From real materials to model Hamiltonians with density matrix downfolding

(Converting a many-electron problem to a fewer-electron one)

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Florida State University

Based on
HJC, H. Zheng, L. K. Wagner J. Chem. Phys. (2015)
H.Zheng*, **HJC***, K. Williams, B. Busemeyer, L. K. Wagner, Front. Phys (2018)

SciDAC-DOE

Bluewaters

INT, Univ. Washington, Quantum Monte Carlo workshop, August 2018

Quantum many body problem

$$H\,\psi = E\,\psi$$

full H, approximate ψ

$$H = -\frac{1}{2}\sum_i \nabla_i^2 - \sum_{I,i} \frac{Z_I}{|r_I - r_i|} + \sum_{i,j,i<j} \frac{1}{|r_i - r_j|}$$

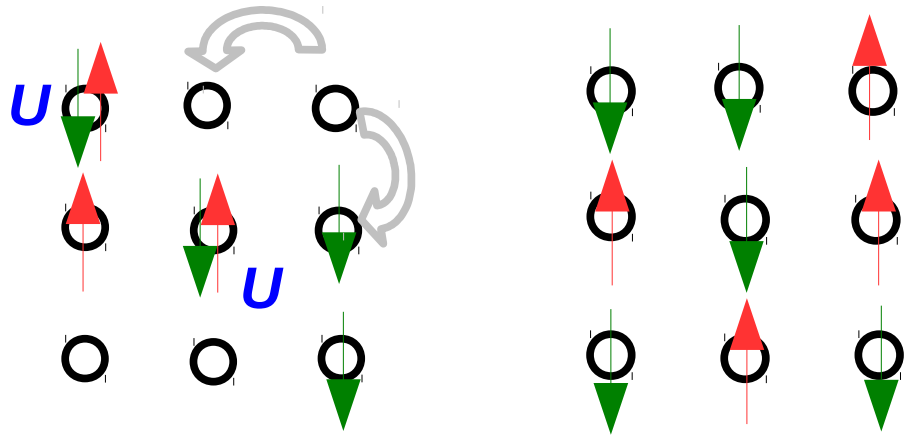
The real thing. Deals with **all electrons** (eg. Fionn's talk)**.**

Hilbert space large, so **smaller systems**.

How do we know we have an "exotic" phase? (eg. spin liquid etc)

Approximate "effective" *H*

$$H_{\text{Hubbard}} = -t \sum_{\langle i,j\rangle,\sigma} c^\dagger_{i,\sigma} c_{j,\sigma} + U \sum_i n^i_\uparrow n^i_\downarrow$$



Deals with **valence electrons** only (physically insightful): eg. many models of high Tc superconductivity

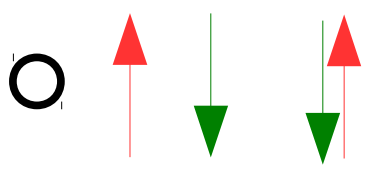
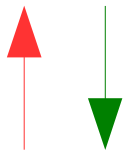
Smaller Hilbert space locally, more conducive for **larger scale simulations**

Several new diagnostics to characterize exotic phases

Models: hard to solve exactly

$$\tilde{H}\,\psi = E\,\psi$$

$$\psi = \sum_{q_1, q_2 \cdots q_N} \psi^{q_1 q_2 \cdots q_N} |q_1 q_2 q_N\rangle$$

q is  or 

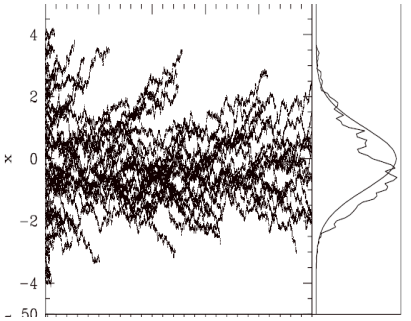
(depends on model)

The Hilbert space is **HUGE**!

N=100 spins ⇨ 10^{16} PB

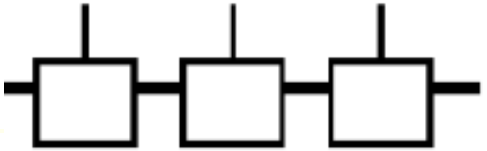
IBM has largest storage array of 120 PB

But many recent advances

ψ = 

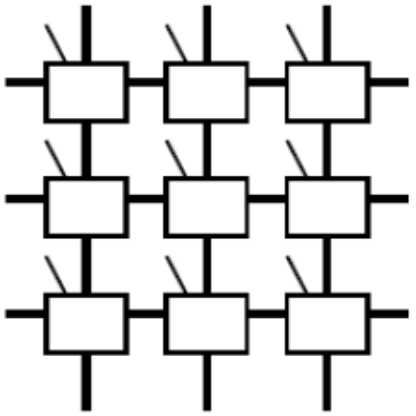
Quantum Monte Carlo (sign problem or trial wavefunction bias)

Ceperley, Becca, Sorella, Scalapino, Scalettar, Zhang, Alavi, Umrigar, Sandvik, Prokof'ev.....

$\psi \approx$ 

Can be made exact

Matrix Product State (MPS / DMRG)

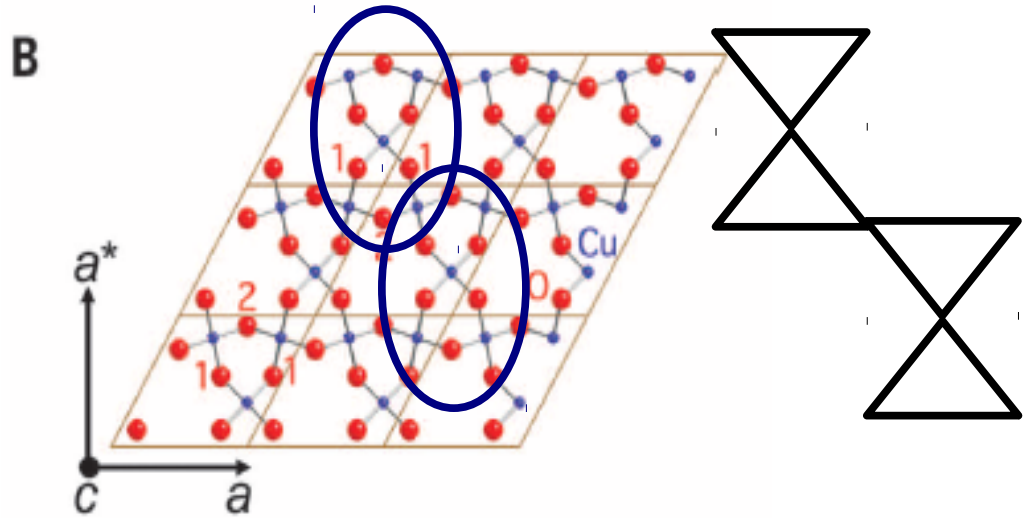


Tensor Product/Network State (TP/NS)

Wilson, White, Ostlund, Nishino, Vidal, Xiang, Verstraete, Cirac

Others: DMFT (Kotliar, Georges,Millis), DMET (Knizia, Chan)

Example of what the "model world" is interested in
2D kagome magnet: experimental realization Herbertsmithite



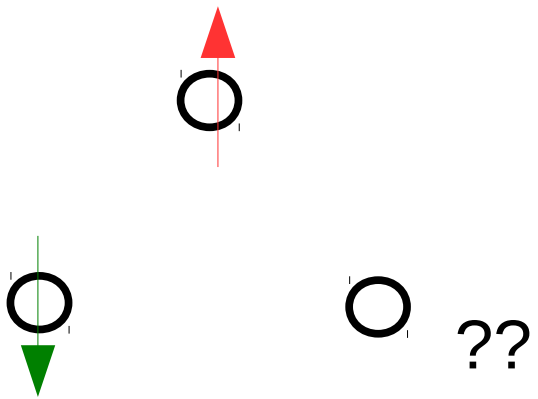
Every copper surrounded by four oxygens much like the high temperature cuprates.

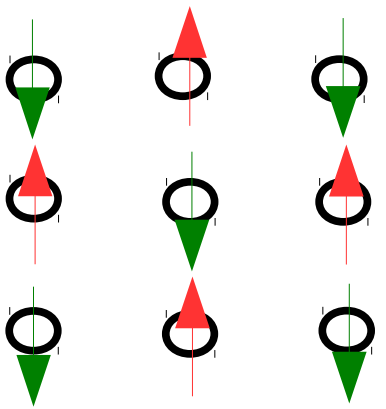
Coppers form a kagome lattice rather than a square lattice.

Both Mott insulators but low energy physics different.

Fu, Imai, Han, Y.S. Lee (Science 2015)

$$H = \sum_{i,j} J_{ij} S_i \cdot S_j$$

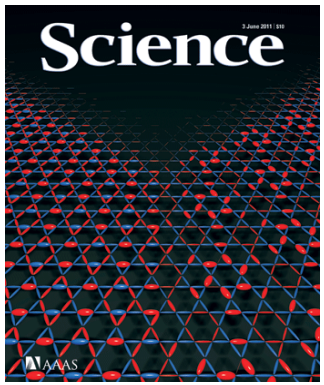




Frustrated

Un - frustrated

Kagome phase diagram: many competing phases with similar energy

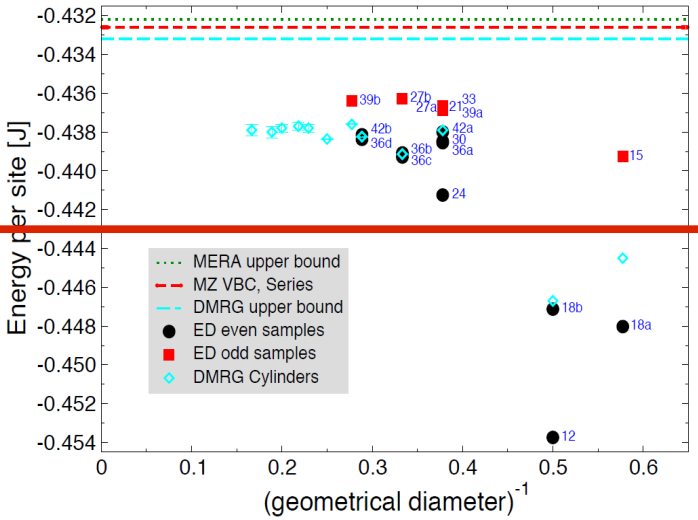


Yan, Huse, White (2011)

Quantum spin liquid is a phase of matter with
(1) no symmetry breaking, **no local order parameter**

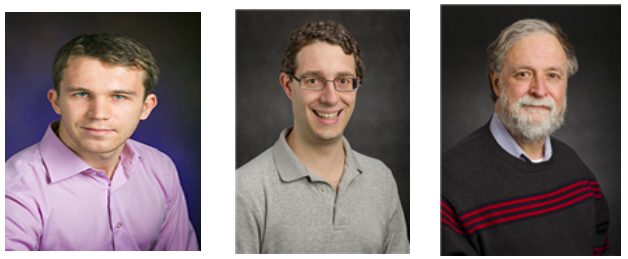
(2) **topological properties**/fractional anyonic excitations : quantum computation?

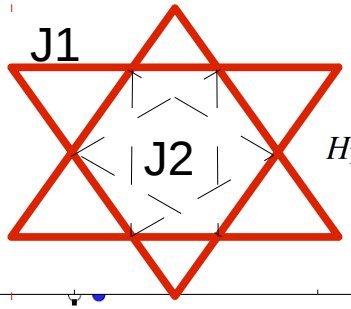
(3) very high multireference character



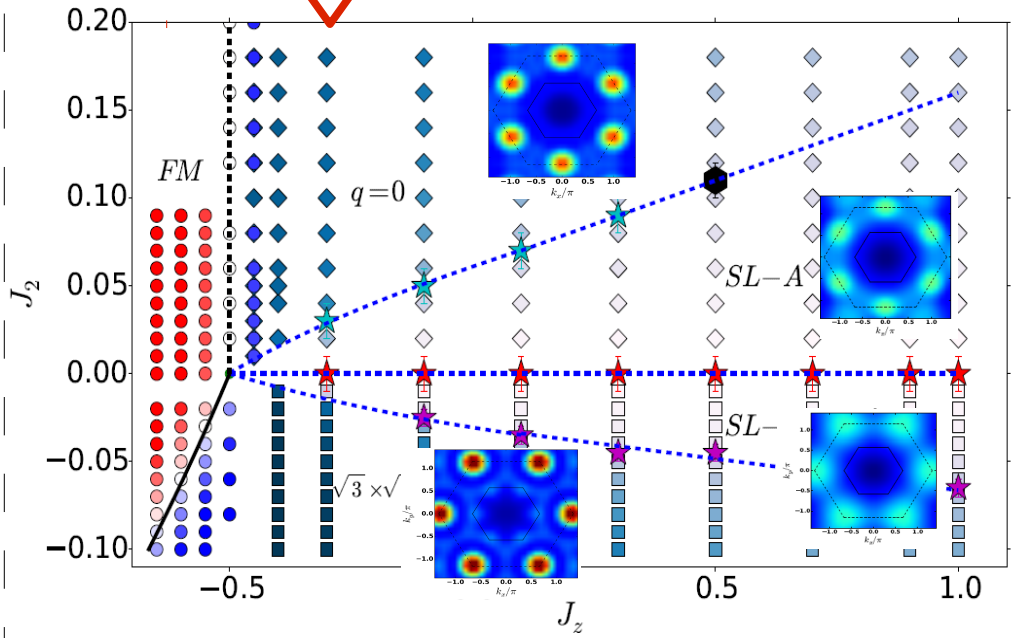
Many competitive phases (Marston Zeng state: 36 site unit cell)
Energy difference between candidates is 0.006 J per site

