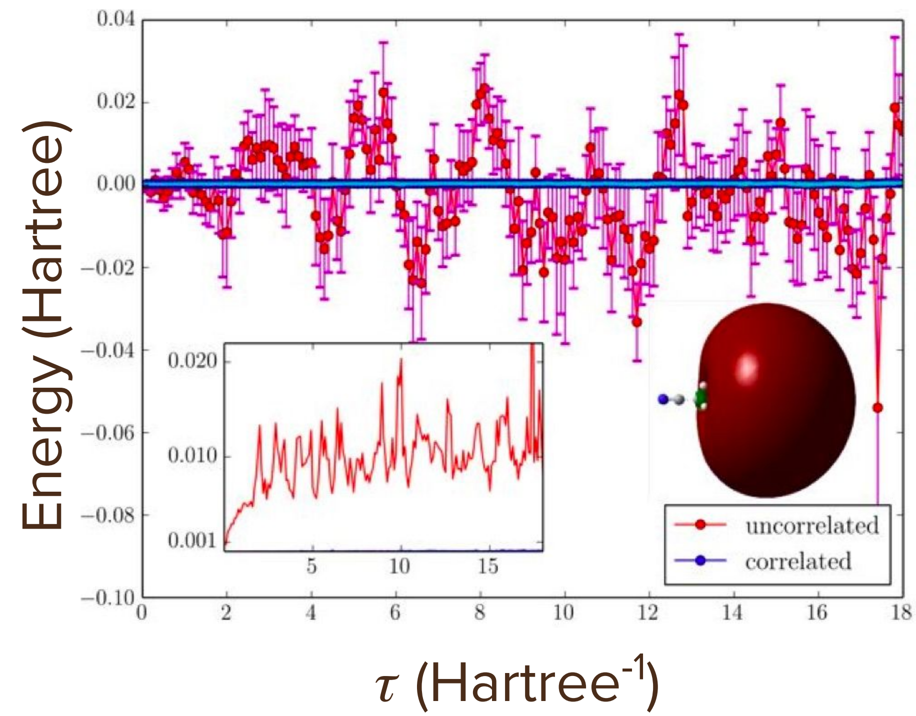
BUT, ALSO USEFUL IN CHEMISTRY…

Dipole-Bound anions bind an excess electron far from their nuclei via their dipole moments.

- **Critical Dipole Moment:** >1.625 D
- **Average Distance Between Electron and Neutral Core:** 10-100s Å
- **Molecular Electron Binding Energies:** >10s cm^{-1}



$C_3H_2O_3^-$



E. Fermi and E. Teller, *Physical Review* (1947); H. Hao, K. Jordan, and B. Rubenstein, *JPCL* (2018).

BUT, ALSO USEFUL IN CHEMISTRY…

Smaller Error Bars via AFQMC than DMC for Significantly Less Cost…

Table 1. EBEs and Dipole Moments of Selected Species from Experiment and Self-Consistent Field [HF], Coupled Cluster [CCSD(T)], DMC, and C-AFQMC Calculations

		EBE (cm^{-1})				
	dipole moment (D)	experiment	ΔSCF[a]	CCSD(T)[a]	DMC[b]	C-AFQMC[c]
SO	1.55[62]	not bound	−3.84	−4.13	−308.20 ± 70.82	−4.54 ± 0.64
HCN	2.98[62]	13[63]	11.00	7.44	46.17 ± 45.30	10.80 ± 2.95
CH_2CHCN	3.87[62]	56−87[12,64]	43.30	61.87	106.63 ± 58.12	65.70 ± 11.03
CH_3CN	3.92[62]	93−145[12,64]	50.83	103.00	93.83 ± 36.21	95.85 ± 9.73
C_3H_2	4.14[65]	170 ± 50[66]	54.61	162.08	151.22 ± 64.25[d]	132.45 ± 9.43[e]
$C_3H_2O_3$	4.55[62]	194 ± 24[67]	103.13	163.31	213.98 ± 116.15	157.70 ± 17.96

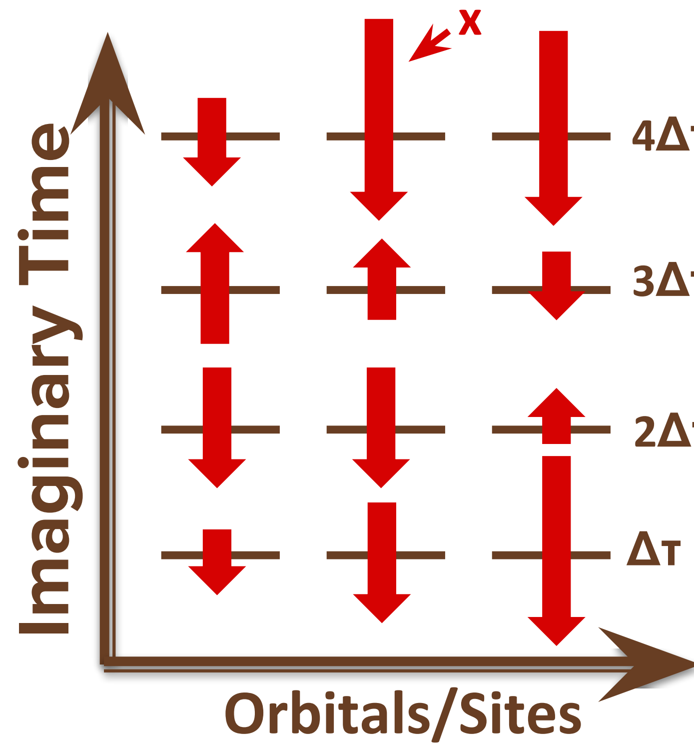
Note: Perhaps, More Accurate DMC Calculations Could Be Achieved…

H. Hao, K. Jordan, and B. Rubenstein, JPCL (2018).

THE MATH BEHIND THE ALGORITHM

Auxiliary Field Quantum Monte Carlo

At a practical level, AFQMC simulations sample a Gaussian-distributed set of fields, much as in a classical MC simulation of the Ising model.



