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Gutzwiller method with machine learning and quantum computing

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2019-11-04

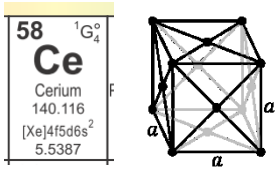
2019 Fall Workshop

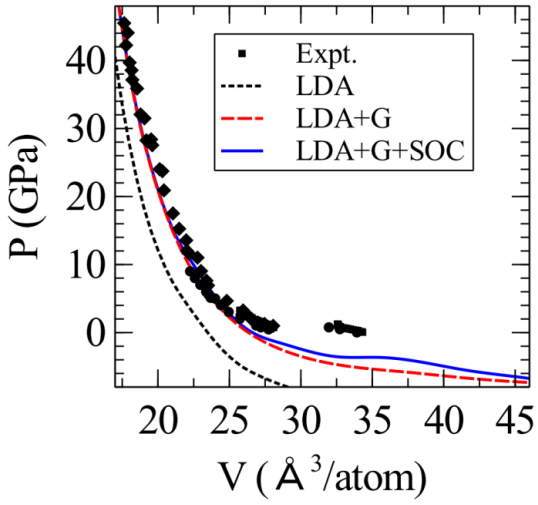
Center for Computational Materials Sciences

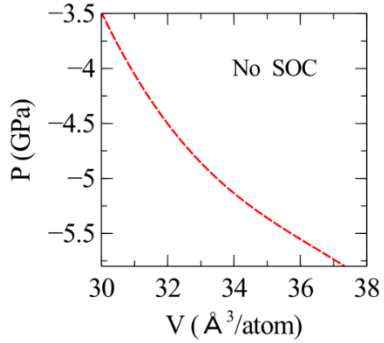
Outline

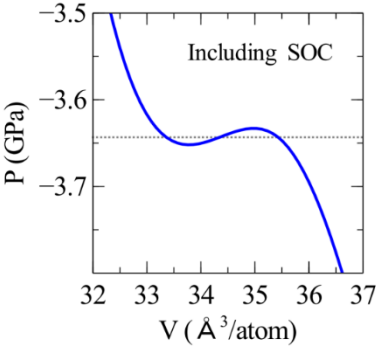
- Achievements of DFT+G calculations
- Analytical Jacobian of Gutzwiller solver:
  a) Formulation
  b) The significance
  c) Implementation and benchmarking
- Hybrid quantum-classical simulation project

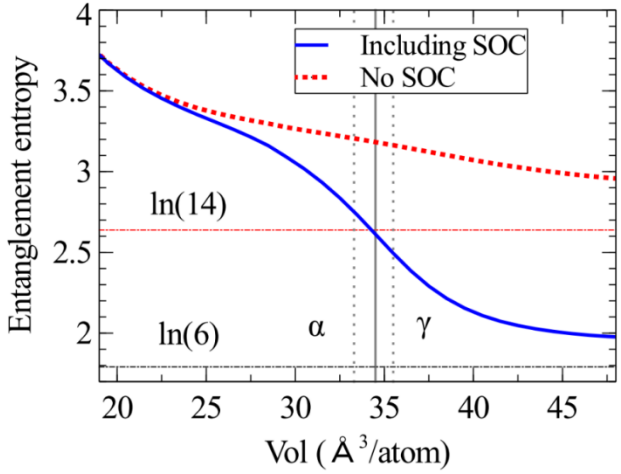
Kondo physics and spin-orbit interaction governing Ce volume collapse transition







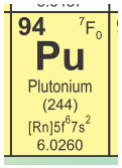


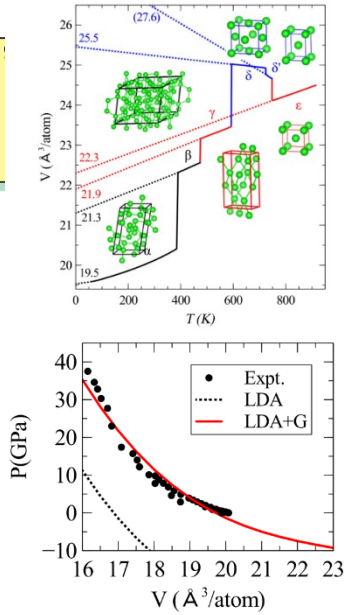


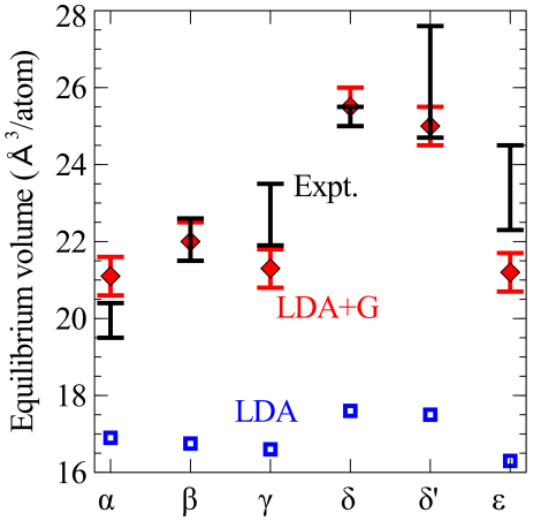
- A sharp crossover transition of the f-electron entanglement entropy
- Decent description of the equation of state
- Volume collapse transition only in the presence of spin-orbit interaction.

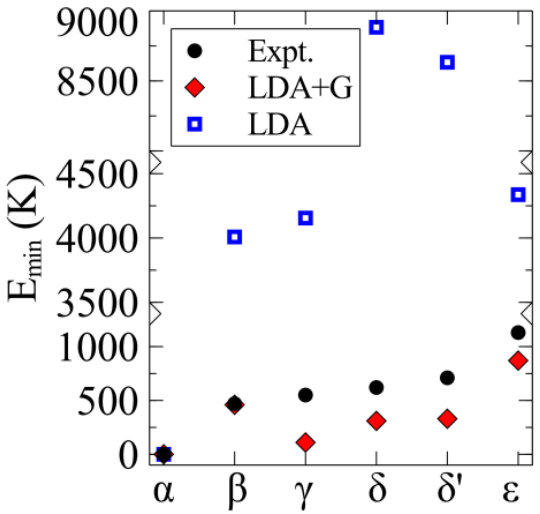
N. Lanatà, Y.-X. Yao*, C.-Z. Wang, K.-M. Ho, J. Schmalian, K. Haule, and G. Kotliar, *Phys. Rev. Lett.* **111**, 196801 (2013).
N. Lanatà*, Y.-X. Yao*, C.-Z. Wang, K.-M. Ho, and G. Kotliar, *Phys. Rev. B (R)* **90**, 161104 (2014).