(J=200 K) 0.006*200 = 1.2 K = 0.1 meV





$$H_{XXZ} = \sum_{\langle i,j \rangle} J_{xy}\left(S_i^x S_j^x + S_i^y S_j^y\right) + J_z S_i^z S_j^z$$

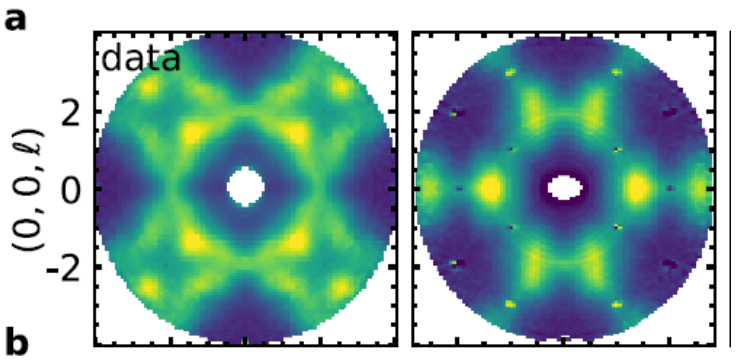


HJC, D. Kochkov, K. Kumar, B.Clark, E. Fradkin, Phys. Rev. Lett (2018)

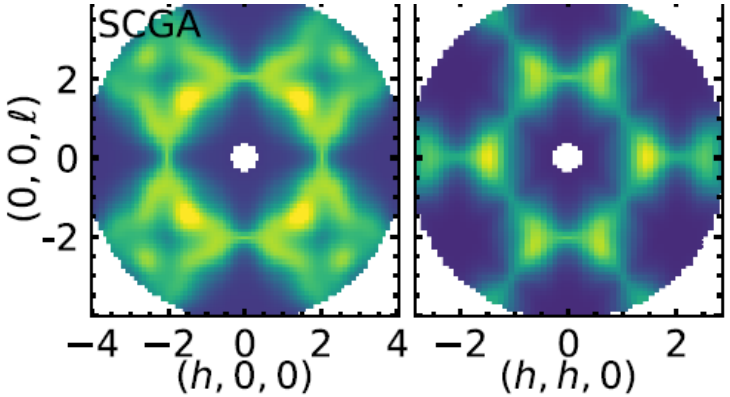
Where does the "real material" lie in the phase diagram?

Flowchart for strongly correlated models

Fit Experimental data: one personal "success" story for frustrated $NaCaNi_2F_7$



Fit magnetic couplings to STATIC structure factor (typically 0.1 meV to 10 meV)

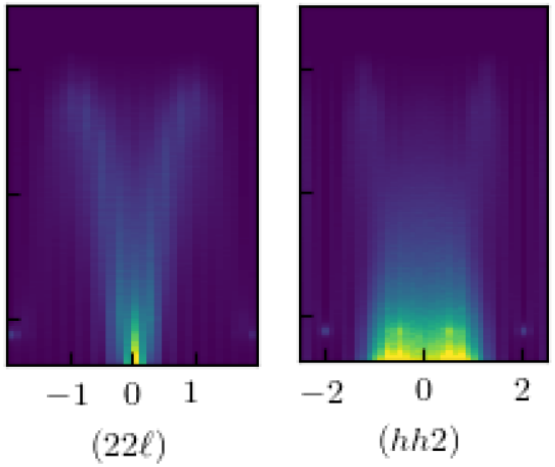


EXPT 1

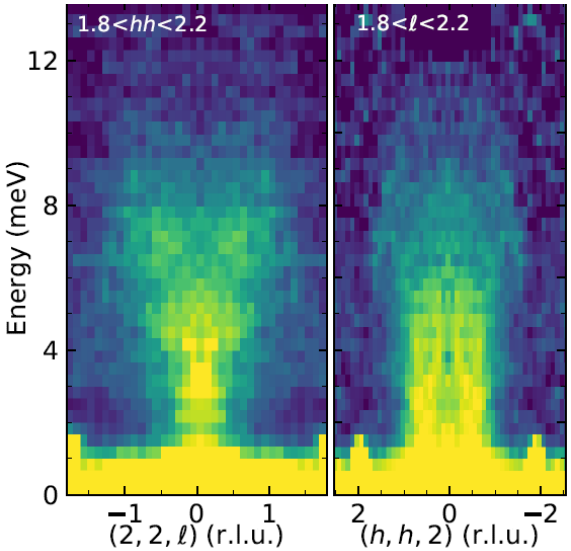
Plumb, **HJC,** et al, arXiv:1711.07509, to appear (2018)

Lattice model only of magnetic ions

Calculations with classical and semiclassical model methods (pyrochlore – 3d version of kagome)



make prediction for DYNAMIC properties (classical Monte Carlo + molecular dynamics or semiclassical spin wave theory)



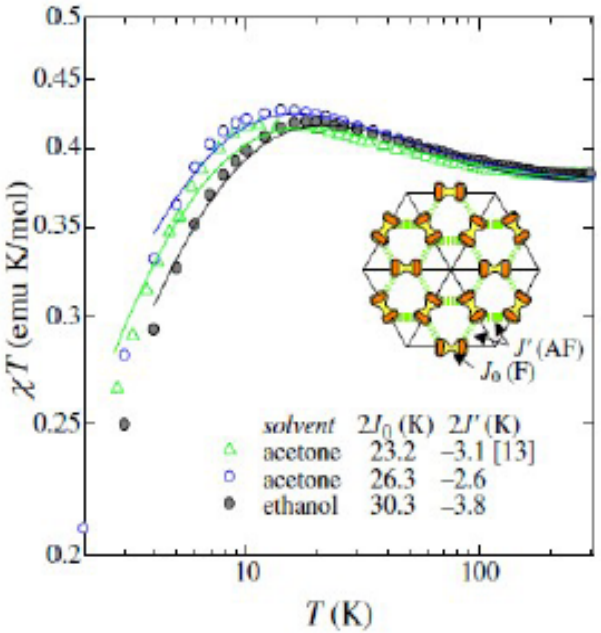
EXPT 2

Indications for a quantum spin liquid (quantum model solution itself needs more work to be sure ….)

S. Zhang*, **HJC*,** Plumb, Moessner,Tchernyshyov, to be submitted (2018)

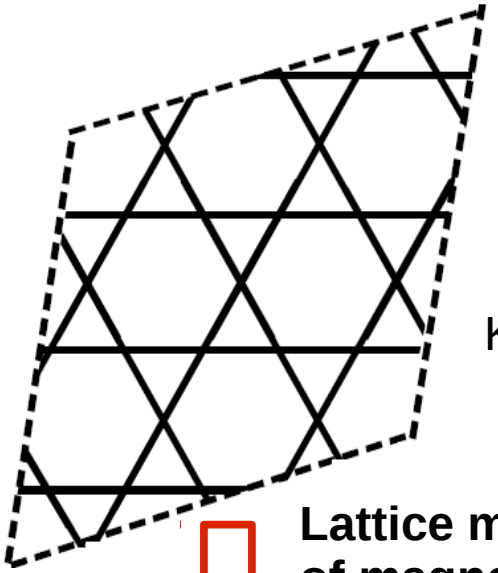
Flowchart for strongly correlated models

Fit Experimental data to get effective Hamiltonian – not always predictive



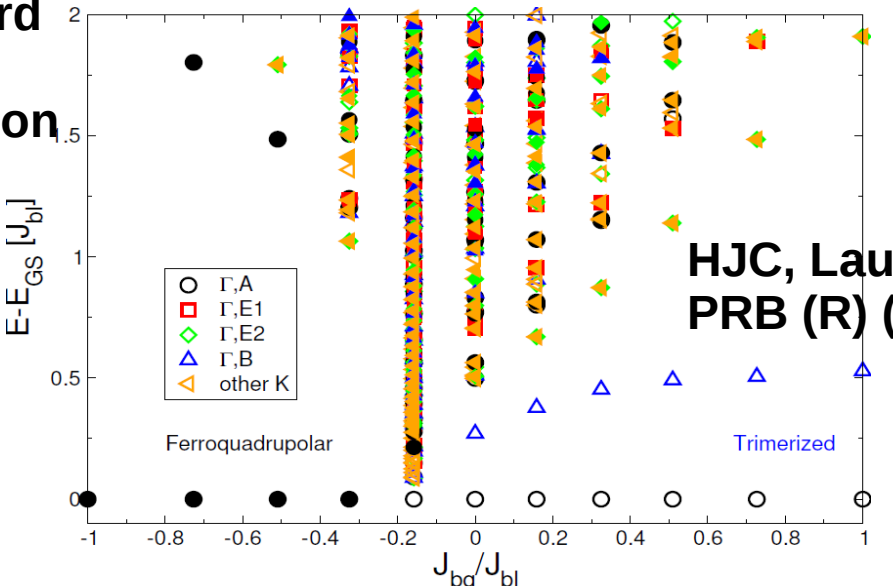
Awaga, JPSJ (2010)

Fit magnetic coupling to high temperature data (assume same model for low T)



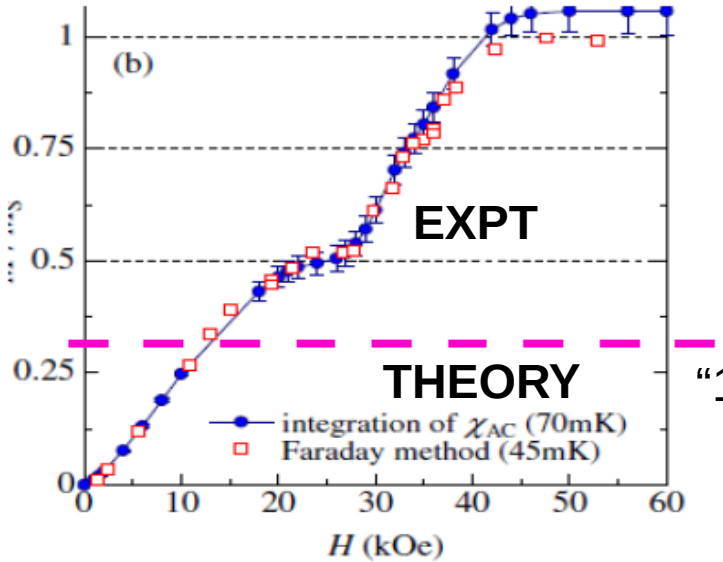
Kagome

Lattice model only of magnetic ions (make a phase diagram in coupling space)



HJC, Lauchli PRB (R) (2015)

Work very hard
Be right
Make prediction



"1/3 plateau"

Magnetization measurement

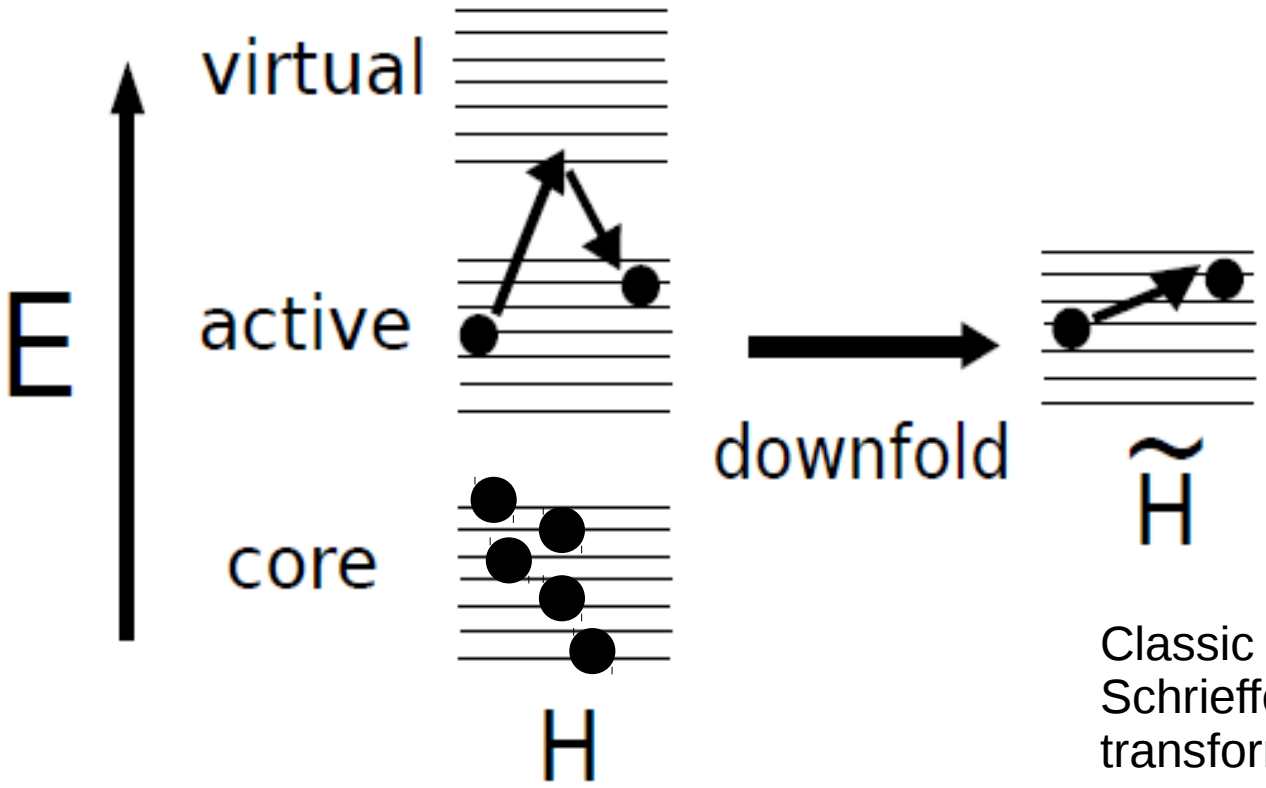
As theorists, want to minimize dependence on experiments so, the questions are…