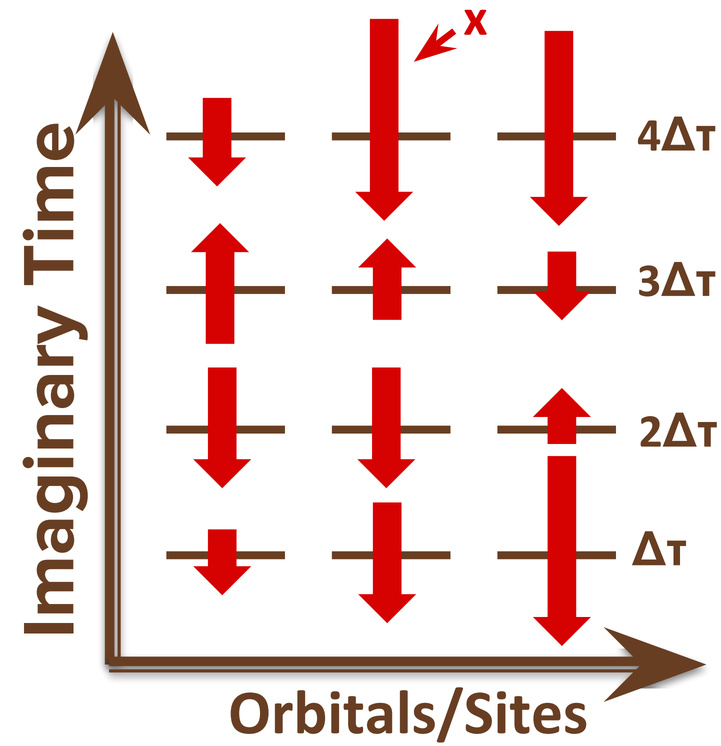
S. Zhang and H. Krakauer, Physical Review Letters (2003); M. Motta and S. Zhang, ArXiv:1711.02242 (2017).

Auxiliary Field Quantum Monte Carlo

Ground State Projection:

$$\boxed{|\Psi_0\rangle} = \lim_{n\to\infty} \left(e^{-\Delta\tau\hat{H}}\right)^n |\Psi_T\rangle$$

Exact Ground State Wave Function



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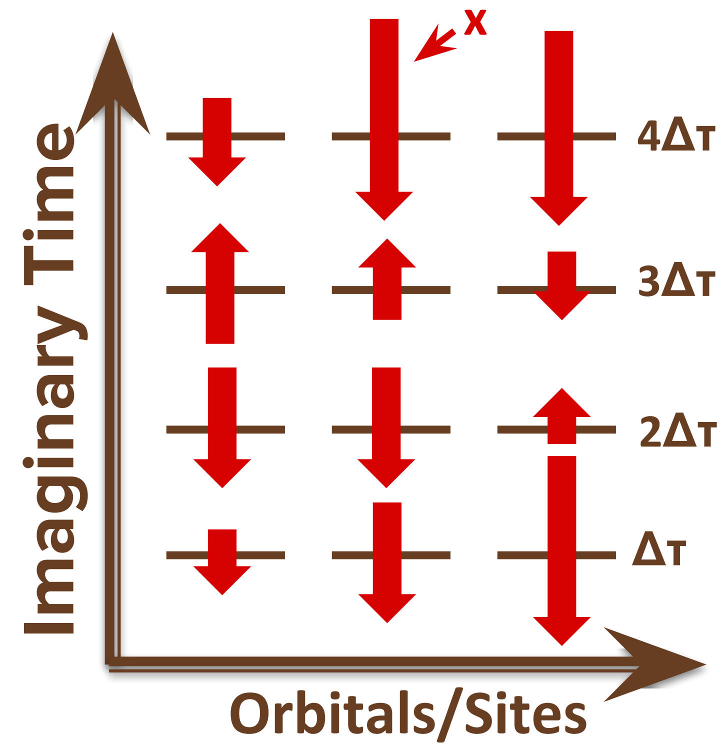
Exact Ground State Wave Function

Trial Wave Function
(HF, Non-Interacting, DFT, CASSCF...)



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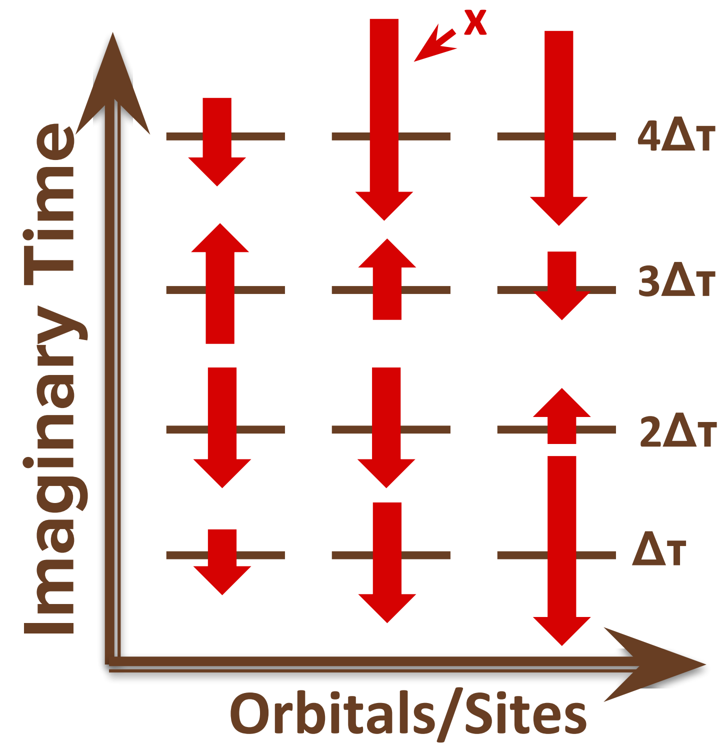
Exact Ground State Wave Function

Projection Operator

Trial Wave Function
(HF, Non-Interacting, DFT, CASSCF...)