Correlation effects balance competition between Peierls effect and Madelung interaction







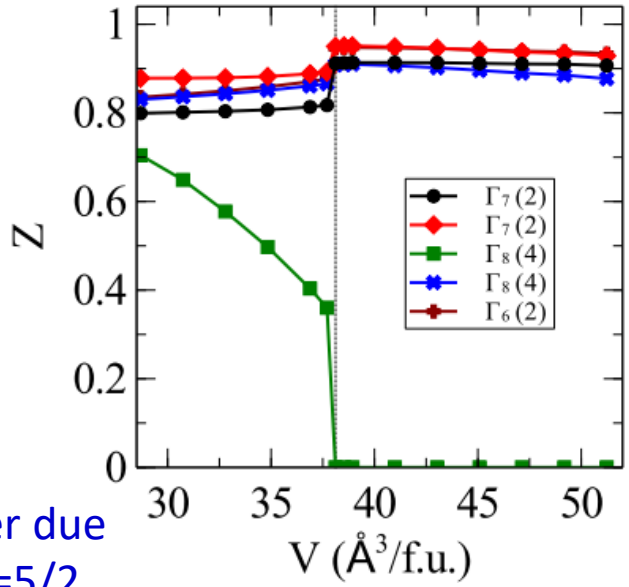


- Remarkably improved descriptions of all six phases of Pu, including equation of state, equilibrium volumes, relative energies.
- Correlation effects are crucial to balance the competition between electrostatic Madelung effect (for closed pack structure) and Peierls effect (for low symmetry).

N. Lanatà*, Y. -X. Yao*, C.-Z. Wang, K.-M. Ho, and G. Kotliar, *Phys. Rev. X* **5**, 011008 (2015).

UO_2: Selective Mott localized orbitals

Z: Kinetic energy renormalization factor



Mott localized orbitals:

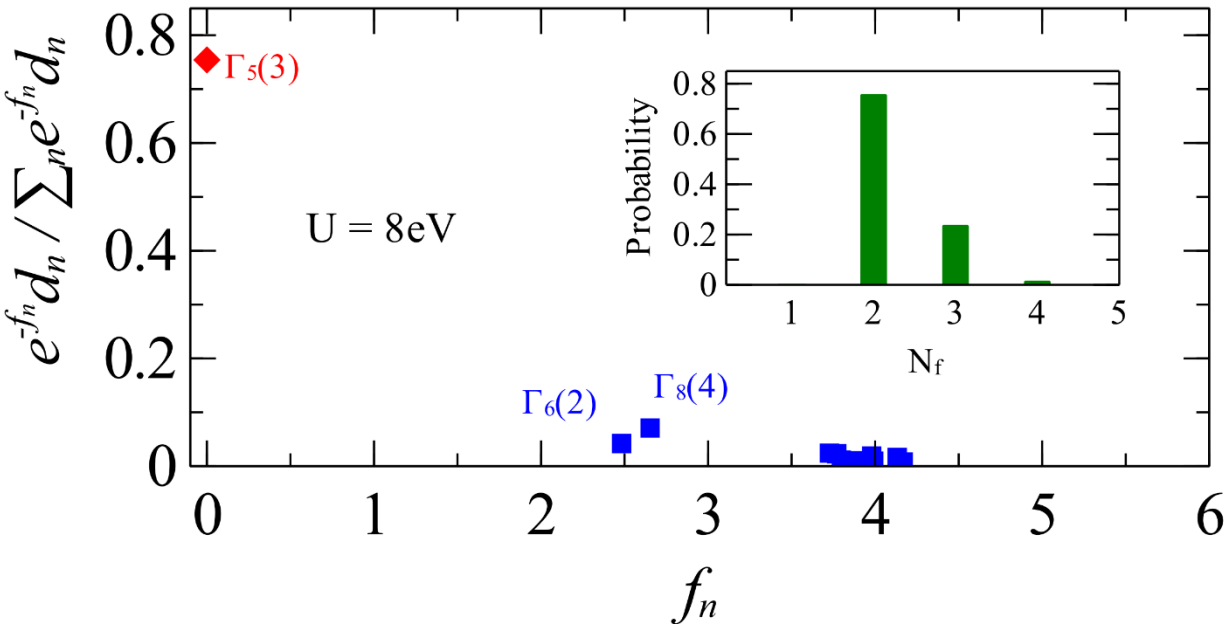
$$|1\rangle \simeq 0.939\,|\Gamma_8^{(1)}, 5/2, +\rangle + 0.343\,|\Gamma_8^{(2)}, 7/2, -\rangle$$
$$|2\rangle \simeq 0.939\,|\Gamma_8^{(1)}, 5/2, -\rangle + 0.343\,|\Gamma_8^{(2)}, 7/2, +\rangle$$
$$|3\rangle \simeq 0.939\,|\Gamma_8^{(2)}, 5/2, +\rangle + 0.343\,|\Gamma_8^{(1)}, 7/2, -\rangle$$
$$|4\rangle \simeq 0.939\,|\Gamma_8^{(2)}, 5/2, -\rangle + 0.343\,|\Gamma_8^{(1)}, 7/2, +\rangle$$

Mott localized states have considerably mixed J^2 character due to the crystal field effect (not a simple picture of all the J=5/2 orbitals localized).

Nicola Lanata*, Yongxin Yao*, Xiaoyu Deng, Vladimir Dobrosavljevic, and Gabriel Kotliar, *PRL* **118**, 126401 (2017)

UO_2: Multiplet structure

local reduced density matrix $\hat{\rho}_f \equiv e^{-\hat{F}}/\mathrm{Tr}[e^{-\hat{F}}]$



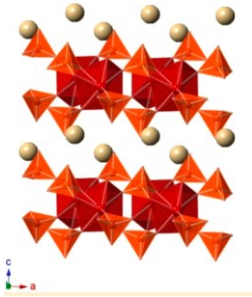
Most probable local configuration $f2$ Γ_5 triplet, consistent with experiment.

Nicola Lanata*, Yongxin Yao*, Xiaoyu Deng, Vladimir Dobrosavljevic, and Gabriel Kotliar, *PRL* **118**, 126401 (2017)

Multiplet structure in *f*-block chromates

w_i	0.88	0.06	0.04	0.002
N_i	6	7	5	6
J_i	0	3.5	2.5	6

$CsAm(CrO_4)_2$

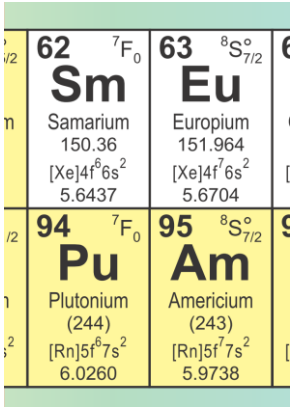


w_i	0.921	0.069	0.007	0.004
N_i	6	7	5	6
J_i	0	3.5	2.5	6

$CsEu(CrO_4)_2$

w_i	0.93	0.017	0.015	0.012
N_i	5	6	6	6
J_i	2.5	2	6	3

$CsSm(CrO_4)_2$



- Dominant multiplet state correlates with valence.
- Smaller dominant multiplet weight in Am-compound implies relatively stronger *f*-covalency.