- Is electronic structure likely to be “super accurate” to resolve small energy scales in solids (especially strongly correlated Mott insulators)?
  Answer: Who knows the future, but currently it is not

- Does one need to fully solve the many electron problem (obtain eigenstates) to understand the important low-energy physics of a problem?
  Answer: Not necessarily

- Can electronic structure tell us important physics that helps build relevant useful models (especially for solids) and helps diagnose what is right or wrong with them?
- **Answer: This is what the talk is about. I will show that QMC is quite useful for this purpose.**

What exactly do we mean by "effective Hamiltonian"? posing the problem

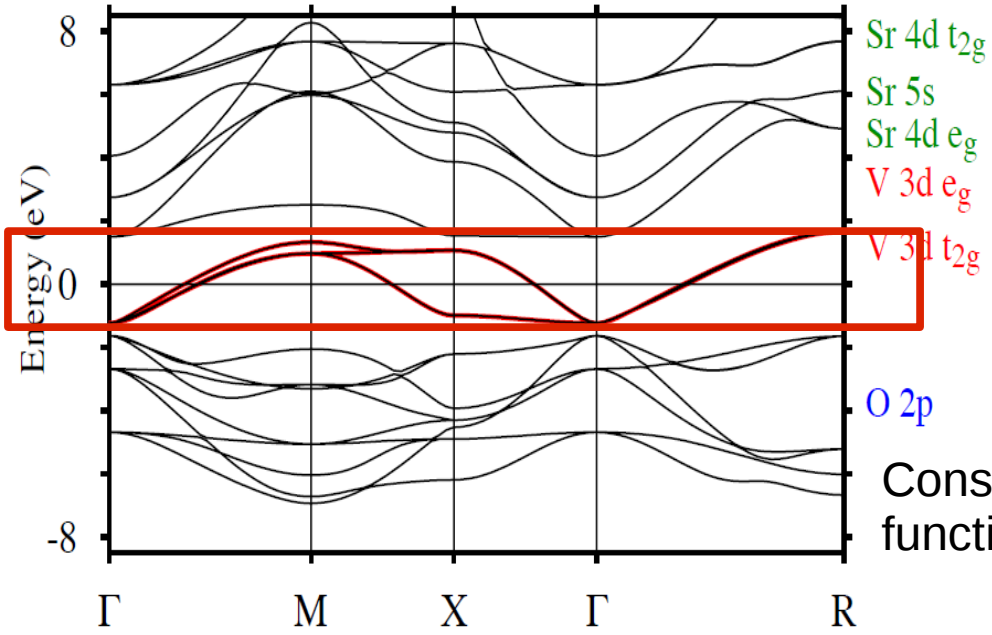


Classic example is the Schrieffer Wolff transformation

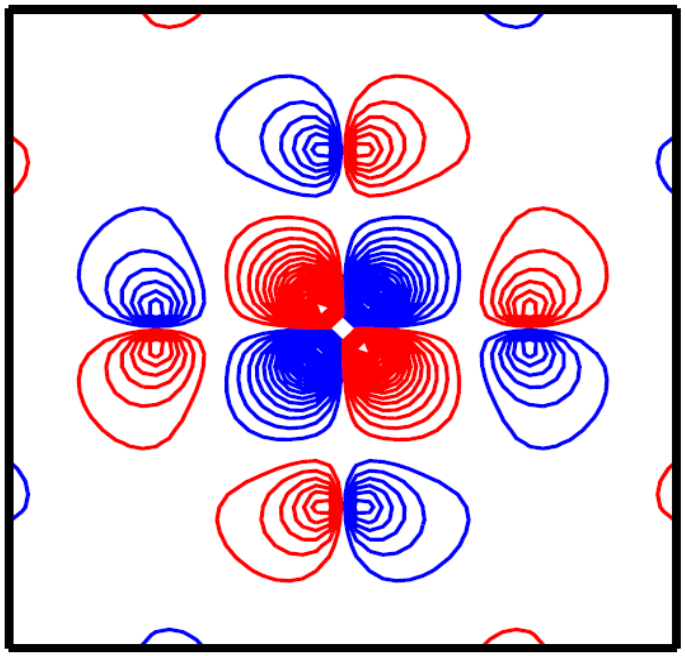
What is typically done to get a model?

Density functional theory

Courtesy E.Pavirini



Construct Wannier functions



Get hoppings “t” (integral of the kinetic energy projected in Wannier basis)
O. Andersen, R. Martin, Saha-Dasgupta, Valenti...

Hubbard U (Interactions) ? Use Post DFT method, constrained RPA
(Imada, Ariyasetiawan, Kotliar, Georges, Biermann, Casula, Werner, Valenti, Jeschke....)

How do we know whether these approximations are good or bad?

Our viewpoint for effective Hamiltonian determination

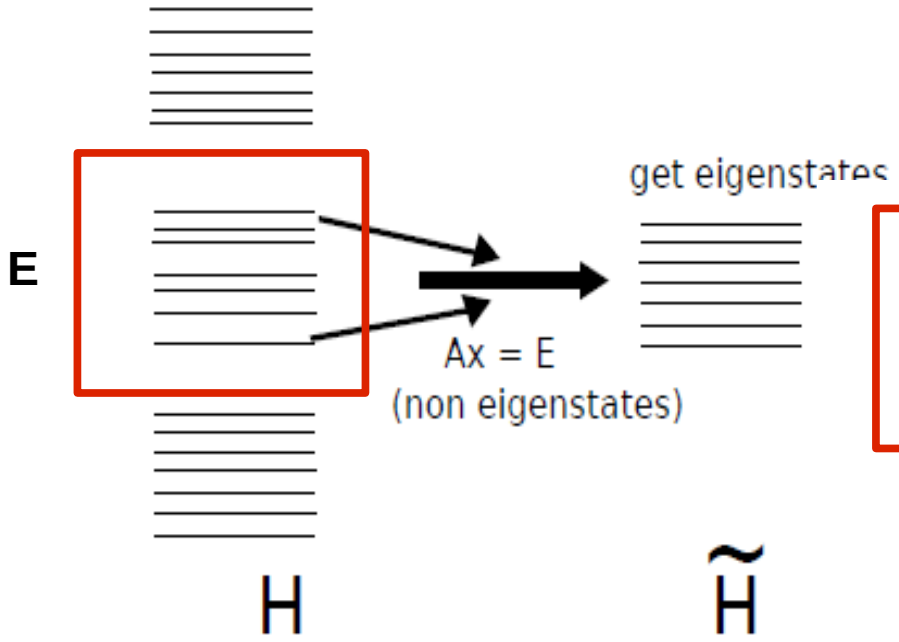
- Why treat kinetic and potential parts of Hamiltonian differently?
- Use information from accurate wavefunctions which do not care about this distinction
- Method must have internal consistency checks – is the model good or bad?
- Model is an “auxiliary system” with different electron number, so have to “match properties” instead of wavefunctions
- (several variants in other contexts: Ceperley, HJC, Henley, Wagner, White, Chan...)

These ideas motivated our first work: **H.J. Changlani, H. Zheng, L.K. Wagner, J. Chem. Phys (2015)**

Posing the problem precisely

Ab initio density matrix downfolding (AI-DMD)

Given a set of low energy wavefunctions **(not necessarily eigenstates)** how does one determine or "learn" the effective Hamiltonian parameters



Reconstruction problem

$$\tilde{H} = C + \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_{ijkl} V_{ijkl} c_i^\dagger c_j^\dagger c_l c_k$$

Finally solve

$$\tilde{H}\psi = E\psi$$

Our criterion :

$$\langle c_i^\dagger c_j \rangle_{\text{Model}} = \langle c_i^\dagger c_j \rangle_{\text{Ab-initio}}$$

$$\langle c_i^\dagger c_j^\dagger c_l c_k \rangle_{\text{Model}} = \langle c_i^\dagger c_j^\dagger c_l c_k \rangle_{\text{Ab-initio}}$$

DMD scheme for effective Hamiltonians

Given a "good" one particle basis

For a single state

$$\tilde{E}_s \equiv \langle H \rangle_s = C + \sum_{ij} t_{ij} \langle c_i^\dagger c_j \rangle + \sum_{ijkl} V_{ijkl} \langle c_i^\dagger c_j^\dagger c_l c_k \rangle$$

TRUE whether state is eigenstate or NOT

For many states

$$\begin{pmatrix} \tilde{E}_1 \\ \tilde{E}_2 \\ \tilde{E}_3 \\ \cdots \\ \cdots \\ \cdots \\ \cdots \\ \tilde{E}_M \end{pmatrix} = \begin{pmatrix} 1 & \langle c_i^\dagger c_j \rangle_1 & .. & \langle c_i^\dagger c_j^\dagger c_l c_k \rangle_1 & .. \\ 1 & \langle c_i^\dagger c_j \rangle_2 & .. & \langle c_i^\dagger c_j^\dagger c_l c_k \rangle_2 & .. \\ 1 & \langle c_i^\dagger c_j \rangle_3 & .. & \langle c_i^\dagger c_j^\dagger c_l c_k \rangle_3 & .. \\ 1 & \langle c_i^\dagger c_j \rangle_4 & .. & \langle c_i^\dagger c_j^\dagger c_l c_k \rangle_4 & .. \\ 1 & .... & .. & .. & .. \\ 1 & .... & .. & .. & .. \\ 1 & \langle c_i^\dagger c_j \rangle_M & .. & \langle c_i^\dagger c_j^\dagger c_l c_k \rangle_M & .. \end{pmatrix} \begin{pmatrix} C \\ t_{ij} \\ .. \\ V_{ijkl} \\ .. \end{pmatrix}$$

Energies **Matrix of density matrices** **Parameters**

AI-DMD scheme for effective Hamiltonians

$$\begin{pmatrix} \tilde{E}_1 \\ \tilde{E}_2 \\ \tilde{E}_3 \\ \cdots \\ \cdots \\ \cdots \\ \cdots \\ \tilde{E}_M \end{pmatrix} = \begin{pmatrix} 1 & \langle c_i^\dagger c_j \rangle_1 & .. & \langle c_i^\dagger c_j^\dagger c_l c_k \rangle_1 & .. \\ 1 & \langle c_i^\dagger c_j \rangle_2 & .. & \langle c_i^\dagger c_j^\dagger c_l c_k \rangle_2 & .. \\ 1 & \langle c_i^\dagger c_j \rangle_3 & .. & \langle c_i^\dagger c_j^\dagger c_l c_k \rangle_3 & .. \\ 1 & \langle c_i^\dagger c_j \rangle_4 & .. & \langle c_i^\dagger c_j^\dagger c_l c_k \rangle_4 & .. \\ 1 & .... & .. & .. & .. \\ 1 & .... & .. & .. & .. \\ 1 & \langle c_i^\dagger c_j \rangle_M & .. & \langle c_i^\dagger c_j^\dagger c_l c_k \rangle_M & .. \end{pmatrix} \begin{pmatrix} C \\ t_{ij} \\ .. \\ V_{ijkl} \\ .. \end{pmatrix}$$

E = Energies **A = Matrix of density matrices** **x = Parameters**

$$\mathbf{E} = A\mathbf{x}$$

$$\mathcal{N} \equiv ||A\mathbf{x} - \mathbf{E}||^2$$ **Minimize difference**

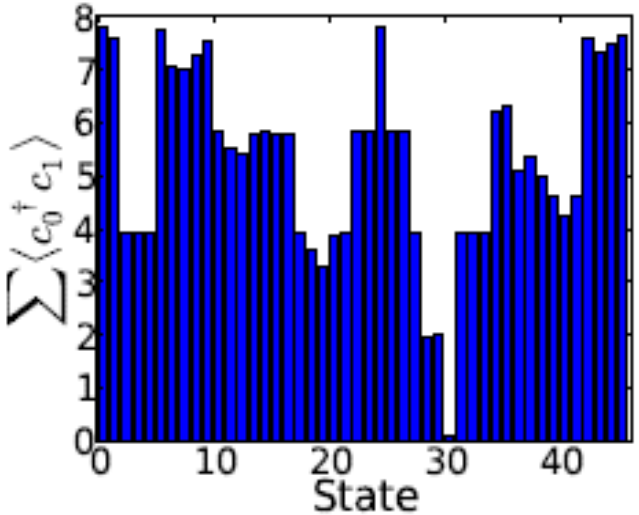
H.J.Changlani, H. Zheng, L.K. Wagner, JCP (2015)