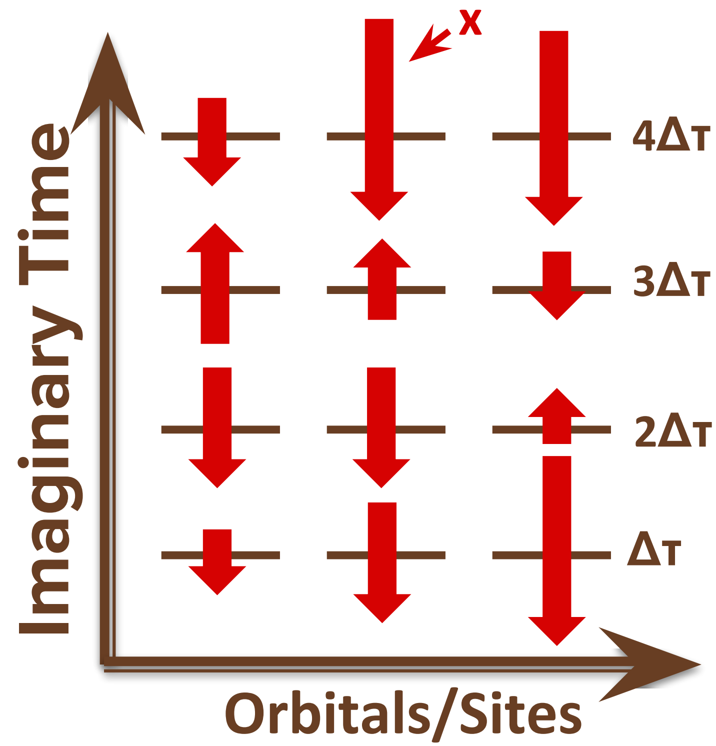
S. Zhang and H. Krakauer, Physical Review Letters (2003); M. Motta and S. Zhang, ArXiv:1711.02242 (2017).

Auxiliary Field Quantum Monte Carlo

Ground State Projection:

$$|\Psi_0\rangle = \lim_{n\to\infty} \left(\underbrace{\boxed{e^{-\Delta\tau \hat{H}}}}_{\text{Projection Operator}} \right)^n |\Psi_T\rangle$$

But, This Is The Exponential of a **Two-Body** Operator! (And, We Can't Express This As a Matrix)



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Auxiliary Field Quantum Monte Carlo

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Projection Operator

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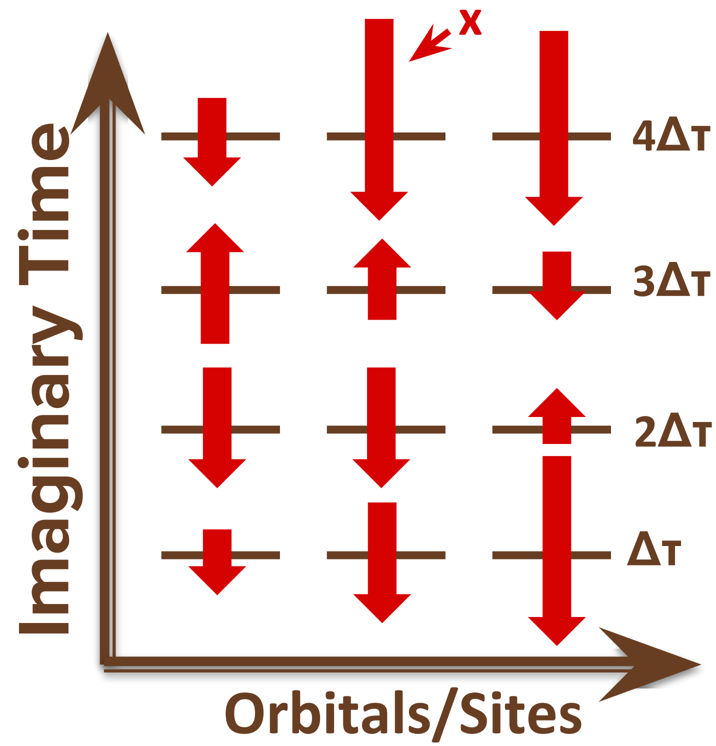
$$|\Phi'\rangle = e^{\hat{A}}|\Phi\rangle$$

One-Body Operator

Thouless's Theorem



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Auxiliary Field Quantum Monte Carlo

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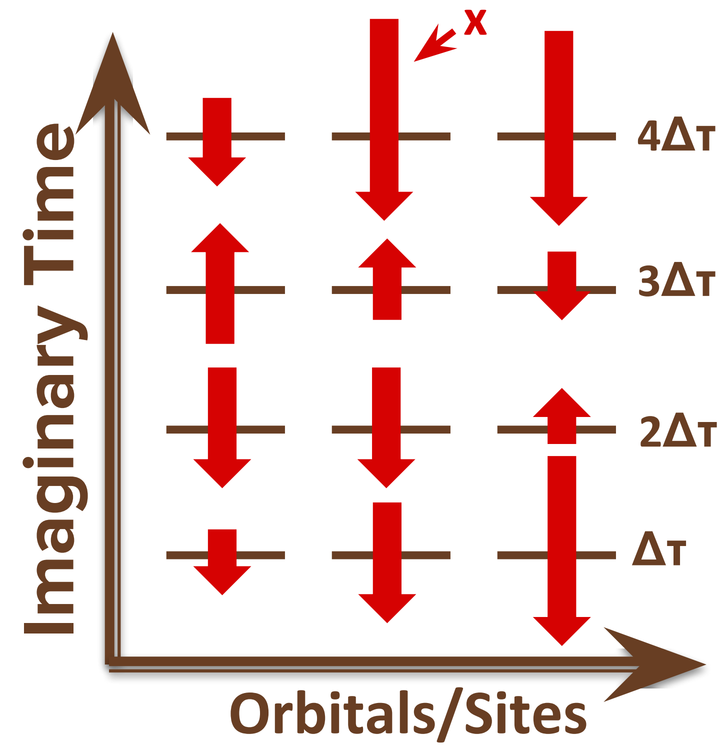
Suzuki-Trotter Factorization:

$$e^{-\Delta\tau\hat{H}} \approx e^{-\Delta\tau\hat{K}/2} e^{-\Delta\tau\hat{V}} e^{-\Delta\tau\hat{K}/2}$$

One-Body Operators

Two-Body Operators



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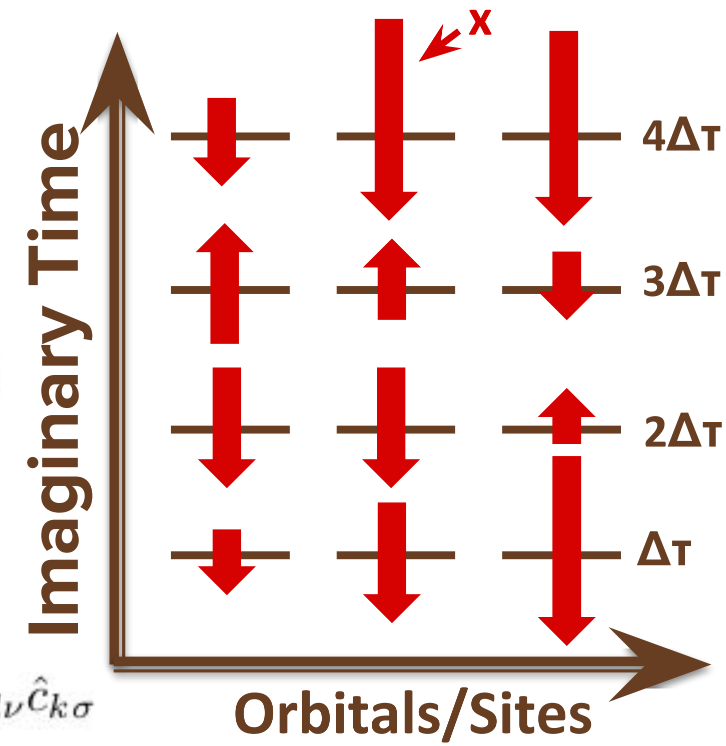
$$e^{-\Delta\tau\hat{H}} \approx e^{-\Delta\tau\hat{K}/2}e^{-\Delta\tau\hat{V}}e^{-\Delta\tau\hat{K}/2}$$

Ab Initio Hamiltonian (Hard!):

$$\hat{H} = \sum_{\sigma}\sum_{ij}^{N} T_{i\sigma,j\sigma}\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + \frac{1}{2}\sum_{\sigma\nu}\sum_{ijkl}^{N} V^{\sigma\nu\sigma\nu}_{ijkl}\hat{c}^\dagger_{i\sigma}\hat{c}^\dagger_{j\nu}\hat{c}_{l\nu}\hat{c}_{k\sigma}$$



S. Zhang and H. Krakauer, Physical Review Letters (2003); M. Motta and S. Zhang, ArXiv:1711.02242 (2017).

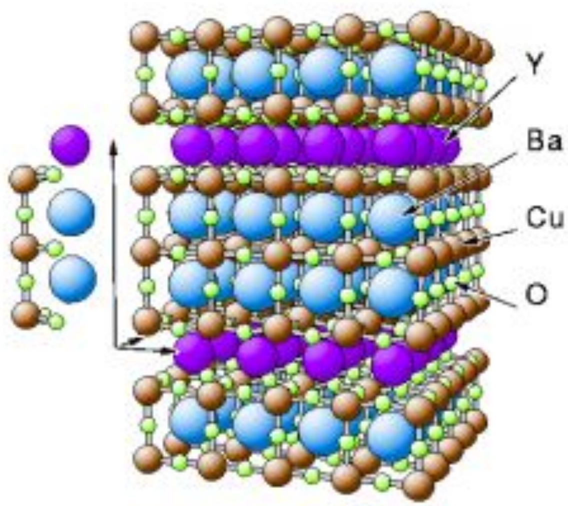
THE HUBBARD MODEL

THE HUBBARD MODEL

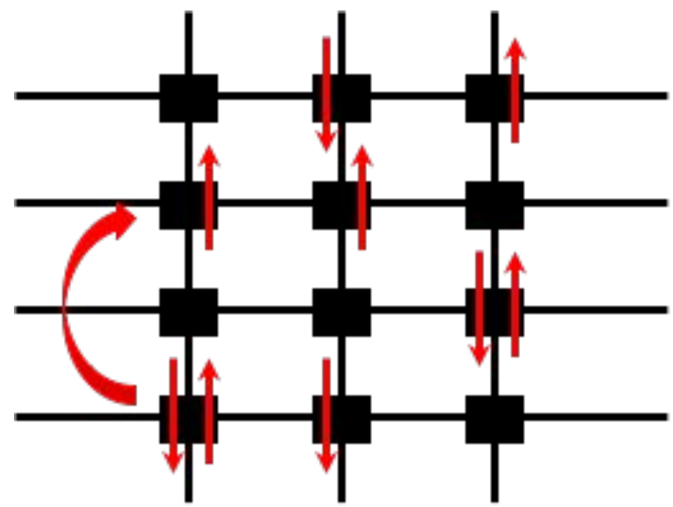
The Theorist's Lab Rat

Site Basis!