Shane S. Galley, Alexandra A. Arico, Tsung-Han Lee, Xiaoyu Deng, Yong-Xin Yao, Joseph M. Sperling, Vanessa Proust, Julia S. Storbeck, Vladimir Dobrosavljevic, Jennifer N. Neu, Theo Siegrist, Ryan E. Baumbach, Thomas E. Albrecht-Schmitt, Nikolas Kaltsoyannis, and Nicola Lanatà, *J. Am. Chem. Soc.* 1**40**, 1674-1685 (2018).

Quantifying *f*-covalency

- Unique feature of handling multiple solutions on equal footing, including multiple (orbital-selective) Mott phases in Gutzwiller ansatz, allowing quantitative unbiased estimation of *f*-electron contribution to covalent bonding.
- Define the *f*-covalent bonding energy

$$\Delta Ecov \equiv E_{gs} - EFull_{Mott}$$

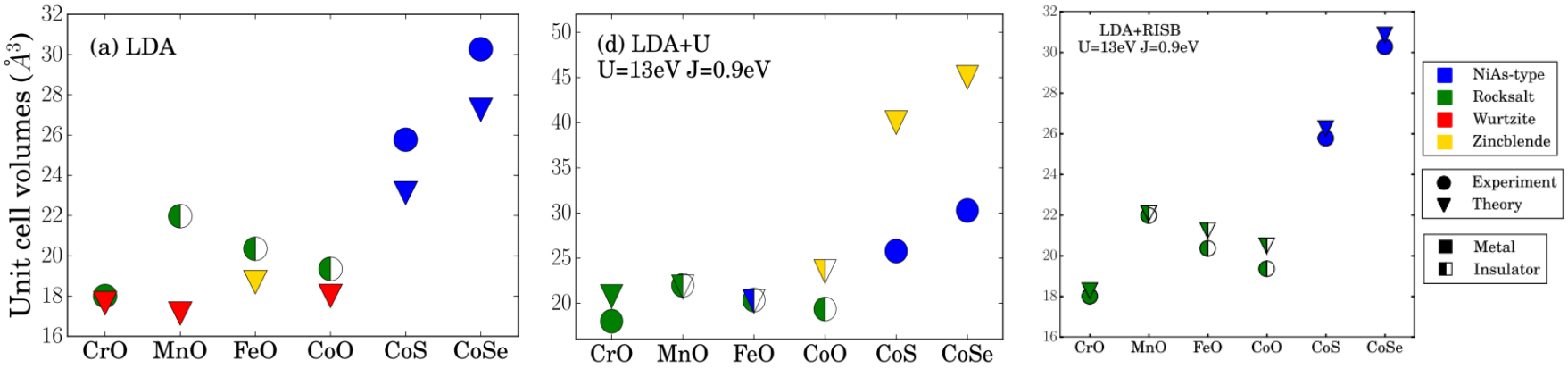
Note for full Mott phase: $|\Psi\rangle = |\Psi_f\rangle \otimes |\Psi_{env}\rangle$

	$CsAm(CrO_4)_2$	$CsEu(CrO_4)_2$	$CsSm(CrO_4)_2$
ΔE_{cov} (eV/f.u.)	1.85	0.76	0.67

- 5*f*-electron covalency contributions to chemical bonds are non-negligible.
- Covalency effects are more important in α -$CsAm(CrO_4)_2$ than others.

Shane S. Galley, Alexandra A. Arico, Tsung-Han Lee, Xiaoyu Deng, Yong-Xin Yao, Joseph M. Sperling, Vanessa Proust, Julia S. Storbeck, Vladimir Dobrosavljevic, Jennifer N. Neu, Theo Siegrist, Ryan E. Baumbach, Thomas E. Albrecht-Schmitt, Nikolas Kaltsoyannis, and Nicola Lanatà, *J. Am. Chem. Soc.* 1**40**, 1674-1685 (2018).

Ground state structure and electronic phases



LDA fails to predict

- ground state structure (rocksalt) of oxides
- insulating state.

- LSDA+U (or GGA+U) generally improves LDA
- Will still predict wrong crystal structures.

DFT+G calculations yield overall good description of ground state structure, electronic states and equilibrium volume.

N. Lanatà, T.-H. Lee, Y.-X. Yao, V. Stevanović, and V. Dobrosavljević, *Npj Computational Materials* **5**, 30 (2019).

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Generic Hubbard Model and Gutzwiller Ansatz

$$\hat{H} = \sum_{\mathbf{k}} \sum_{ij} \sum_{\alpha\beta\sigma} \epsilon_{\mathbf{k}i\alpha j\beta} \hat{c}^{\dagger}_{\mathbf{k}i\alpha\sigma} \hat{c}_{\mathbf{k}j\beta\sigma} + \sum_{\mathbf{R}} \sum_{i\alpha \in corr} \hat{H}^{loc}_{i} \left[\left\{ \hat{c}^{\dagger}_{\mathbf{R}i\alpha\sigma} \right\}, \left\{ \hat{c}_{\mathbf{R}i\alpha\sigma} \right\} \right]$$

Gutzwiller wave function

$$|\Psi_G\rangle \equiv \mathcal{P} |\Psi_0\rangle = \prod_{\mathbf{R}, i \in corr} \mathcal{P}_{\mathbf{R}i} |\Psi_0\rangle$$

Gutzwiller correlator

$$\mathcal{P}_{\mathbf{R}i} = \sum_{\Gamma\Gamma'} \Lambda_{i\Gamma\Gamma'} |\Gamma_{\mathbf{R}i}\rangle \langle \Gamma'_{\mathbf{R}i}|$$

$$|\Gamma_{\mathbf{R}i}\rangle = \left(c^{\dagger}_{\mathbf{R}i1}\right)^{n_1(\Gamma_{\mathbf{R}i})} \cdots \left(c^{\dagger}_{\mathbf{R}iM}\right)^{n_M(\Gamma_{\mathbf{R}i})} |0\rangle$$

Expectation values

Renormalized nonlocal one-particle density matrix:

$$\left\langle \Psi_G \left| \hat{c}^\dagger_{i\alpha} \hat{c}_{j\beta} \right| \Psi_G \right\rangle = \mathcal{R}^\dagger_{a\alpha} \mathcal{R}_{\beta b} \left\langle \Psi_0 \left| \hat{f}^\dagger_{ia} \hat{f}_{jb} \right| \Psi_0 \right\rangle$$