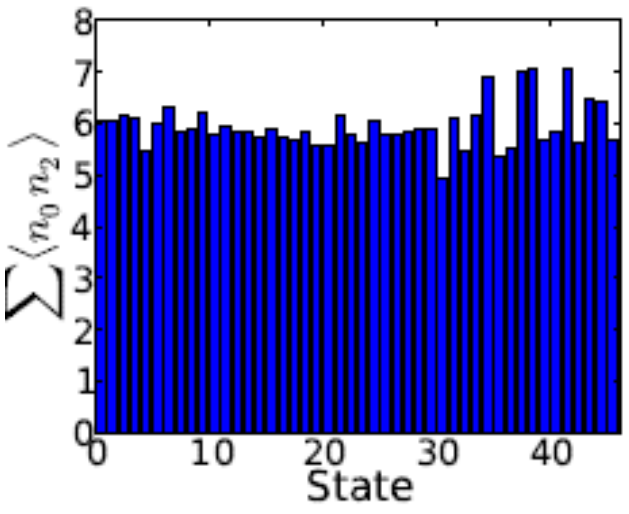
AI-DMD scheme for effective Hamiltonians

Energy must vary with variation in density matrices to be “relevant”

$$\begin{pmatrix} \tilde{E}_1 \\ \tilde{E}_2 \\ \tilde{E}_3 \\ \cdots \\ \cdots \\ \cdots \\ \cdots \\ \tilde{E}_M \end{pmatrix} = \begin{pmatrix} 1 & \langle c_i^\dagger c_j \rangle_1 & .. & \langle c_i^\dagger c_j^\dagger c_l c_k \rangle_1 & .. \\ 1 & \langle c_i^\dagger c_j \rangle_2 & .. & \langle c_i^\dagger c_j^\dagger c_l c_k \rangle_2 & .. \\ 1 & \langle c_i^\dagger c_j \rangle_3 & .. & \langle c_i^\dagger c_j^\dagger c_l c_k \rangle_3 & .. \\ 1 & \langle c_i^\dagger c_j \rangle_4 & .. & \langle c_i^\dagger c_j^\dagger c_l c_k \rangle_4 & .. \\ 1 & .... & .. & .. & .. \\ 1 & .... & .. & .. & .. \\ 1 & \langle c_i^\dagger c_j \rangle_M & .. & \langle c_i^\dagger c_j^\dagger c_l c_k \rangle_M & .. \end{pmatrix} \begin{pmatrix} C \\ t_{ij} \\ .. \\ V_{ijkl} \\ .. \end{pmatrix}$$

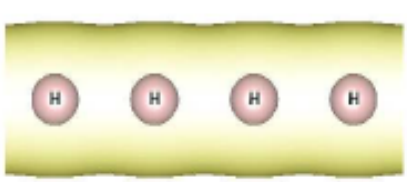
E = Energies **A = Matrix of density matrices** **x = Parameters**



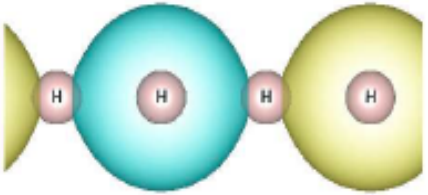


We need a "good" (often local) one particle basis (*i*)

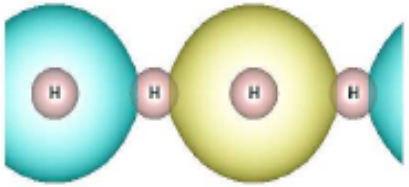
Ab initio density matrix downfolding (AI-DMD)



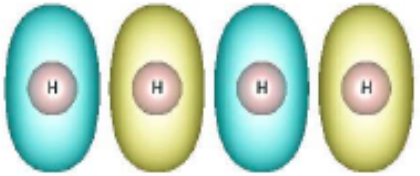
(a) KS 1



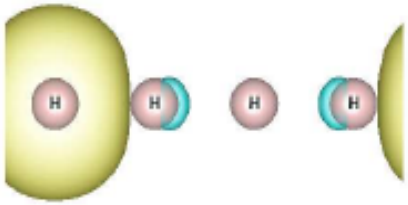
(b) KS 2



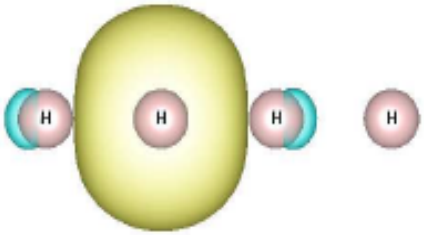
(c) KS 3



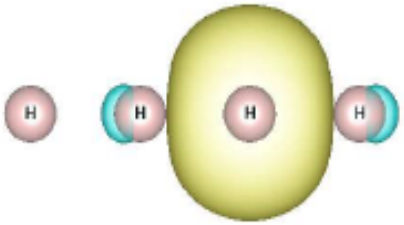
(d) KS 4



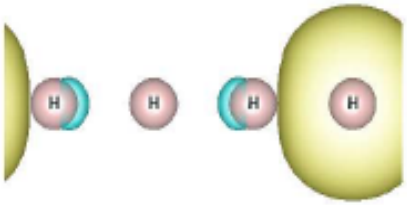
(e) Wannier 1



(f) Wannier 2



(g) Wannier 3



(h) Wannier 4

Examples I will talk about

- A pedagogical toy model that highlights the main ideas (no QMC, everything can be exactly solved) – 3-band Hubbard model to 1-band Hubbard model

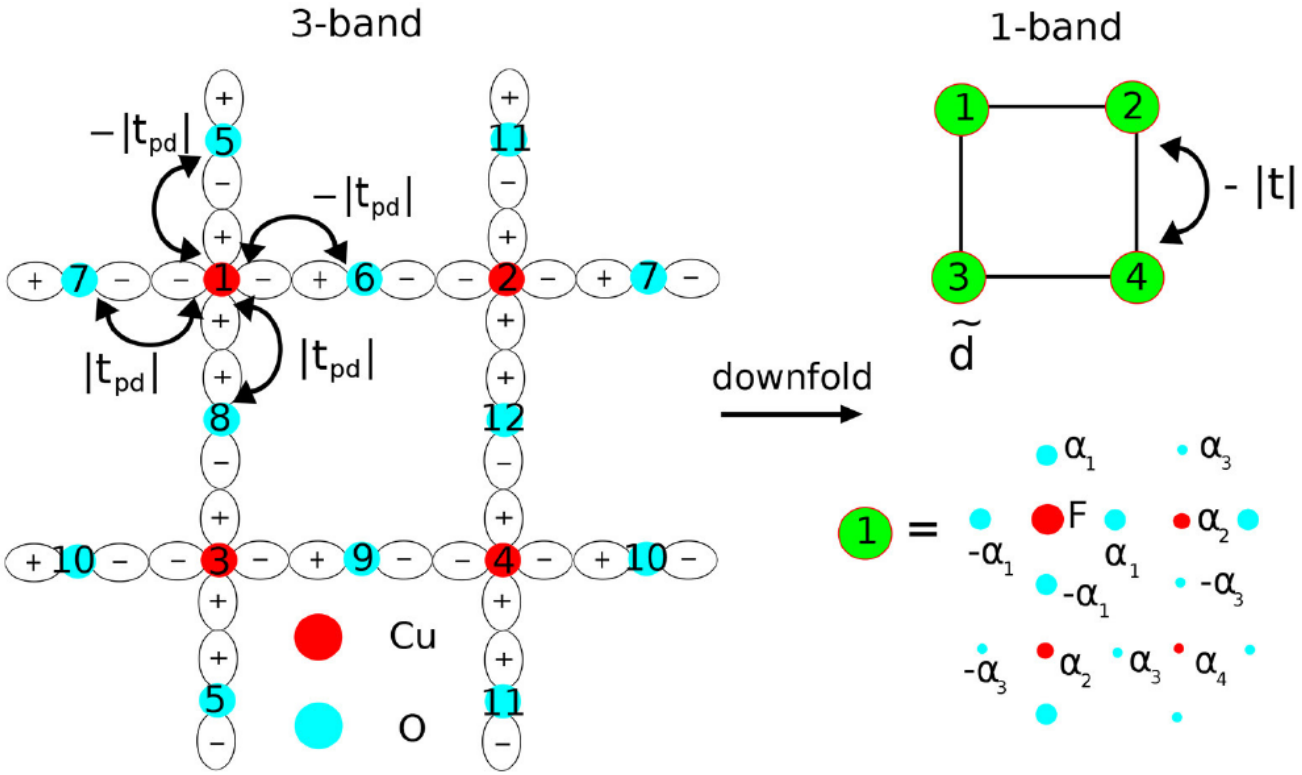
- Benzene molecule with QMC – effective one orbital per site –

- QMC on graphene

- Transition metals, as a futuristic (preliminary) application

Increasing complexity

Example 1: (Toy) Three to one band model at half filling



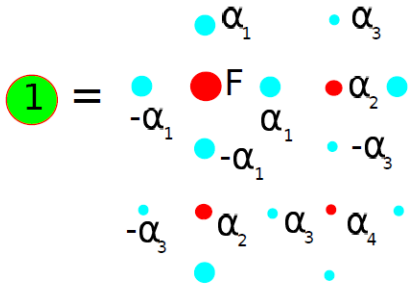
$$H = \epsilon_p \sum_{j\in p,\eta} n_{j,\eta} + \epsilon_d \sum_{i\in d,\eta} n_{i,\eta} + t_{pd} \sum_{\langle i\in d, j\in p\rangle,\eta} \mathrm{sgn}(p_i, d_j)\left(c^\dagger_{i,\eta} c_{j,\eta} + \mathrm{h.c.}\right)$$

$$+U_p \sum_{j\in p} n_{j,\uparrow} n_{j,\downarrow} + U_d \sum_{i\in d} n_{i,\uparrow} n_{i,\downarrow} + V_{pd} \sum_{\langle i\in p, j\in d\rangle} n_j n_i \,, \qquad \Delta \equiv \epsilon_p - \epsilon_d$$

$$H = E_0 - t \sum_{\langle i,j\rangle,\eta} \tilde{d}^\dagger_{i,\eta} \tilde{d}_{j,\eta} + U \sum_i \tilde{n}^i_\uparrow \tilde{n}^i_\downarrow$$

Example 1: Three to one band model – what are the optimal orbitals?

$$\tilde{d}_{i,\eta} = \sum_j T_{ij} c_{j,\eta}$$

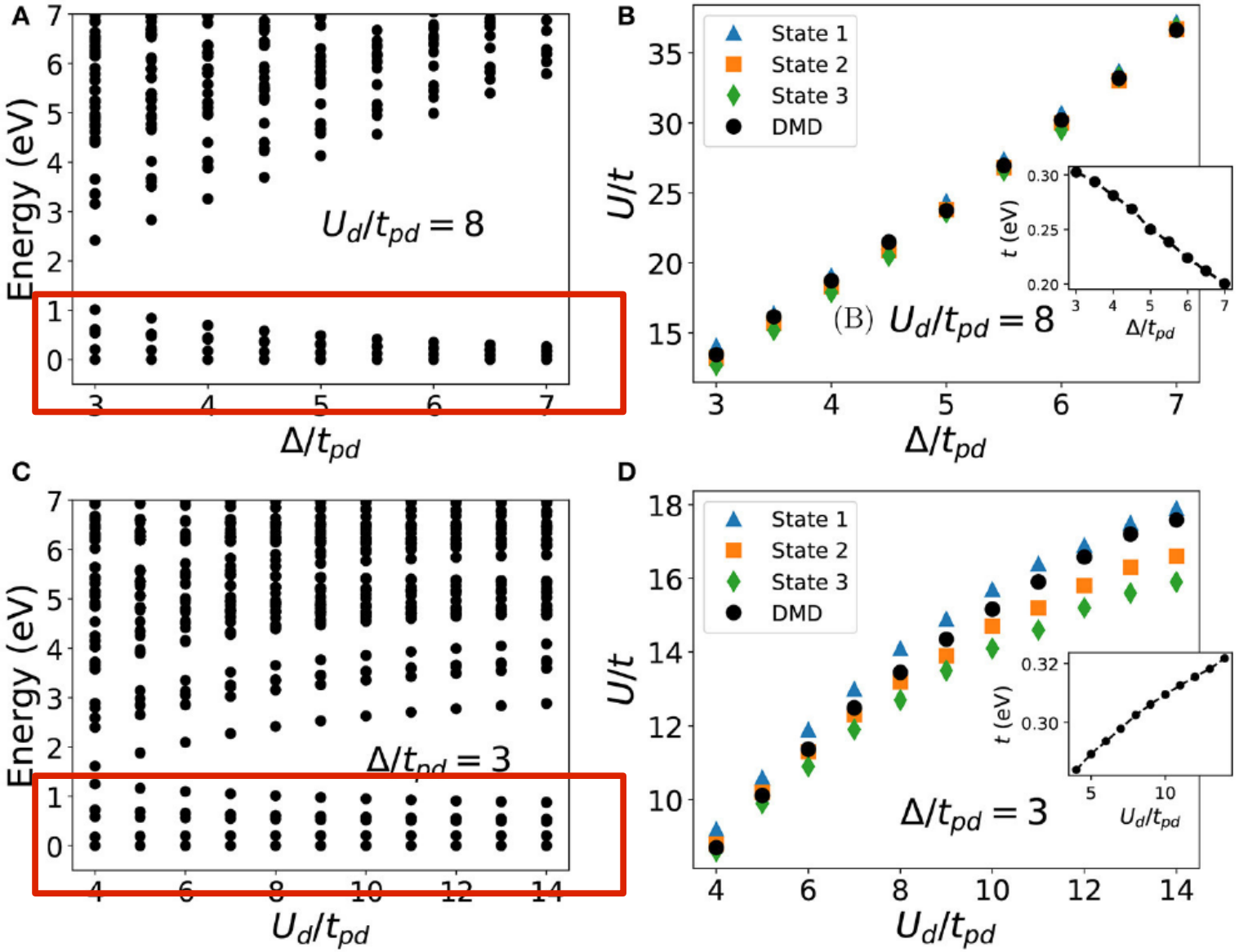


$$\langle \tilde{d}^{\dagger}_{i,\eta} \tilde{d}_{j,\eta} \rangle_s = \sum_{mn} T^*_{im} \langle {c_{m,\eta}}^{\dagger} c_{n,\eta} \rangle_s T_{jn} \ ,$$

$$\langle \tilde{n}_{i,\uparrow} \tilde{n}_{i,\downarrow} \rangle_s = \sum_{jkmn} T^*_{ij} T^*_{im} \langle {c_{j,\uparrow}}^{\dagger} {c_{m,\downarrow}}^{\dagger} c_{n,\downarrow} c_{k,\uparrow} \rangle_s T_{in} T_{ik}$$

$$C = \sum_s \sum_\eta \left(\sum_i \langle \tilde{d}^{\dagger}_{i,\eta} \tilde{d}_{i,\eta} \rangle_s - N_\eta \right)^2 + \sum_{mn} (\left(\mathbf{T}\mathbf{T}^{\dagger} \right)_{mn} - \delta_{mn})^2$$