$$\hat{H}_{Hubbard} = -T \sum_{\langle ij \rangle \sigma} \left(\hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + H.C. \right) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$



Map to
Single-Band
Model



YBaCuO (Superconductor)

2D Lattice Model

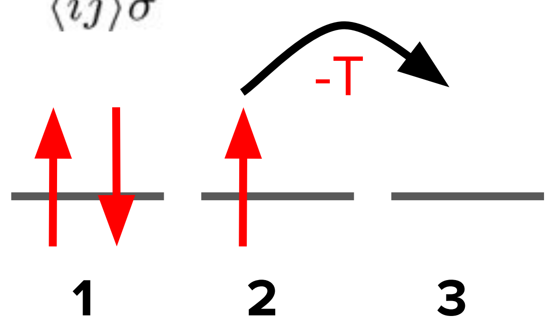
THE HUBBARD MODEL

The Theorist's Lab Rat

$$\hat{H}_{Hubbard} = -T \sum_{\langle ij \rangle \sigma} \left(\hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + H.C. \right) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

Kinetic ("Hopping") Term

$$-T \sum_{\langle ij \rangle \sigma} \left(\hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + H.C. \right)$$



$$K_{\uparrow} = \begin{array}{c c} & \begin{array}{ccc} \mathbf{1} & \mathbf{2} & \mathbf{3} \end{array} \\ \begin{array}{c} \mathbf{1} \\ \\ \mathbf{3} \end{array} & \begin{bmatrix} 0 & -T & -T \\ -T & 0 & -T \\ -T & -T & 0 \end{bmatrix} \end{array}$$

With Periodic Boundary Conditions

THE HUBBARD MODEL

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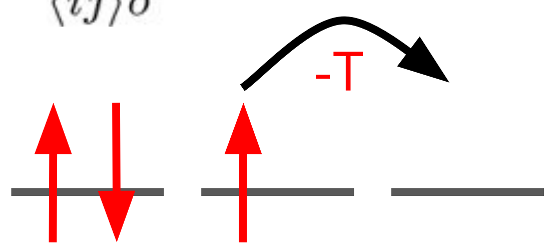
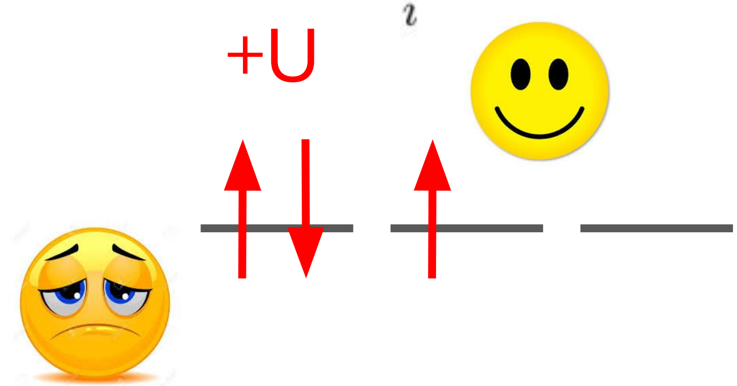


Electron Repulsion Term

$$U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$



(BACK TO) THE MATH BEHIND THE ALGORITHM

Auxiliary Field Quantum Monte Carlo

Ground State Projection:

$$|\Psi_0\rangle = \lim_{n\to\infty}\left(e^{-\Delta\tau\hat{H}}\right)^n |\Psi_T\rangle$$

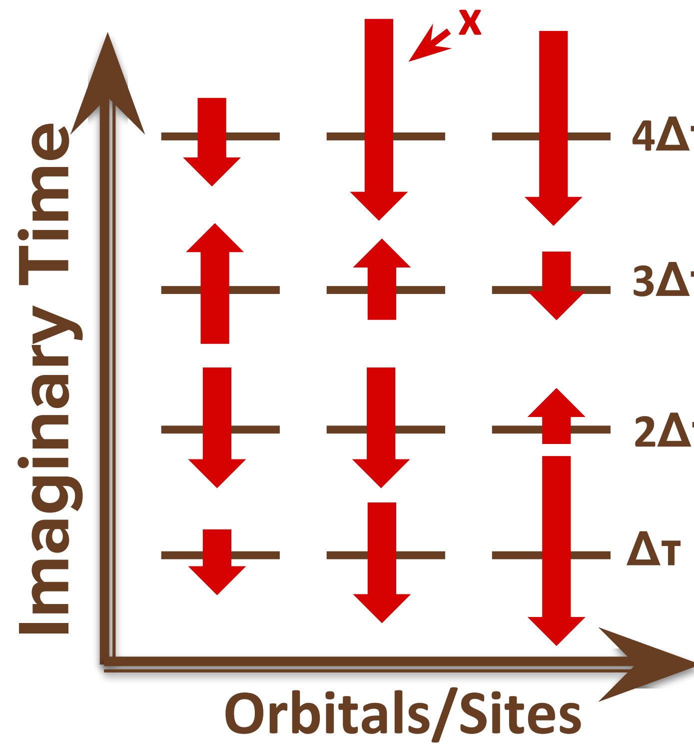
Suzuki-Trotter Factorization:

$$e^{-\Delta\tau\hat{H}} \approx e^{-\Delta\tau\hat{K}/2} e^{-\Delta\tau\hat{V}} e^{-\Delta\tau\hat{K}/2}$$

For Hubbard(!):

$$e^{-\Delta\tau\hat{K}} = e^{-\Delta\tau t\sum_{ij,\sigma}(\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}+\hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma})}$$

$$e^{-\Delta\tau\hat{V}} = e^{-\Delta\tau U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}}$$