Renormalized local reduced many-body density matrix:

$$\varrho^G \equiv \phi\phi^\dagger = \Lambda \varrho^0 \Lambda^\dagger$$

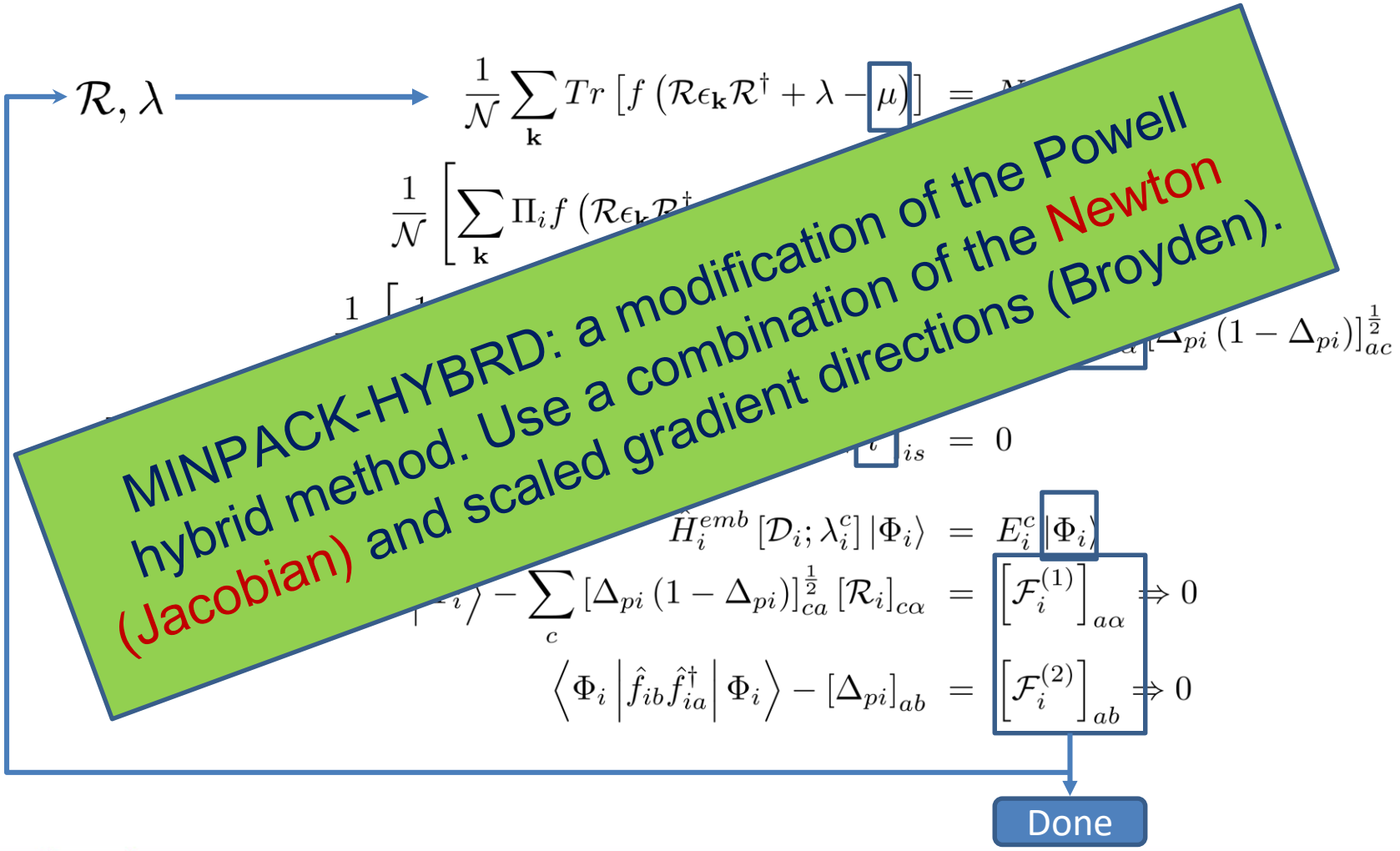
$$\varrho^0_{\Gamma\Gamma'} \equiv \langle \Psi_0 | \Gamma \rangle \langle \Gamma' | \Psi_0 \rangle$$

$$\phi = \Lambda \sqrt{\varrho^0}$$

Expectation value of any local operator

$$\left\langle \Psi_G \left| \hat{O}_l \right| \Psi_G \right\rangle = Tr \left[\phi\phi^\dagger O_l \right]$$

Gutzwiller nonlinear equations



MINPACK-HYBRD: a modification of the Powell hybrid method. Use a combination of the Newton (Jacobian) and scaled gradient directions (Broyden).

Gutzwiller Embedding Hamiltonian

$$\hat{H}^{emb}\left[\mathcal{D};\lambda^{c}\right] \equiv \hat{H}^{loc}\left[\left\{\hat{c}_{\alpha}^{\dagger}\right\},\left\{\hat{c}_{\alpha}\right\}\right] + \sum_{a\alpha}\left(\mathcal{D}_{a\alpha}\hat{c}_{\alpha}^{\dagger}f_{a} + H.c.\right) + \sum_{ab}\lambda_{ab}^{c}\hat{f}_{b}\hat{f}_{a}^{\dagger}$$

Quadratic + quartic terms

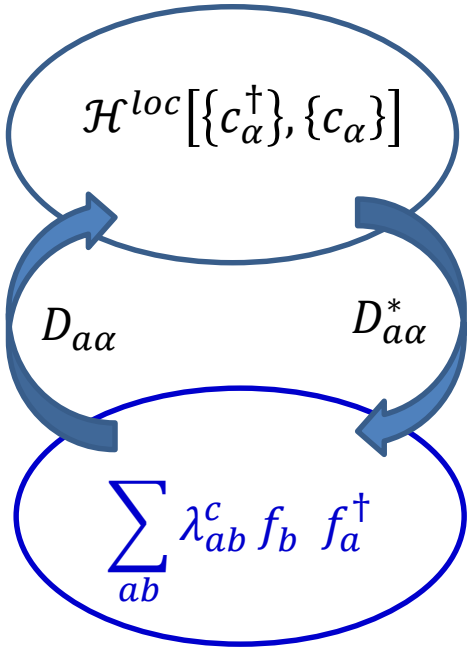
- The number of bath orbitals is exactly equal to the number of impurity orbitals.
- Solve the grounds state of the model at “half-filling”:

  1) Exact diagonalization ➔ $|\Phi\rangle$

  2) DMRG, …, ➔ $|\Phi\rangle$

However, what we need is some reduced information of $|\Phi\rangle$: $\vec{f}(\{D,\lambda\}) = DM$

3) Machine learning



ML mapping function and derivative

Represent local single particle matrices in the symmetry-adapted orthonormal Hermitian matrix basis

$$\{h_{is} : [g_{in}, h_{is}] = 0 \ \forall g \in G_i\}$$

$$\begin{aligned}
\Delta_{pi} &= \sum_s d_{is}^p \ {}^t h_{is} \\
\lambda_i &= \sum_s l_{is} \ h_{is} \\
\lambda_i^c &= \sum_s l_{is}^c \ h_{is} \\
\mathcal{R}_i &= \sum_s r_{is} \ h_{is} \\
\mathcal{D}_i &= \sum_s d_{is} \ h_{is}
\end{aligned}$$

The ML mapping function

$$\left\{ \left\langle \Phi_i \left| \hat{c}_{i\alpha}^\dagger \hat{f}_{ia} \right| \Phi_i \right\rangle, \left\langle \Phi_i \left| \hat{f}_{ib} \hat{f}_{ia}^\dagger \right| \Phi_i \right\rangle \right\} = f\left(\{l_{is}^c, d_{is}\}\right)$$