Example 1: Three to one band model, (renormalized) effective parameters



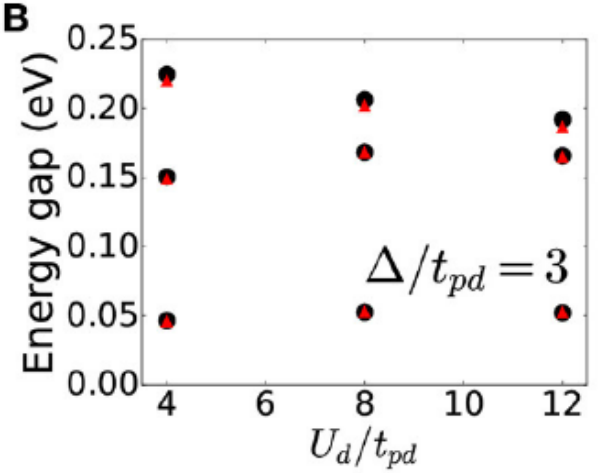
Example 1: Three to one band model, Multi-scale prediction

- Obtain effective parameters for a 4 unit cell system from downfolding
- Check their transferability/predictive power on a 8 unit cell system by checking energy gaps
- Hilbert space of the 3-band 8 unit cell system is 112 million (Lanczos)
- Hilbert space of the 1-band 8 unit cell system is 4900 (exact diag)

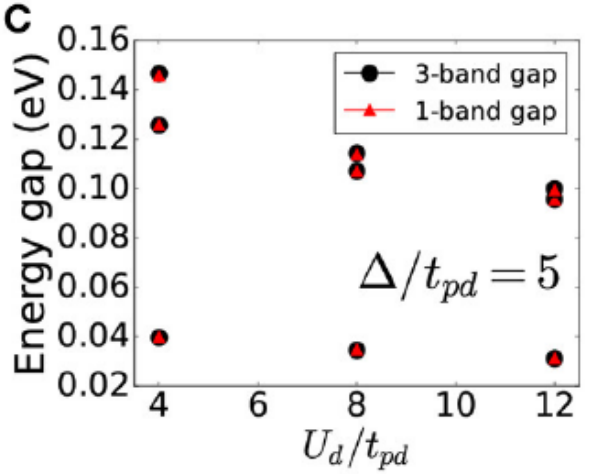
A

Δ/t_{pd}	U_d/t_{pd}	t (eV)	U/t
3.0	4.0	0.2839	8.698
3.0	8.0	0.3025	13.45
3.0	12.0	0.3155	16.58
5.0	4.0	0.2326	15.08
5.0	8.0	0.2501	23.75
5.0	12.0	0.2647	29.89

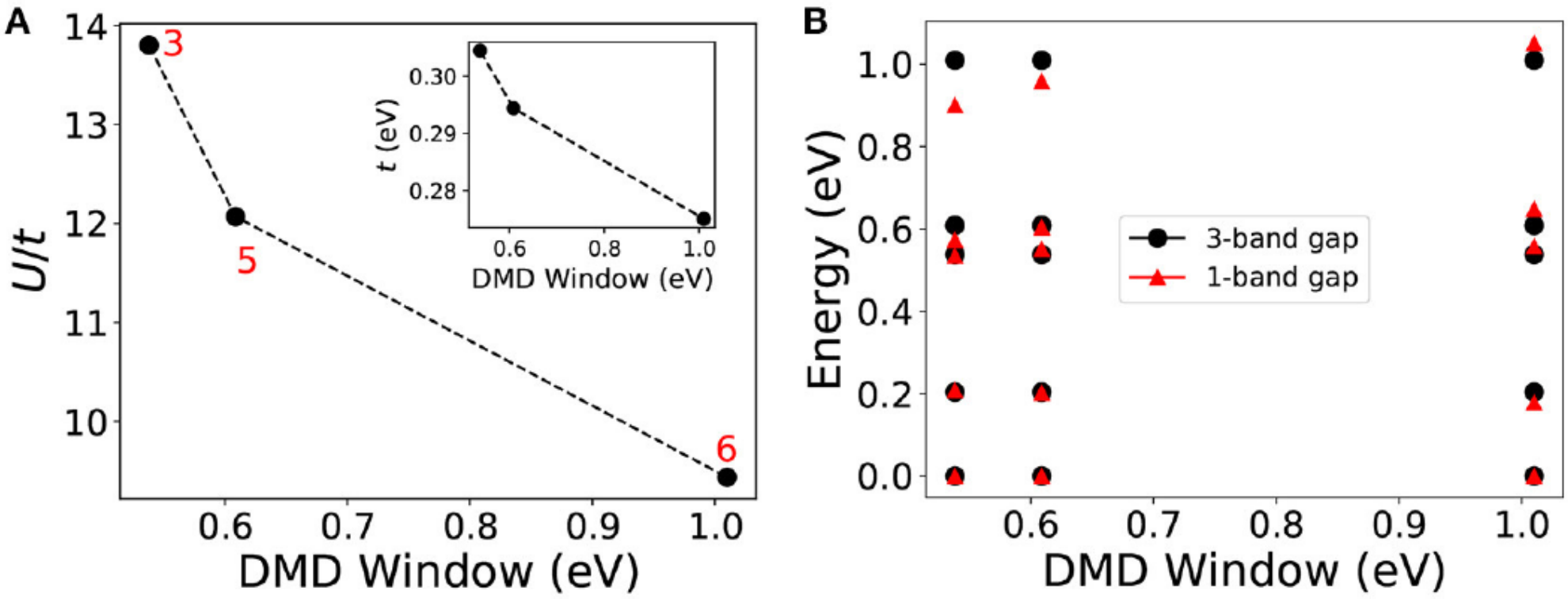
B



C



Example 1: Three to one band model – Parameters are energy window dependent



The parameters depend on the energy window of interest, much like what the renormalization group has taught us.

Quantum Monte Carlo in a nutshell

What?

Stochastic sampling of many electron configurations

Optimize many-body wavefunction:

$$\psi_T(r_1, r_2, ...r_N) = \mathcal{J} \sum_i d_i D_i$$

Jastrow: Introduces electron correlation

Determinants (HF or DFT)

Variational Monte Carlo
(sample trial wf, often not chemically accurate)

Projector (Diffusion) Monte Carlo:
(exact but sign problem)

Diffusion Monte Carlo with nodal constraint
(systematic error, but very accurate)

Why?

Scalable, esp. important for solids

Accuracy improvable
(by improving wavefunctions)

Can calculate observables
(correlation functions, structure factor)

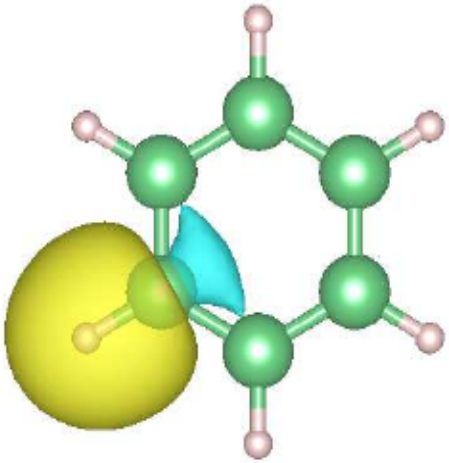
$$\langle c_i^\dagger c_j \rangle \langle c_i^\dagger c_j^\dagger c_l c_k \rangle$$

Refs: Ceperley, Alder, Umrigar, Nightingale, Mitas, Foulkes...

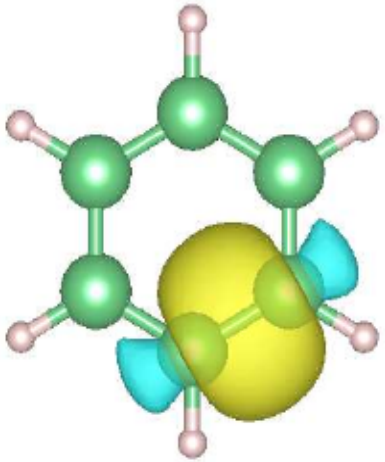
QWALK software: Wagner, Bajdich, Mitas, JCP (2009)

Example 2: Benzene molecule

One particle orbitals



Occupancy 0.99



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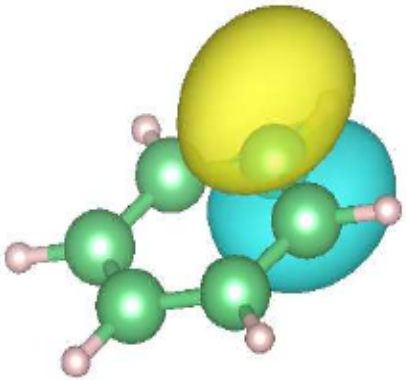
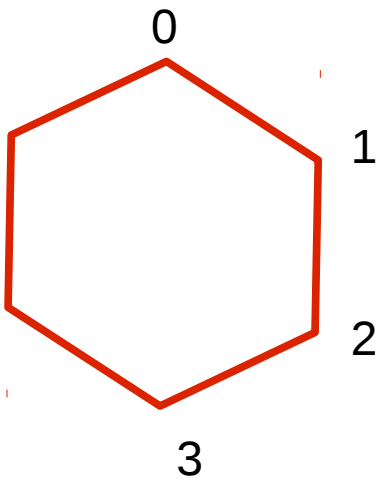


Occupancy 0.5



$$H = -t \sum_{ij} c^{\dagger}_{i,\sigma} c_{j,\sigma} + \text{h.c.} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}$$

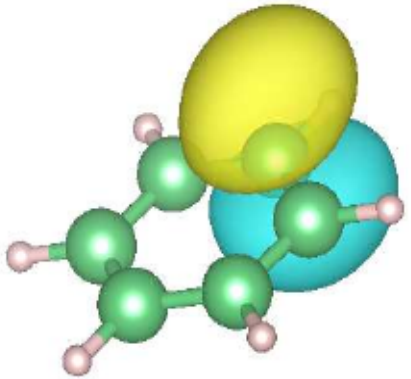
Hubbard

$$H = -\sum_{ij} t_{ij} c^{\dagger}_{i,\sigma} c_{j,\sigma} + \text{h.c.} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow} + \sum_{ij} V_{ij} n_i n_j$$

Extended Hubbard (PPP)

Example 2: Benzene molecule

Testing the one particle basis



Full ab-initio calculation : 30 electrons (eg. 15 u, 15 d)

“Effective” Lattice model: 6 electrons (eg. 3 u, 3 d)