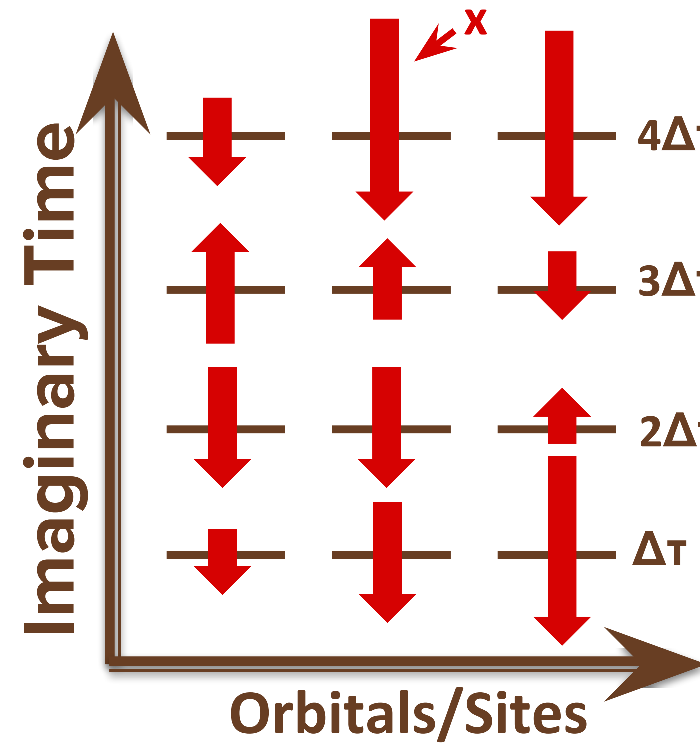


S. Zhang and H. Krakauer, Physical Review Letters (2003); M. Motta and S. Zhang, ArXiv:1711.02242 (2017).

HUBBARD-STRATONOVICH TRANSFORM

Gaussian Integral:

$$1 = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-1/2(x \pm y)^2} dx.$$



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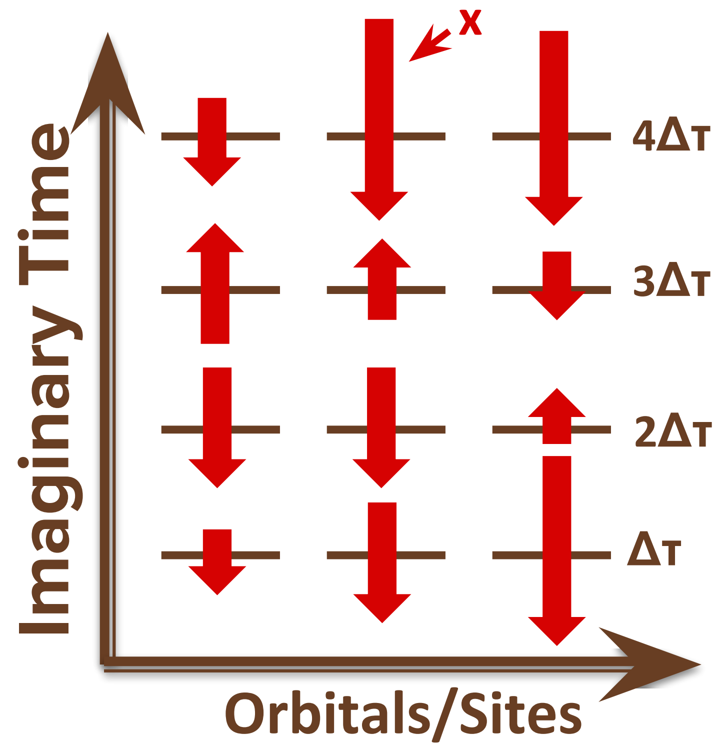
$$e^{y^2/2} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-1/2(x^2 \pm 2xy)} dx.$$



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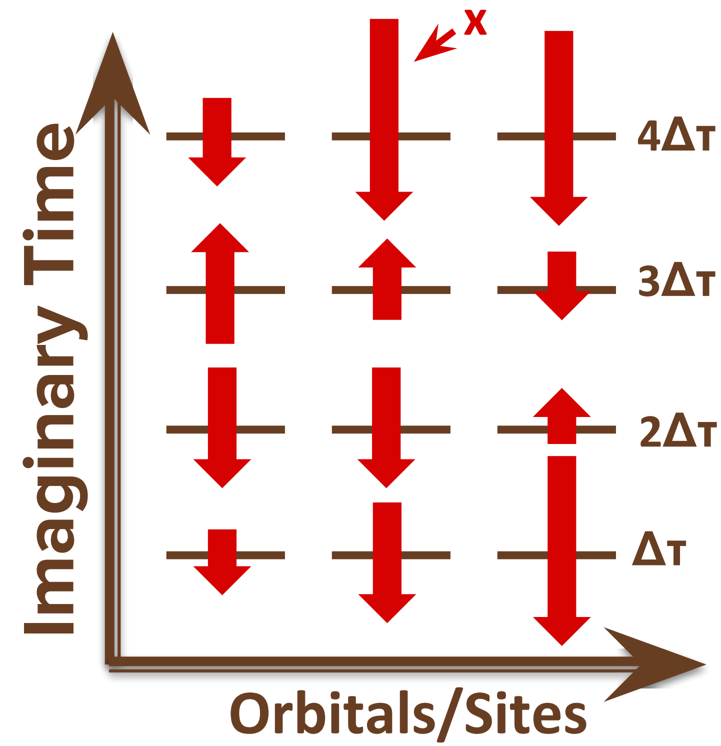
General *Continuous* Transform:

$$e^{-(\Delta\tau/2)\lambda\hat{v}^2} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-x^2/2} e^{x\sqrt{-\Delta\tau\lambda}\hat{v}}$$