The analytical derivatives

$$\frac{\partial f[\langle \Phi_i | \hat{c}_{i\alpha}^\dagger \hat{f}_{ia} | \Phi_i \rangle]}{\partial l_{is'}^c}, \frac{\partial f[\langle \Phi_i | \hat{c}_{i\alpha}^\dagger \hat{f}_{ia} | \Phi_i \rangle]}{\partial d_{is'}}$$

$$\frac{\partial f[\langle \Phi_i | \hat{f}_{ib} \hat{f}_{ia}^\dagger | \Phi_i \rangle]}{\partial l_{is'}^c}, \frac{\partial f[\langle \Phi_i | \hat{f}_{ib} \hat{f}_{ia}^\dagger | \Phi_i \rangle]}{\partial d_{is'}}$$

$$\text{KRG: } f[\mathbf{x}] = \sum_i y_i e^{-\gamma \sum_j \left| x_j - s_j^{(i)} + 0^+ \right|}$$

Nitty-Gritties: full Jacobian matrix

$$\frac{1}{\mathcal{N}}\sum_{\mathbf{k}} Tr\left[f\left(\mathcal{R}\epsilon_{\mathbf{k}}\mathcal{R}^{\dagger}+\lambda-\mu\right)\right] = N_e$$

$$\frac{1}{\mathcal{N}}\left[\sum_{\mathbf{k}} \Pi_i f\left(\mathcal{R}\epsilon_{\mathbf{k}}\mathcal{R}^{\dagger}+\lambda-\mu\right)\Pi_i\right]_{ba} = \left[\Delta_{pi}\right]_{ab}$$

$$\frac{1}{\mathcal{N}}\sum_{c}\left[\Delta_{pi}\left(1-\Delta_{pi}\right)\right]^{-\frac{1}{2}}_{ac}\left[\frac{1}{R_i}\sum_{\mathbf{k}} \Pi_i f\left(\mathcal{R}\epsilon_{\mathbf{k}}\mathcal{R}^{\dagger}+\lambda-\mu\right)\Pi_i\right]_{ac} = \left[\mathcal{D}_i\right]_{a\alpha}$$

$$-\sum_{cb\alpha}\frac{\partial}{\partial d^{p}_{is}}\left[\Delta_{pi}\left(1-\Delta_{pi}\right)\right]^{\frac{1}{2}}_{cb}\left[\mathcal{D}_i\right]_{b\alpha}\left[\mathcal{R}_i\right]_{c\alpha} - c.c. - l_{is} = l^{c}_{is}$$

$$\hat{H}^{emb}_{i}\left[\mathcal{D}_i;\lambda^{c}_{i}\right]\left|\Phi_i\right\rangle - E^{c}_{i}\left|\Phi_i\right\rangle = 0$$

$$\sum_{c}\left[\Delta_{pi}\left(1-\Delta_{pi}\right)\right]^{-\frac{1}{2}}_{ca}\left\langle\Phi_i\left|\hat{c}^{\dagger}_{i\alpha}\hat{f}_{ic}\right|\Phi_i\right\rangle - \left[\mathcal{R}_i\right]_{a\alpha} = \left[\mathcal{F}^{(1)}_{i}\right]_{a\alpha}\Rightarrow 0$$

$$\left\langle\Phi_i\left|\hat{f}_{ib}\hat{f}^{\dagger}_{ia}\right|\Phi_i\right\rangle - \left[\Delta_{pi}\right]_{ab} = \left[\mathcal{F}^{(2)}_{i}\right]_{ab}\Rightarrow 0$$

Second order derivatives of a matrix function?

Nicola Lanata'

$$\frac{\partial\left[\mathcal{F}^{(1)}_{i}\right]_{a\alpha}}{\partial r\left(l\right)_{i's'}} = \sum_{c}\left(\frac{\partial\left(\left[\Delta_{pi}\left(1-\Delta_{pi}\right)\right]^{-\frac{1}{2}}_{ca}\right)}{\partial r\left(l\right)_{i's'}}\left\langle\Phi_i\left|\hat{c}^{\dagger}_{i\alpha}\hat{f}_{ic}\right|\Phi_i\right\rangle\right.$$

$$\left.+\left[\Delta_{pi}\left(1-\Delta_{pi}\right)\right]^{-\frac{1}{2}}_{ca}\left(\frac{\partial\left\langle\Phi_i\left|\hat{c}^{\dagger}_{i\alpha}\hat{f}_{ic}\right|\Phi_i\right\rangle}{\partial l^{c}_{is''}}\frac{\partial l^{c}_{is''}}{\partial r\left(l\right)_{i's'}}+\frac{\partial\left\langle\Phi_i\left|\hat{c}^{\dagger}_{i\alpha}\hat{f}_{ic}\right|\Phi_i\right\rangle}{\partial d_{is''}}\frac{\partial d_{is''}}{\partial r\left(l\right)_{i's'}}\right)\right)-\frac{\partial r_{is}}{\partial r\left(l\right)_{i's'}}$$

$$\frac{\partial\left[\mathcal{F}^{(2)}_{i}\right]_{ab}}{\partial r\left(l\right)_{i's'}} = \sum_{c}\left(\frac{\partial\left\langle\Phi_i\left|\hat{f}_{ib}\hat{f}^{\dagger}_{ia}\right|\Phi_i\right\rangle}{\partial l^{c}_{is''}}\frac{\partial l^{c}_{is''}}{\partial r\left(l\right)_{i's'}}+\frac{\partial\left\langle\Phi_i\left|\hat{f}_{ib}\hat{f}^{\dagger}_{ia}\right|\Phi_i\right\rangle}{\partial d_{is''}}\frac{\partial d_{is''}}{\partial r\left(l\right)_{i's'}}\right)-\frac{\partial\left[\Delta_{pi}\right]_{ab}}{\partial r\left(l\right)_{i's'}}$$

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Analytical Jacobian for large system simulation

$$\mathbf{J} = \begin{bmatrix} \dfrac{\partial \mathbf{f}}{\partial x_1} & \cdots & \dfrac{\partial \mathbf{f}}{\partial x_n} \end{bmatrix} = \begin{bmatrix} \dfrac{\partial f_1}{\partial x_1} & \cdots & \dfrac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \dfrac{\partial f_m}{\partial x_1} & \cdots & \dfrac{\partial f_m}{\partial x_n} \end{bmatrix}$$

Numerical Jacobian evaluation requires number of function evaluations proportional to dimension of the solution vector, which soon becomes dominant in systems of large size or low symmetry!