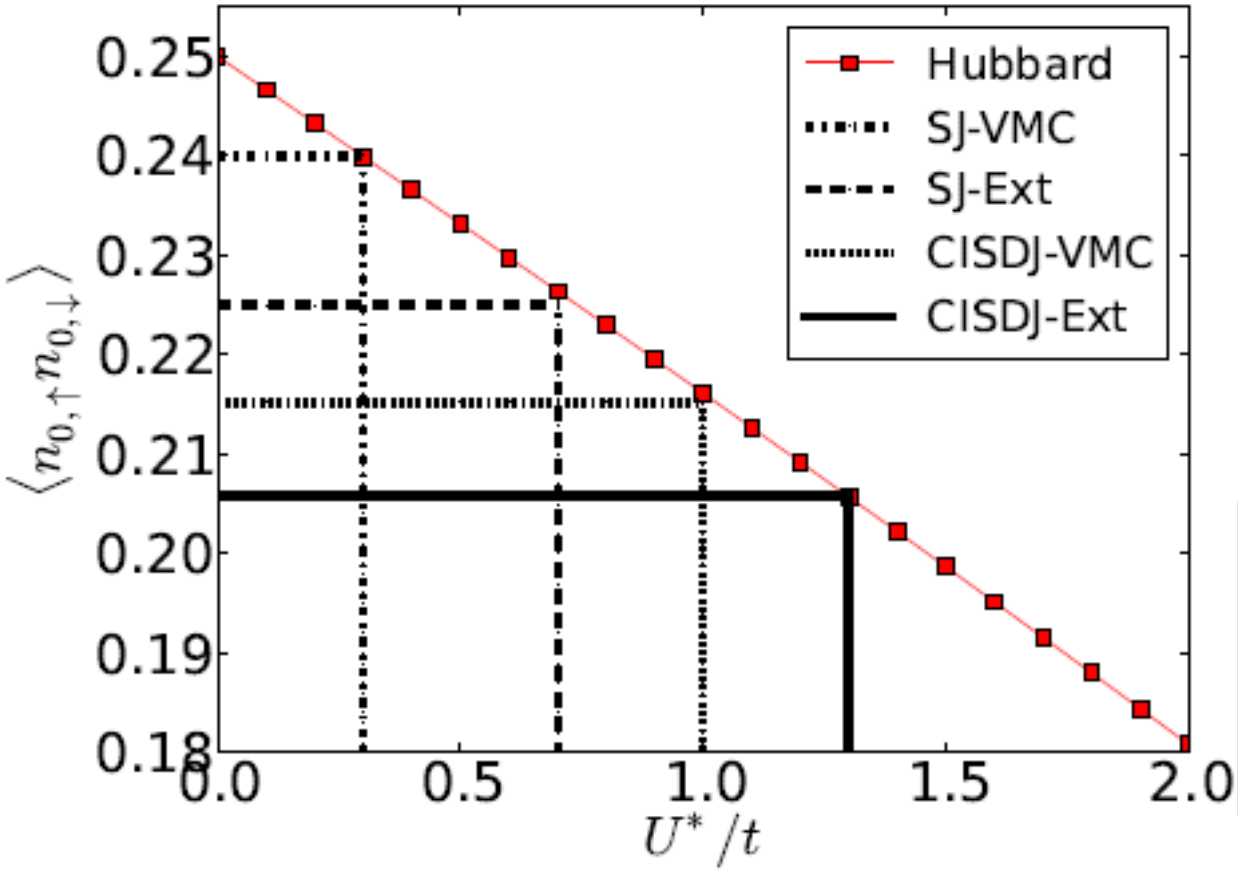
Spin	DFT	SJ-VMC	SJ-DMC	CISDJ-VMC	CISDJ-DMC	$N_\uparrow, N_\downarrow$	Used in Fit?
0	-37.6303	-37.6229(6)	-37.7213(9)	-37.6352(6)	-37.7259(9)	2.96,2.96	Yes
1	-37.4634	-37.4546(6)	-37.5555(7)	-37.4814(6)	-37.5707(7)	3.94,1.98	Yes
				-37.4561(6)	-37.5479(6)	3.94,1.98	Yes
				-37.4531(6)	-37.5470(6)	3.94,1.98	Yes
2	-37.3203	-37.2987(6)	-37.3974(7)	-37.3141(6)	-37.4020(7)	4.92,1.00	Yes
3	-37.0378	-37.0116(4)	-37.1074(7)	-37.0118(4)	-37.1083(7)	4.88,0.02	No

Energy Units: Ha

Example 2: Benzene molecule

Hubbard model, double occupancy

$$H_{\text{Hubbard}} = -t \sum_{\langle i,j \rangle,\sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}$$



SJ = Slater-Jastrow
(1 determinant)

CISD-J = Multidet - Jastrow

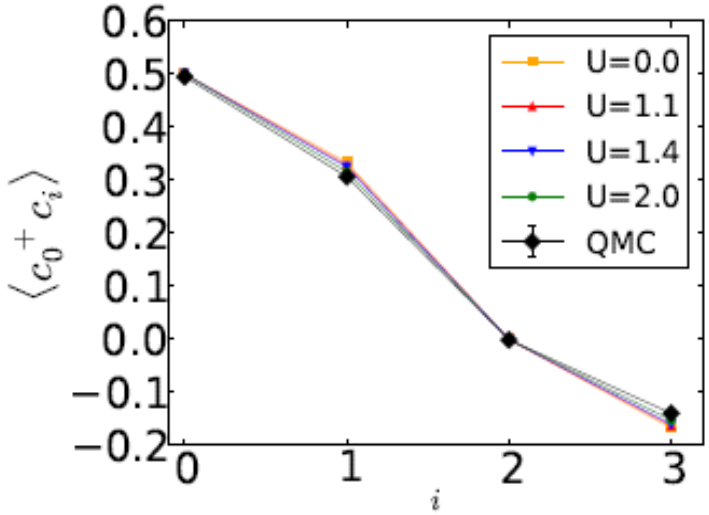
Why is U hard to get?

U depends very sensitively on the level of correlation In the wavefunction

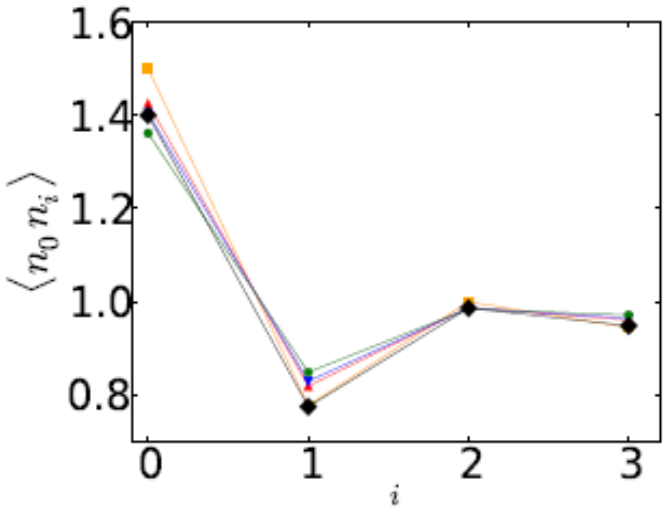
Half filled ground state (S=0)

Example 2: Benzene molecule

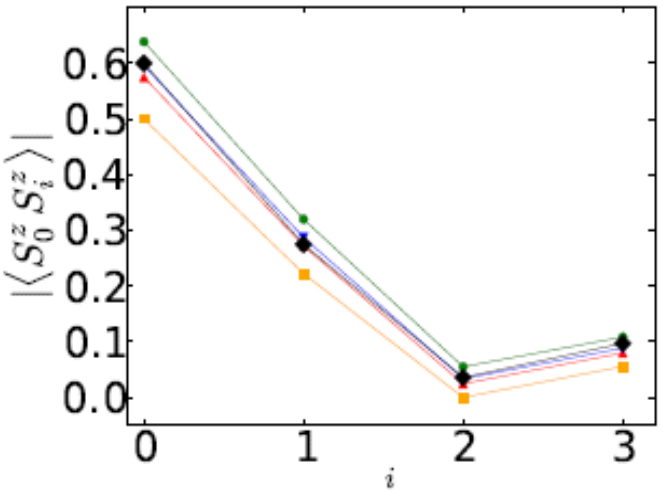
Comparison of model vs ab-initio correlation functions in ground state



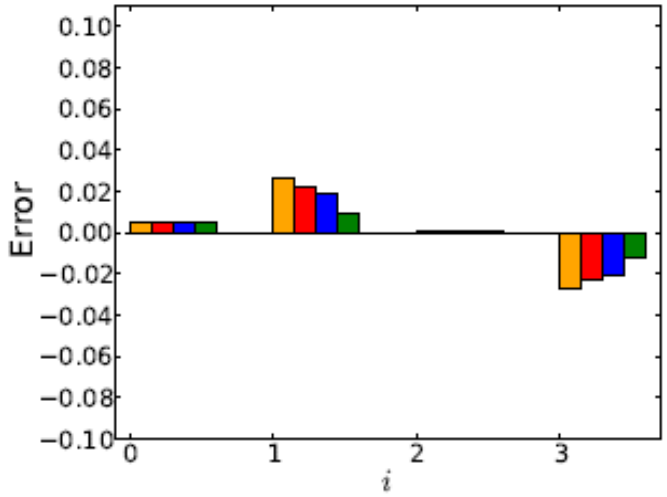
(a)



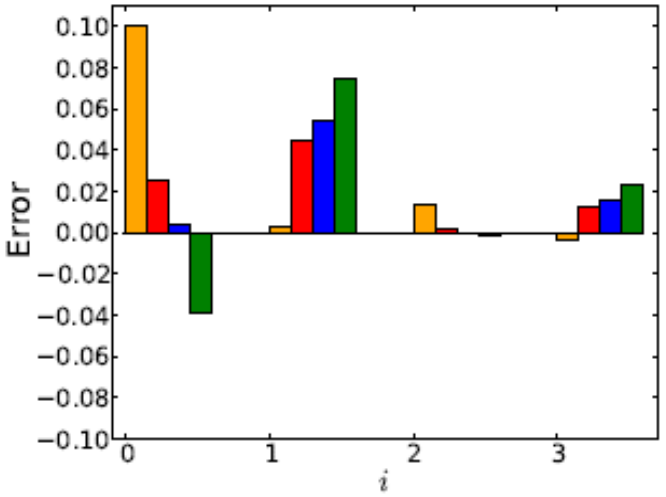
(b)



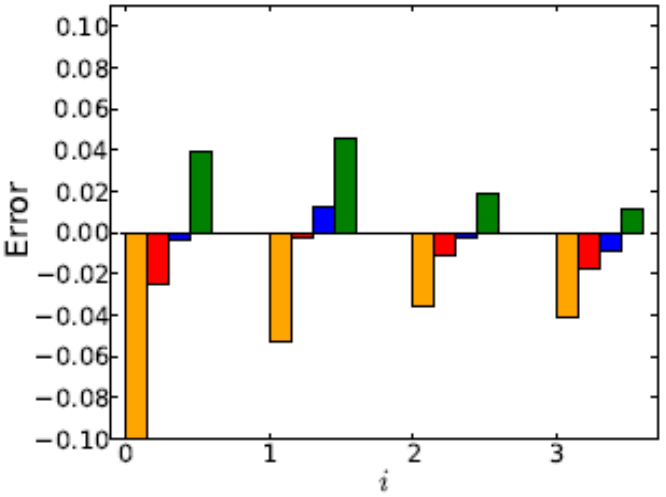
(c)



(d)



(e)

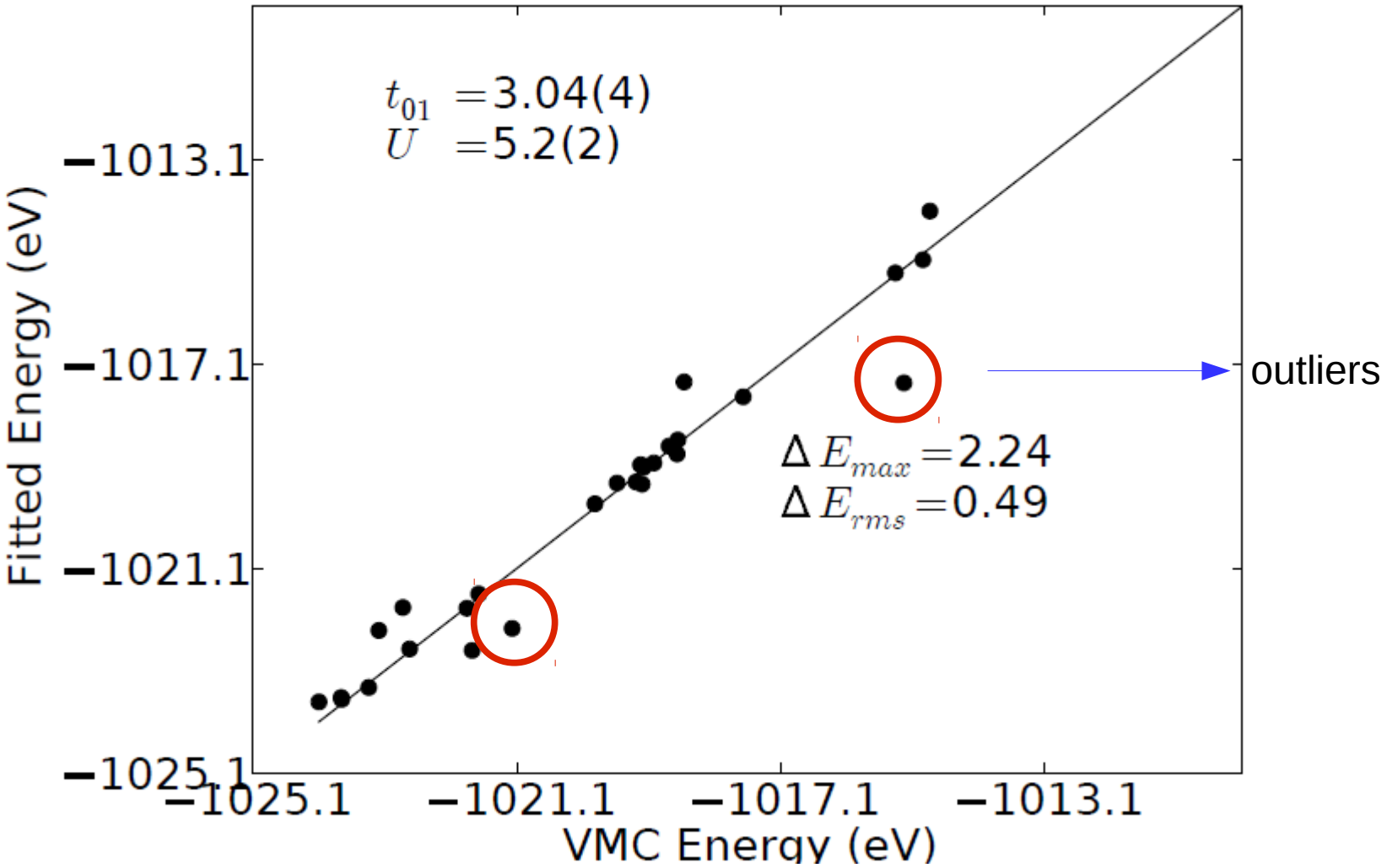


(f)