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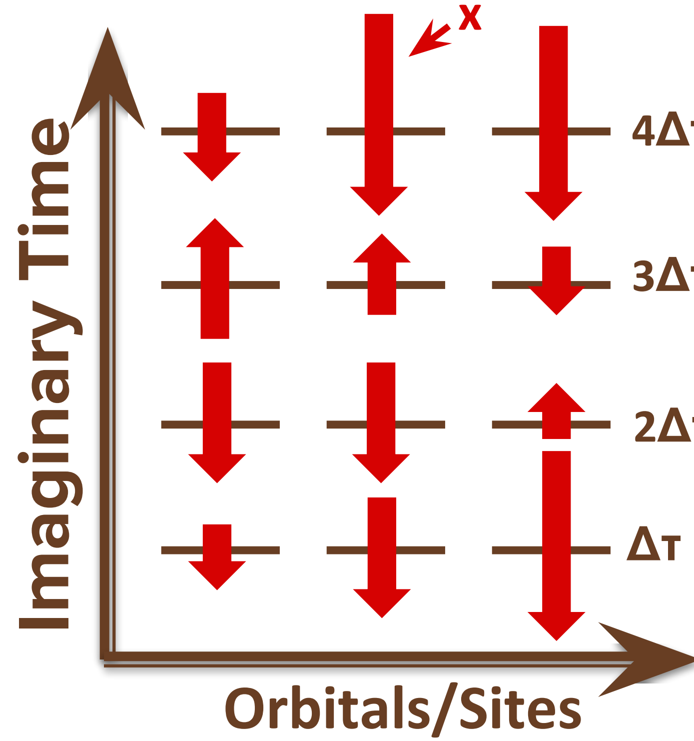
Need to Rewrite As Square:

$$e^{-\Delta\tau\hat{V}} = e^{-\Delta\tau U \sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}}$$



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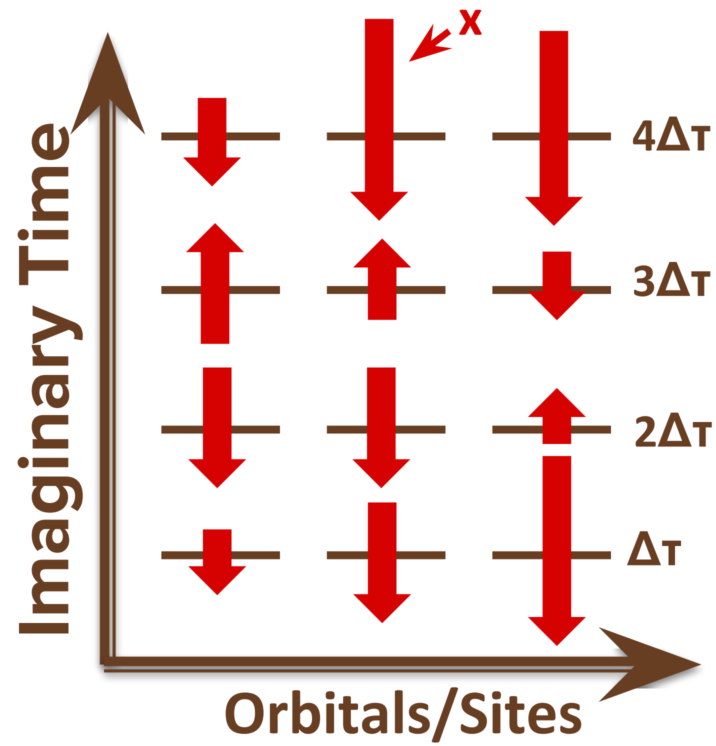
Need to Rewrite As Square:

$$e^{-\Delta\tau\hat{V}} = e^{-\Delta\tau U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}}$$

$$\hat{n}_\uparrow\hat{n}_\downarrow = -\frac{(\hat{n}_\uparrow - \hat{n}_\downarrow)^2}{2} + \frac{(\hat{n}_\uparrow + \hat{n}_\downarrow)}{2}$$

$$e^{-\Delta\tau\hat{V}} = \prod_i e^{\Delta\tau U(\hat{n}_{i\uparrow}-\hat{n}_{i\downarrow})^2/2} e^{-\Delta\tau U(\hat{n}_{i\uparrow}+\hat{n}_{i\downarrow})/2}$$



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HUBBARD-STRATONOVICH TRANSFORM

Do HS Transform:

$$e^{-\Delta\tau\hat{V}} = \prod_i e^{\Delta\tau U(\hat{n}_{i\uparrow}-\hat{n}_{i\downarrow})^2/2} e^{-\Delta\tau U(\hat{n}_{i\uparrow}+\hat{n}_{i\downarrow})/2}$$

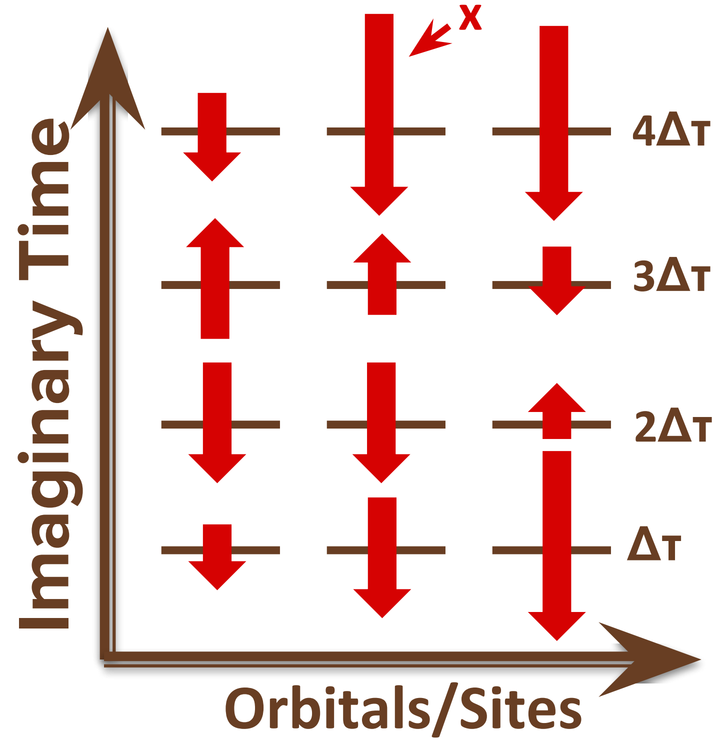
$$e^{-\Delta\tau\hat{V}} = \prod_i e^{-\Delta\tau U(\hat{n}_{i\uparrow}+\hat{n}_{i\downarrow})/2}$$