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Implementation: OOP

```
type,public::bandstru_ob
    !< iso=2 => soc
    integer ispin_in,nspin_in,
    integer n_mott,mode_hk ! m
    !< ne(3). 1: total number
    real(q),pointer :: ek(:,:,
    real(q),allocatable :: norm
    complex(q),pointer :: r(:,
            &d0(:,:,:),nrl(:,:,
    complex(q),pointer :: psi0_
    complex(q),pointer :: vk (
    complex(q),allocatable :: k
    complex(q),allocatable :: k
    type (sym_info) :: sym
    type (k_points) :: kpt

    contains
    procedure::init=>set_bnd_i
    procedure::read_hk0=>read_k
    procedure::rotate_hk0=>rota
    procedure::corr_ebwidth=>ca
    procedure::calc_all=>calc_k
    procedure::rm_hle_from_hk0=
    procedure::calc_fermi=>gut
```

```
type,extends(bandstru_ob),public::bandsder_ob
    real(q),pointer :: fw_der(:,:,:)
    real(q) :: sum_fw_der=0
    real(q),allocatable :: pmupr(:)   ! dmu/dr e
    real(q),allocatable :: pmupl(:)   ! dmu/dlam
    contains
    procedure::calc_derivatives
end type

contains

subroutine calc_derivatives(this,loc,mpi,io)
class(bandsder_ob) :: this
class(localstder_ob) :: loc
class(mpi_ob) :: mpi
integer,intent(in)::io

call loc%init_der()
call set_mu_delta(this%ef,this%kpt%delta)
call set_fermi_wt_derivative(this,mpi,io)
call set_pmupl(this,loc,mpi)
call set_pmupr(this,loc,mpi)
call set_pdm(this,loc,mpi)
call loc%calc_pdm_pp(io)
call loc%calc_pdplr()
call loc%calc_plcplr()
call loc%calc_pdlc_pp(io)
```

Benchmark

0 maxerr = 1.131318
1 maxerr = 1.131318
2 maxerr = 1.131318
3 maxerr = 1.131318
4 maxerr = 1.131319
5 maxerr = 1.131350
6 maxerr = 1.131334
7 maxerr = 1.131251
8 maxerr = 0.253372
9 maxerr = 0.021059
10 maxerr = 0.035637
11 maxerr = 0.045146
12 maxerr = 0.021059
13 maxerr = 0.021060
14 maxerr = 0.021071
15 maxerr = 0.021043
16 maxerr = 0.015036
17 maxerr = 0.017871
18 maxerr = 0.005150
19 maxerr = 0.000539
20 maxerr = 1.39e-05
21 maxerr = 2.28e-06

1 maxerr = 1.13131
2 maxerr = 1.13131
3 maxerr = 1.13131
4 maxerr = 1.13131
5 maxerr = 1.13131
6 maxerr = 0.28457
7 maxerr = 0.17625
8 maxerr = 0.04030
9 maxerr = 0.02578
10 maxerr = 0.01943
11 maxerr = 0.01356
12 maxerr = 0.00220
13 maxerr = 0.00166
14 maxerr = 0.00095
15 maxerr = 9.5e-05
16 maxerr = 1.7e-05
17 maxerr = 4.1e-06

0 maxerr = 1.02568
1 maxerr = 1.02568
2 maxerr = 1.02568
3 maxerr = 1.02568
4 maxerr = 1.02568
5 maxerr = 1.02571
6 maxerr = 1.02568
7 maxerr = 1.02571
8 maxerr = 1.02597
9 maxerr = 1.02570
10 maxerr = 1.02597
11 maxerr = 1.02570
12 maxerr = 0.30190
13 maxerr = 0.01960
14 maxerr = 0.03630
15 maxerr = 0.05215
16 maxerr = 0.01960
17 maxerr = 0.01961
18 maxerr = 0.01960
19 maxerr = 0.01961
20 maxerr = 0.01964
21 maxerr = 0.01961
22 maxerr = 0.01964
23 maxerr = 0.01961
24 maxerr = 0.01345
25 maxerr = 0.01372
26 maxerr = 0.00214
27 maxerr = 0.00015
28 maxerr = 9.4e-06
29 maxerr = 7.7e-07

0 maxerr = 1.02625
1 maxerr = 1.02625
2 maxerr = 1.02625
3 maxerr = 1.02625
4 maxerr = 1.02625
5 maxerr = 1.02625
6 maxerr = 0.58126
7 maxerr = 0.39147
8 maxerr = 0.15406
9 maxerr = 0.08180
10 maxerr = 0.06056
11 maxerr = 0.01275
12 maxerr = 0.00481
13 maxerr = 0.00049
14 maxerr = 0.00037
15 maxerr = 0.00152
16 maxerr = 4.5e-07

Outline

- Achievements of DFT+G calculations
- Analytical Jacobian of Gutzwiller solver:
  a) Formulation
  b) The significance
  c) Implementation and benchmarking
- Hybrid quantum-classical simulation project

Questions, comments criticisms to

yxphysics@gmail.com

National Quantum Initiative Act

An Act

To provide for a coordinated Federal program to accelerate quantum research and development for the economic and national security of the United States.

Be it enacted by the Senate and House of Representatives of the United States of America in Congress assembled,

SECTION 1. SHORT TITLE; TABLE OF CONTENTS.

(a) SHORT TITLE.—This Act may be cited as the "National Quantum Initiative Act".

TITLE IV—DEPARTMENT OF ENERGY QUANTUM ACTIVITIES

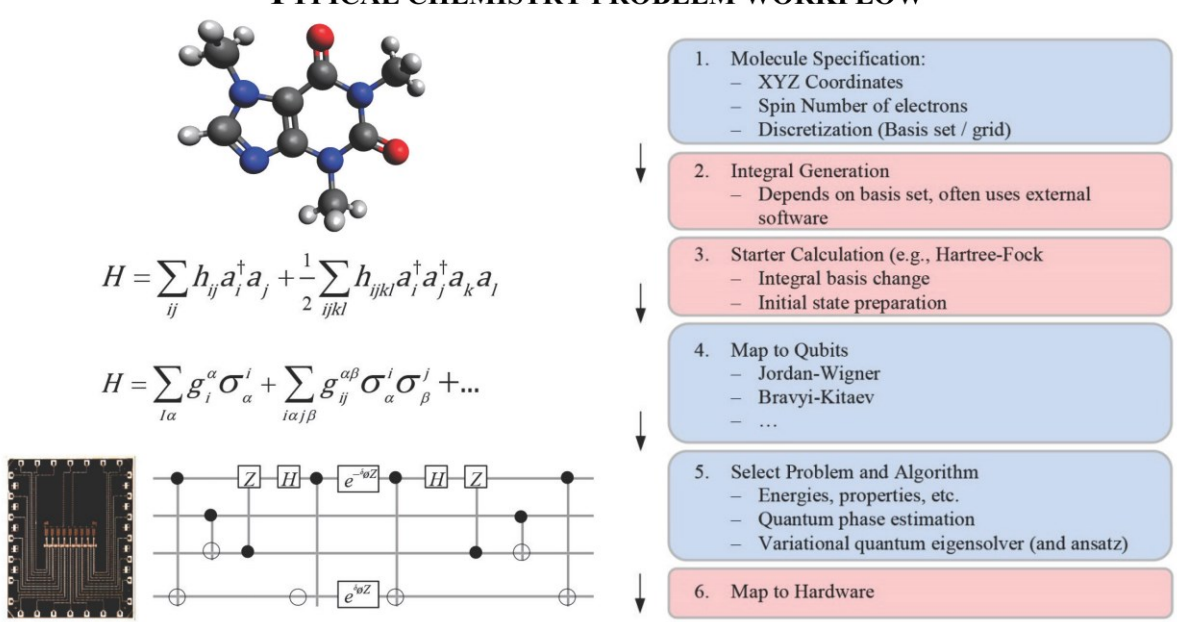
Opportunities for Quantum Computing in Chemical and Materials Sciences