Example 2: Benzene molecule

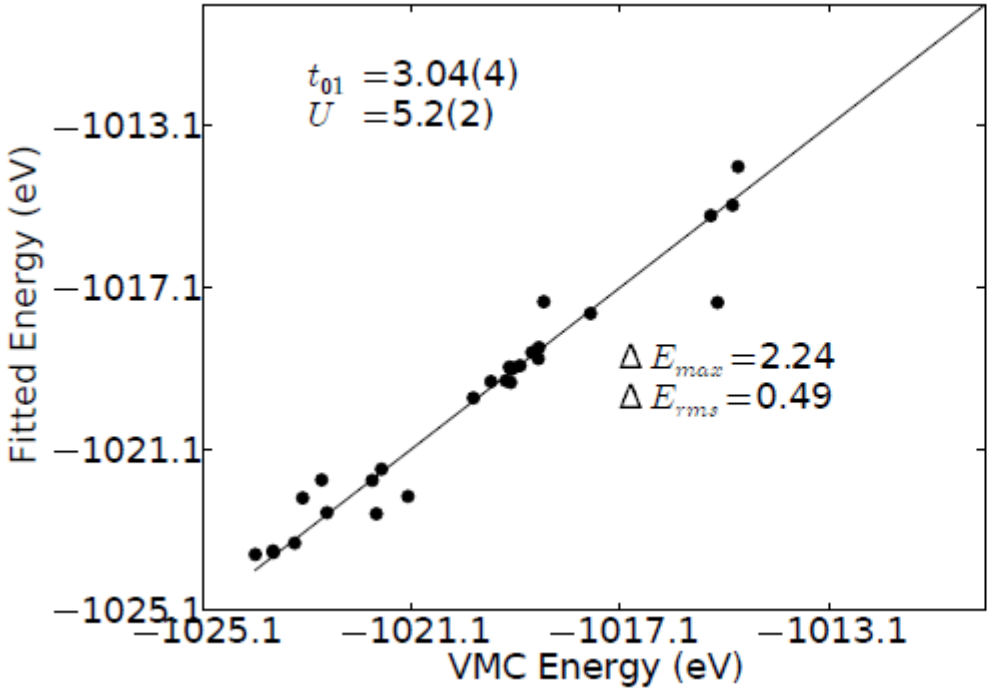
Hubbard model

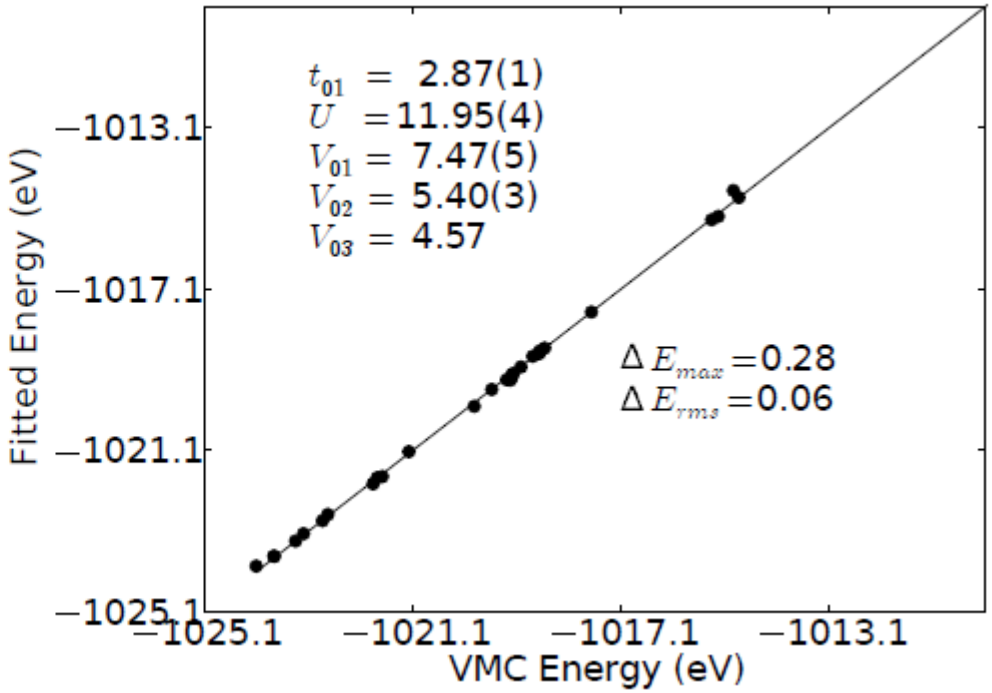
$$\mathbf{E} = A\mathbf{x}$$



Example 2: Benzene molecule

Hubbard and extended Hubbard (PPP) model





Hubbard only

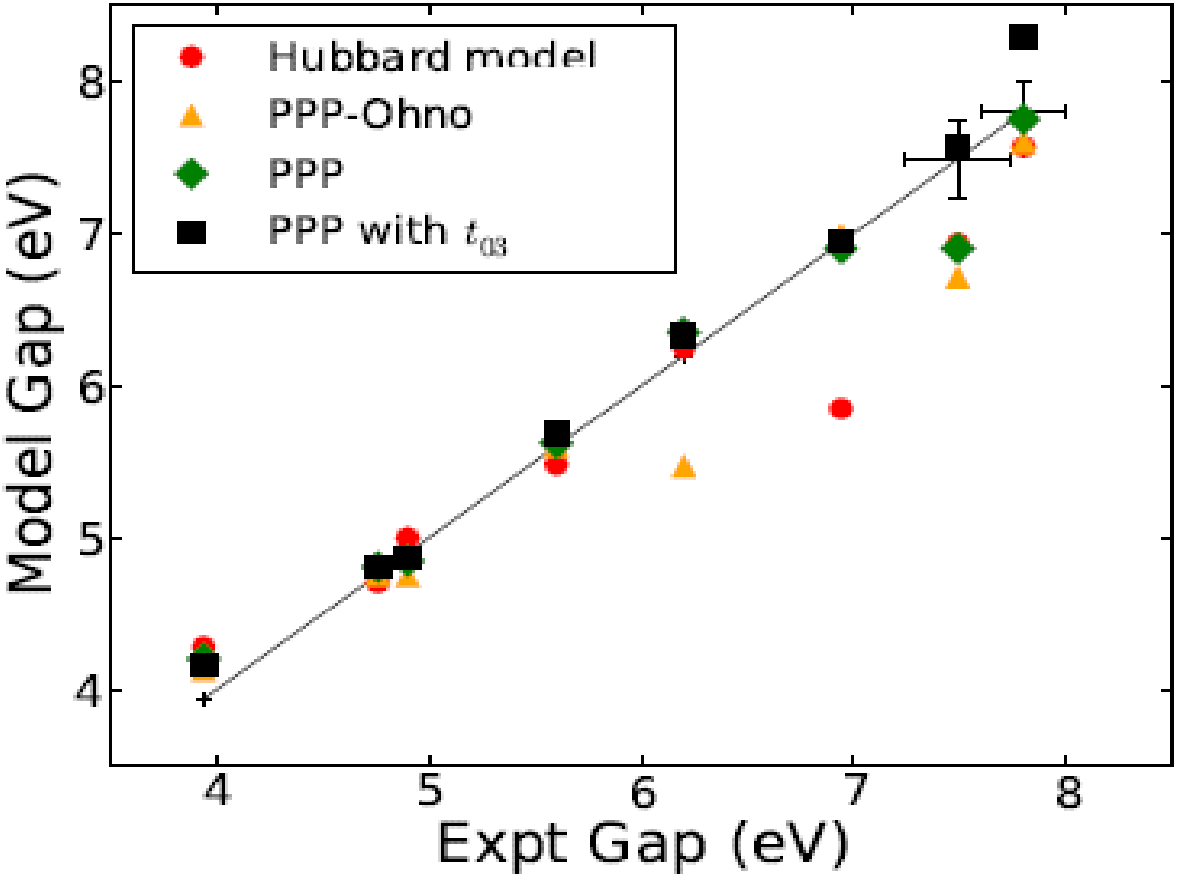
$$H = -t \sum_{ij} c^{\dagger}_{i,\sigma} c_{j,\sigma} + \text{h.c.} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}$$

Extended Hubbard

$$H = -\sum_{ij} t_{ij} c^{\dagger}_{i,\sigma} c_{j,\sigma} + \text{h.c.} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow} + \sum_{ij} V_{ij} n_i n_j$$

Example 2: Benzene molecule

Reconstructing eigenstates by solving lattice model of 6 electrons
+ comparison to experiment

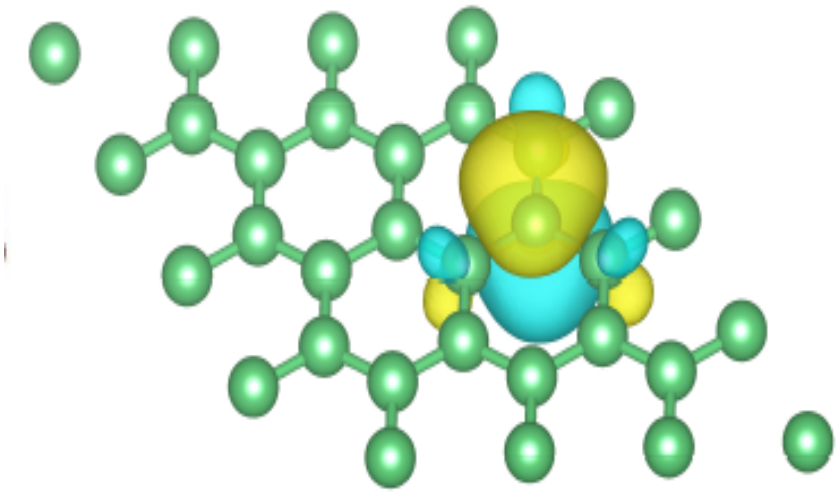


Some subtleties:
Need to calculate parameters from variational and diffusion MC, and extrapolate

Comparable to previous semi-empirical fits + We DO NOT use experimental data!

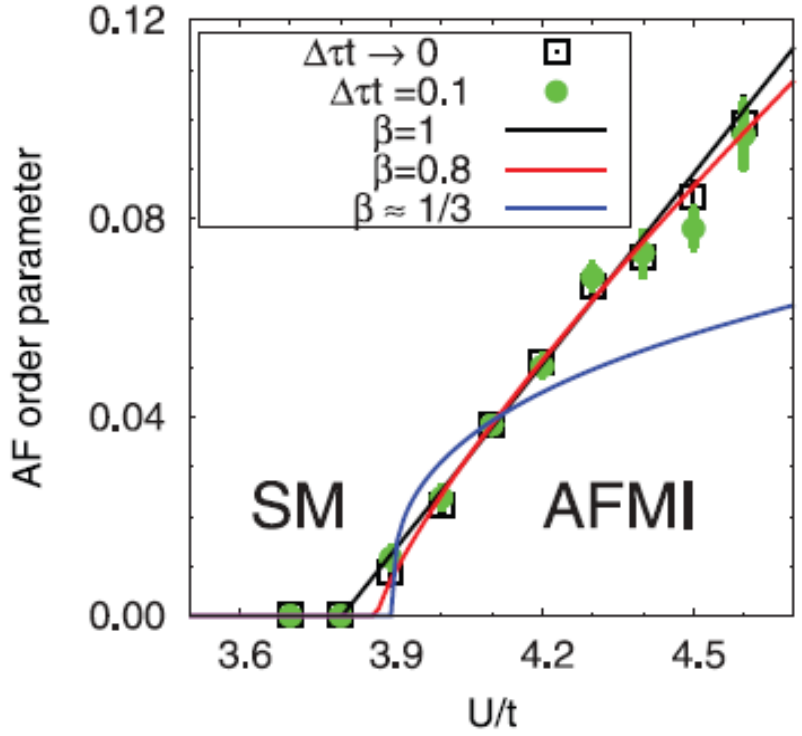
Example 3: Graphene (periodic solid)

What is the "effective" U ?