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx_i e^{-x_i^2/2} e^{x_i\sqrt{\Delta\tau U}(\hat{n}_{i\uparrow}-\hat{n}_{i\downarrow})}$$

Just Becomes a Matrix!

Merge:

$$e^{-\Delta\tau\hat{H}} = \int_{-\infty}^{\infty} d\vec{x}p(\vec{x})\hat{B}(\vec{x})$$



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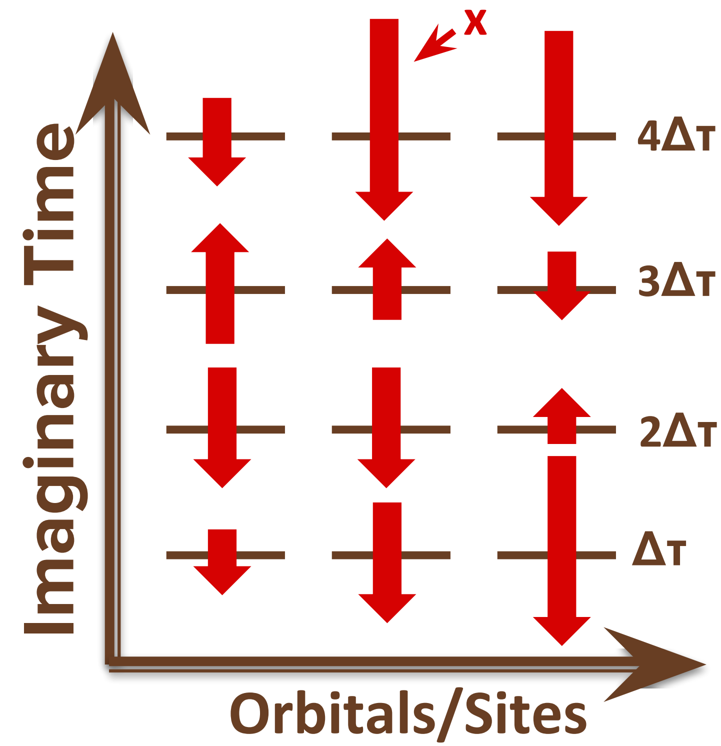
HUBBARD-STRATONOVICH TRANSFORM

What Does Transform Look Like?

$$e^{-\Delta\tau\hat{V}} = \prod_i e^{-\Delta\tau U(\hat{n}_{i\uparrow}+\hat{n}_{i\downarrow})/2} \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx_i e^{-x_i^2/2} e^{x_i\sqrt{\Delta\tau U}(\hat{n}_{i\uparrow}-\hat{n}_{i\downarrow})}$$

Up Potential Matrix

$$\left[e^{-\Delta\tau V}\right]_\uparrow = \begin{bmatrix} e^{-\Delta\tau U} e^{x_1\sqrt{\Delta\tau U}} & 0 & 0 \\ 0 & e^{-\Delta\tau U} e^{x_2\sqrt{\Delta\tau U}} & 0 \\ 0 & 0 & e^{-\Delta\tau U} e^{x_3\sqrt{\Delta\tau U}} \end{bmatrix}$$



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EXERCISES

PART I EXERCISES

- **GOAL: To Understand Propagation in the AFQMC Algorithm**
  - Form the Kinetic Operator and Kinetic Propagator
  - Iteratively Apply It To a Trial Wave Function
  - Measure the Energy (Should Be The Same As ED)

We will take it in steps, since very different than the usual!

PART I EXERCISES

Calculating energies is more complicated than yesterday due to the non-orthogonal Slater determinants you obtain!

$$\langle E_{mixed} \rangle = \frac{\langle \Psi_T | \hat{H} | \Psi \rangle}{\langle \Psi_T | \Psi \rangle}$$

$$\begin{aligned}
\langle E \rangle_{mixed} &= \frac{\langle \Psi_T | \hat{K} | \Psi \rangle}{\langle \Psi_T | \Psi \rangle} \\
&= -t \sum_{\langle i j \rangle \sigma} \frac{\langle \Psi_T | \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \hat{c}^{\dagger}_{j\sigma} \hat{c}_{i\sigma} | \Psi \rangle}{\langle \Psi_T | \Psi \rangle} \\
&= -t \sum_{\langle i j \rangle \sigma} \left(\langle \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} \rangle + \langle \hat{c}^{\dagger}_{j\sigma} \hat{c}_{i\sigma} \rangle \right)
\end{aligned}$$

PART I EXERCISES

Calculating energies is more complicated than yesterday due to the non-orthogonal Slater determinants you obtain!

$$\begin{aligned}\langle \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} \rangle &= \frac{\langle \Psi_T | \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} | \Psi \rangle}{\langle \Psi_T | \Psi \rangle} \\ &= \left[\Psi^{\sigma} \left[\left(\Psi^{\sigma}_T \right)^{\dagger} \Psi^{\sigma} \right]^{-1} \left(\Psi_T \right)^{\dagger} \right]_{ij}\end{aligned}$$

One-Body Density Matrix

Plug This Back Into Previous Expression