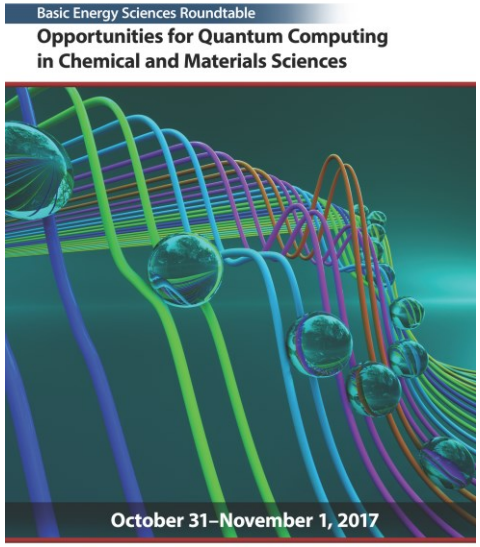
Priority Research Opportunities .....

PRO 1: Controlling the Quantum Dynamics of Nonequilibrium Chemical and Materials Systems .....

PRO 2: Unraveling the Physics and Chemistry of Strongly Correlated Electron Systems

PRO 3: Embedding Quantum Hardware in Classical Frameworks .....





Hybrid Quantum-Classical Approach

PHYSICAL REVIEW X **6,** 031045 (2016)

Hybrid Quantum-Classical Approach to Correlated Materials

Bela Bauer,[1] Dave Wecker,[2] Andrew J. Millis,[3] Matthew B. Hastings,[1,2] and Matthias Troyer[4,2]

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[2]*Quantum Architectures and Computation Group, Microsoft Research, Redmond, Washington 98052, USA*
[3]*Department of Physics, Columbia University in the City of New York, New York, New York 10027, USA*
[4]*Theoretische Physik and Station Q Zurich, ETH Zurich, 8093 Zurich, Switzerland*

(Received 8 October 2015; revised manuscript received 23 August 2016; published 21 September 2016)

Solve discretized AIM:

$$H = H_{\text{imp}} + H_{\text{bath}} + H_{\text{mix}},$$

$$H_{\text{imp}} = \sum_{\alpha\beta} t_{\alpha\beta} c_\alpha^\dagger c_\beta + \sum_{\alpha\beta\gamma\delta} U_{\alpha\beta\gamma\delta} c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta,$$

$$H_{\text{mix}} = \sum_{\alpha i} (V_{\alpha i} c_\alpha^\dagger d_i + \bar{V}_{\alpha i} d_i^\dagger c_\alpha),$$

$$H_{\text{bath}} = \sum_i \epsilon_i d_i^\dagger d_i,$$

- Adiabatic state preparation
- Quantum phase estimation (QPE)
- Measure real time GF

For $N_{s0} = 2\text{–}20$ @0 K:

- Measurements: $10^6 \sim 10^8$
- Deep circuits: $10^6 \sim 10^8$ gates

Noisy Intermediate Quantum Computing

Quantum Computing in the NISQ era and beyond

John Preskill

Institute for Quantum Information and Matter and Walter Burke Institute for Theoretical Physics,
California Institute of Technology, Pasadena CA 91125, USA
30 July 2018

- 50 to a few hundred qubits
- Error rate per two-qubit gate: 0.1% or worse
- Measurement error: 1% or worse
- Circuit to run < 1000 two-qubit gates

Variational Quantum Eigen Solver

an unsung hero of approximate quantum computing

ARTICLE

Received 9 Dec 2013 | Accepted 27 May 2014 | Published 23 Jul 2014

DOI: 10.1038/ncomms5213 OPEN

A variational eigenvalue solver on a photonic quantum processor

Alberto Peruzzo[1,*,†], Jarrod McClean[2,*], Peter Shadbolt[1], Man-Hong Yung[2,3], Xiao-Qi Zhou[1], Peter J. Love[4], Alán Aspuru-Guzik[2] & Jeremy L. O'Brien[1]

Accelerated Variational Quantum Eigensolver

Daochen Wang,* Oscar Higgott, and Stephen Brierley

Riverlane, 3 Charles Babbage Road, Cambridge CB3 0GT, United Kingdom

(Received 18 June 2018; revised manuscript received 18 December 2018; published 12 April 2019)

The theory of variational hybrid quantum-classical algorithms

Jarrod R McClean[1], Jonathan Romero[2], Ryan Babbush[3] and Alán Aspuru-Guzik[2]

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[2] Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA 02138, USA
[3] Google, Venice, CA 90291, USA

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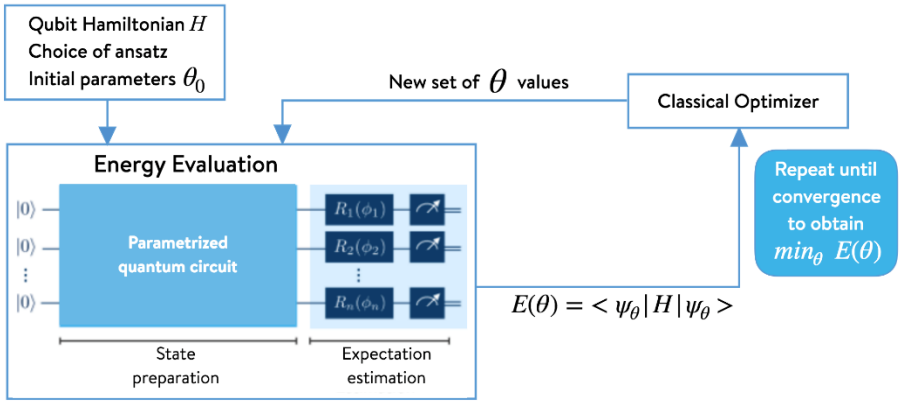
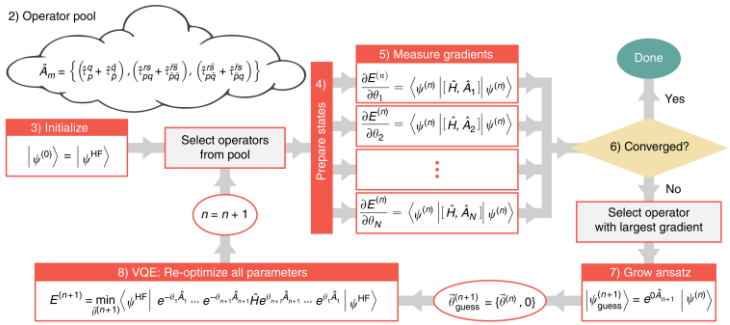
An adaptive variational algorithm for exact molecular simulations on a quantum computer