Wannier function for graphene

Often quoted Hubbard U/t =3.8

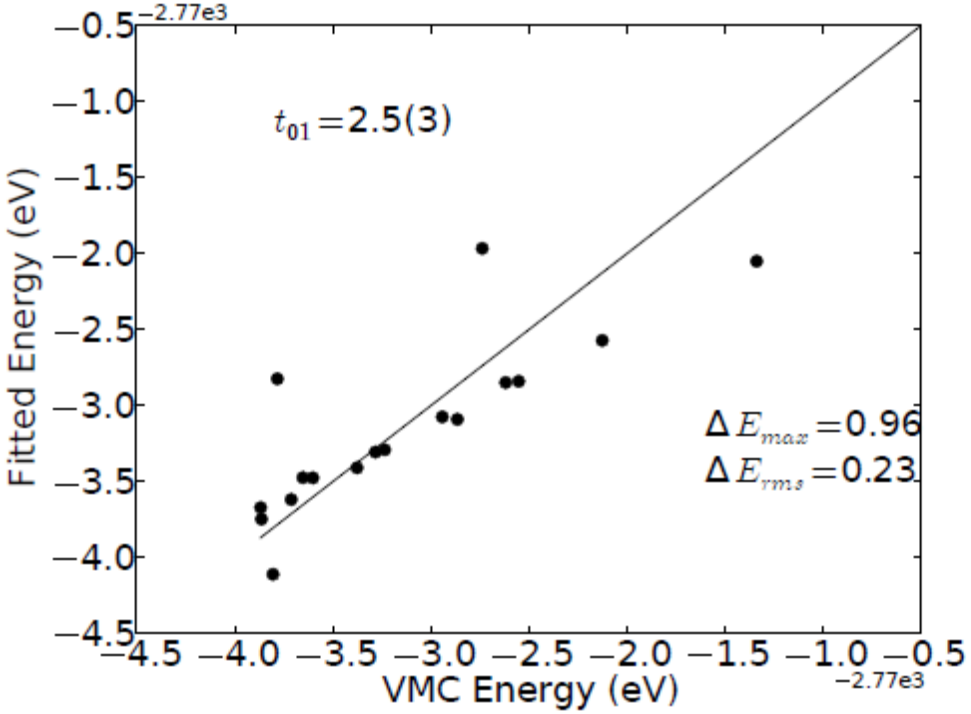


Sorella et al (Nature Scientific Reports 2012)

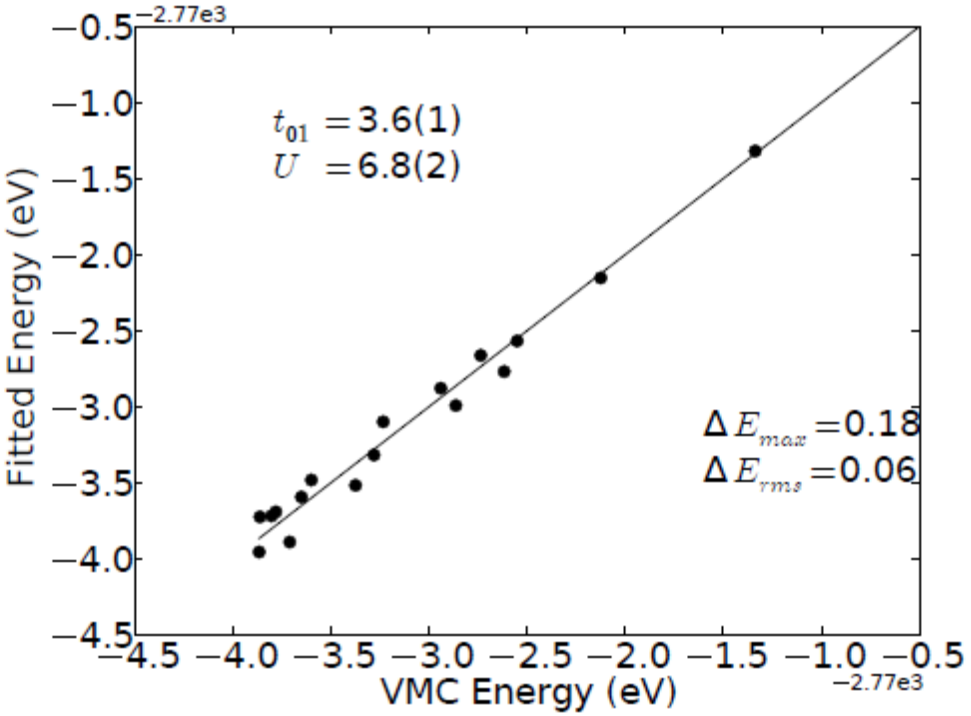
Full ab-initio calculation on 3x3 cell : 72 electrons (eg. 36 u, 36 d)
"Effective" Lattice model on 3x3 cell: 18 electrons (eg. 9 u, 9 d)

Example 3: Graphene (periodic solid)

What is the “effective” U ?

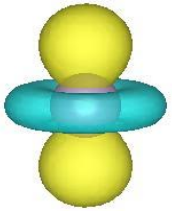


Tight binding model



Hubbard model

Our result U*/t approx 1.3 +/- 0.2 , cRPA result 1.6 +/- 0.2 (PRL 2013)
Graphene is well in semi-metallic phase



Example 4: Transition metal atoms

rotationally symmetric case: Hund's coupling J

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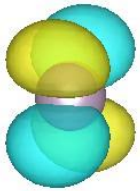

Antiferromagnetism and correlation of electrons in transition metals

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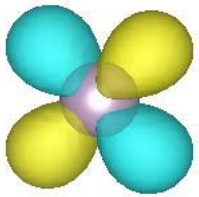
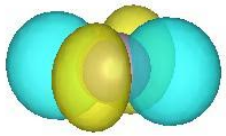
(Received 12 October 1982)



$$H=\sum_{m,n,i,\sigma} t_{mn}a^{\dagger}_{mi\sigma}a_{ni\sigma}+(U+2J)\sum_{m,i} n_{mi\uparrow}n_{mi\downarrow}+U\sum_{\substack{m,i,j,\sigma\\ i<j}} n_{mi\sigma}n_{mj,-\sigma}+(U-J)\sum_{\substack{m,i,j,\sigma\\ i<j}} n_{mi\sigma}n_{mj\sigma}$$

$$-J\sum_{\substack{m,i,j,\sigma\\ i<j}} a^{\dagger}_{mi\sigma}a_{mi,-\sigma}a^{\dagger}_{mj,-\sigma}a_{mj\sigma}+J\sum_{m,i,j} a^{\dagger}_{mi\uparrow}a^{\dagger}_{mi\downarrow}a_{mj\downarrow}a_{mj\uparrow}$$



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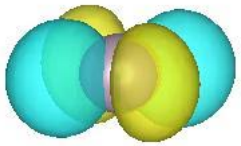

Hubbard-like Hamiltonians for interacting electrons in *s*, *p*, and *d* orbitals

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[1]*Imperial College London, London SW7 2AZ, United Kingdom*
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(Received 20 July 2015; revised manuscript received 2 November 2015; published 1 February 2016)

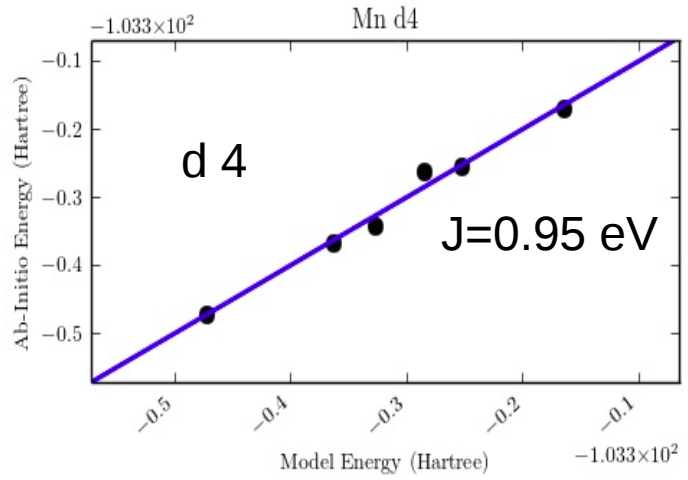
Others: Ohno, Kanamori, Dworin-Narath, Parisier-Pople-Parr, Georges, Kotliar, Imada...

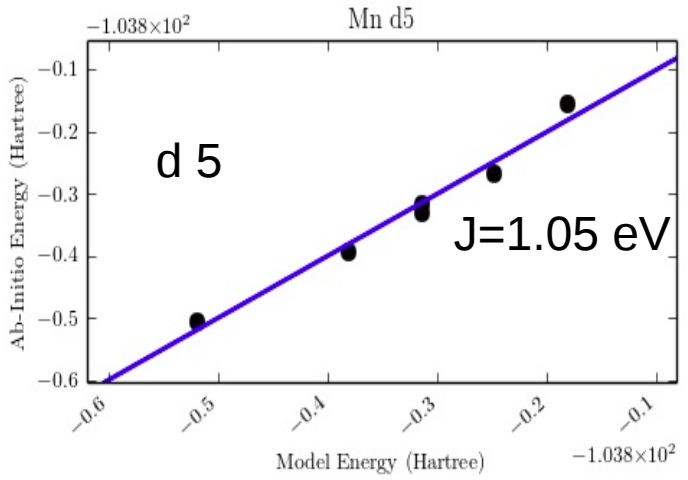
Example 4: Transition metal atoms

rotationally symmetric case: Hund's coupling J

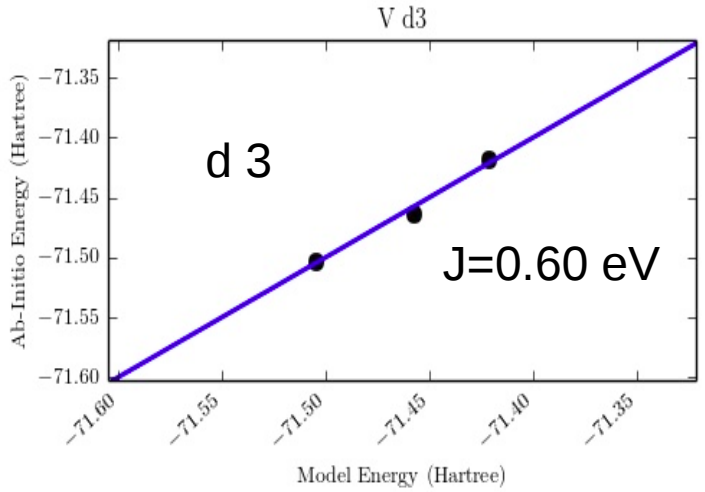
$$H = \sum_{m,n,i,\sigma} t_{mn} a^{\dagger}_{mi\sigma} a_{ni\sigma} + (U+2J) \sum_{m,i} n_{mi\uparrow} n_{mi\downarrow} + U \sum_{\substack{m,i,j,\sigma \\ i<j}} n_{mi\sigma} n_{mj,-\sigma} + (U-J) \sum_{\substack{m,i,j,\sigma \\ i<j}} n_{mi\sigma} n_{mj\sigma}$$
$$- J \sum_{\substack{m,i,j,\sigma \\ i<j}} a^{\dagger}_{mi\sigma} a_{mi,-\sigma} a^{\dagger}_{mj,-\sigma} a_{mj\sigma} + J \sum_{m,i,j} a^{\dagger}_{mi\uparrow} a^{\dagger}_{mi\downarrow} a_{mj\downarrow} a_{mj\uparrow}$$

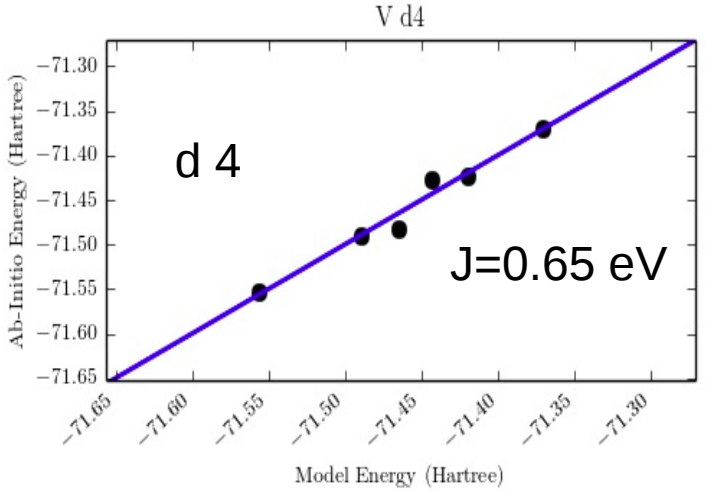
Mn





V





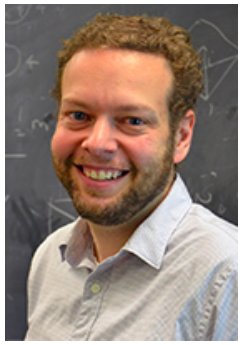
Summary of DMD

$$\begin{pmatrix} \tilde{E}_1 \\ \tilde{E}_2 \\ \tilde{E}_3 \\ \cdots \\ \cdots \\ \cdots \\ \tilde{E}_M \end{pmatrix} = \begin{pmatrix} 1 & \langle c_i^\dagger c_j \rangle_1 & .. & \langle c_i^\dagger c_j^\dagger c_l c_k \rangle_1 & .. \\ 1 & \langle c_i^\dagger c_j \rangle_2 & .. & \langle c_i^\dagger c_j^\dagger c_l c_k \rangle_2 & .. \\ 1 & \langle c_i^\dagger c_j \rangle_3 & .. & \langle c_i^\dagger c_j^\dagger c_l c_k \rangle_3 & .. \\ 1 & \langle c_i^\dagger c_j \rangle_4 & .. & \langle c_i^\dagger c_j^\dagger c_l c_k \rangle_4 & .. \\ 1 & .... & .. & .. & .. \\ 1 & .... & .. & .. & .. \\ 1 & \langle c_i^\dagger c_j \rangle_M & .. & \langle c_i^\dagger c_j^\dagger c_l c_k \rangle_M & .. \end{pmatrix} \begin{pmatrix} C \\ t_{ij} \\ .. \\ V_{ijkl} \\ .. \end{pmatrix}$$

Energies **Matrix of density matrices** **Parameters**

- Model Hamiltonians using wavefunction data
  - main idea is to relate “energies” and “reduced density matrices”
- Look beyond Hubbard-only models, eg. Kanamori form
- Promising but also challenging when many energy scales (FeSe, cuprates)
- *Ab-initio* community can help those studying strongly correlated models

Acknowledgements



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- Cyrus Umrigar
- (late) Christopher Henley
- Garnet Chan
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Thanks for listening!