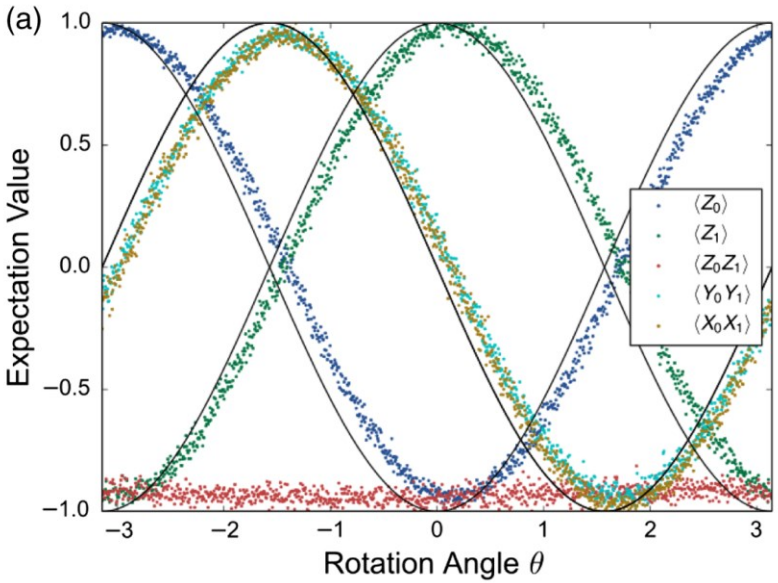
Harper R. Grimsley[1], Sophia E. Economou[2], Edwin Barnes[2] & Nicholas J. Mayhall[1]

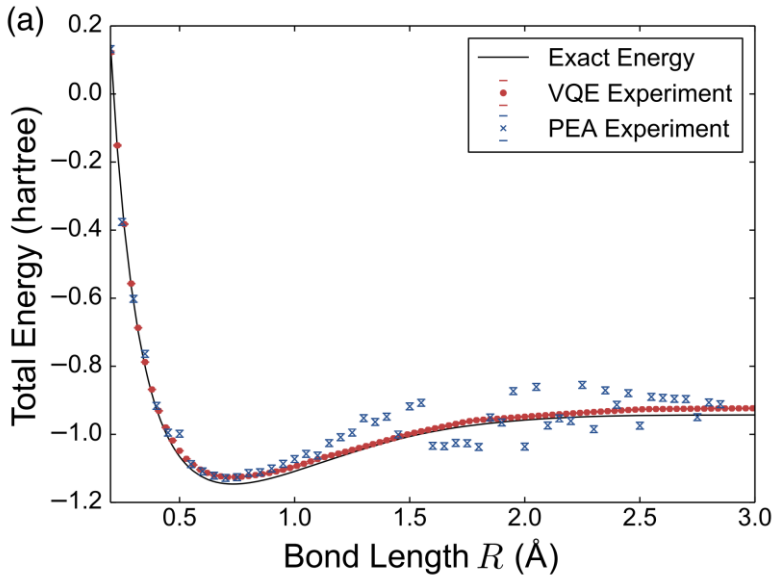




Trade deep circuits with few measurements in QPE for short circuits with more measurements in VQE for error mitigation.

Noise tolerance





PHYSICAL REVIEW X **6,** 031007 (2016)

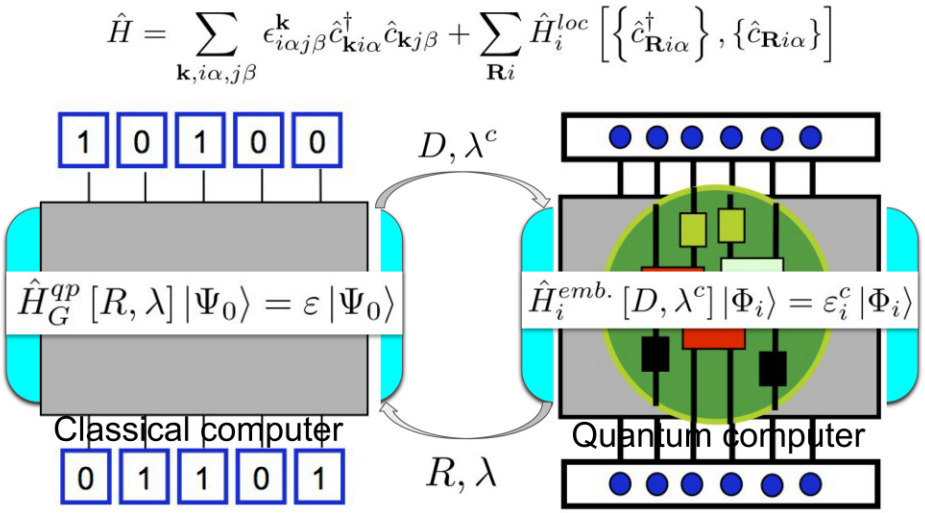
Scalable Quantum Simulation of Molecular Energies

P. J. J. O'Malley,[1,*] R. Babbush,[2,†] I. D. Kivlichan,[3] J. Romero,[3] J. R. McClean,[4] R. Barends,[5] J. Kelly,[5] P. Roushan,[5] A. Tranter,[6,7] N. Ding,[2] B. Campbell,[1] Y. Chen,[5] Z. Chen,[1] B. Chiaro,[1] A. Dunsworth,[1] A. G. Fowler,[5] E. Jeffrey,[5] E. Lucero,[5] A. Megrant,[5] J. Y. Mutus,[5] M. Neeley,[5] C. Neill,[1] C. Quintana,[1] D. Sank,[5] A. Vainsencher,[1] J. Wenner,[1] T. C. White,[5] P. V. Coveney,[7] P. J. Love,[6] H. Neven,[2] A. Aspuru-Guzik,[3] and J. M. Martinis[5,1,‡]

Gutzwiller Embedding Hamiltonian

$$\hat{H}^{emb}\left[\mathcal{D};\lambda^{c}\right]\equiv\hat{H}^{loc}\left[\left\{\hat{c}_{\alpha}^{\dagger}\right\},\left\{\hat{c}_{\alpha}\right\}\right]+\sum_{a\alpha}\left(\mathcal{D}_{a\alpha}\hat{c}_{\alpha}^{\dagger}f_{a}+H.c.\right)+\sum_{ab}\lambda_{ab}^{c}\hat{f}_{b}\hat{f}_{a}^{\dagger}$$

- The number of bath orbitals is exactly equal to the number of impurity orbitals.
- “Dimer” with much sparse Hamiltonian
- Various variational quantum eigen-solver to find the ground state and measure the one-particle density matrix.




Thank you!