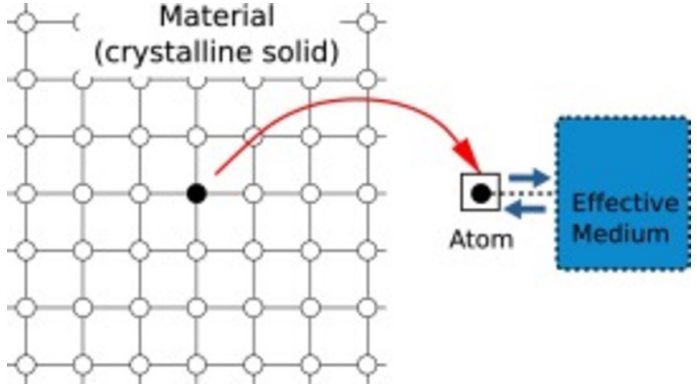
Solving for the ground state of the Anderson impurity model using VQE

Eric Jones

Quantum Applications Engineer

Motivation & Background

Why AIM?
(or impurity models generally?)



$$\hat{H} = \sum_{\substack{\alpha\beta \\ \sigma\sigma'}} \mu_{\alpha\beta\sigma\sigma'} \hat{c}^{\dagger}_{\alpha\sigma} \hat{c}_{\beta\sigma'} + \sum_{\substack{\alpha\beta\gamma\delta \\ \sigma\sigma'}} U_{\alpha\beta\gamma\delta} \hat{c}^{\dagger}_{\alpha\sigma} c^{\dagger}_{\beta\sigma'} \hat{c}_{\gamma\sigma'} \hat{c}_{\delta\sigma}$$
$$+ \sum_{i\alpha\sigma} \left(V_{i\alpha} \hat{f}^{\dagger}_{i\sigma} \hat{c}_{\alpha\sigma} + \text{h.c.} \right) + \sum_{ij\sigma} \epsilon_{ij} \hat{f}^{\dagger}_{i\sigma} \hat{f}_{j\sigma}, \qquad (9)$$

QC CC

Solve AIM (μ, U)	$\boldsymbol{G}_{imp.}(\omega)$ V, ϵ	$\boldsymbol{G}_{imp.}(\omega) = \boldsymbol{G}_{loc.}(\omega)$

Computational Complexity
(N bath, M impurity orbitals)

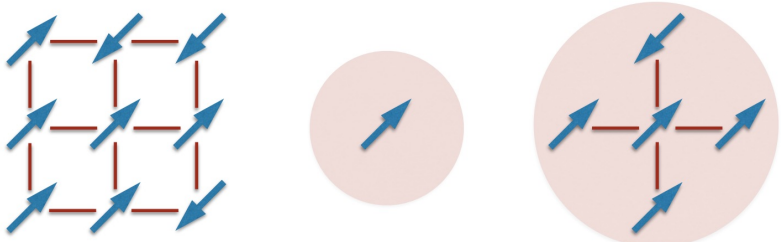
Exact Diagonalization
- ~ exp(M + N)

CTQMC (sign problem!)
- ~ exp(M) poly(N)

NRG/DMRG
- ~ exp(M) / exp(N)

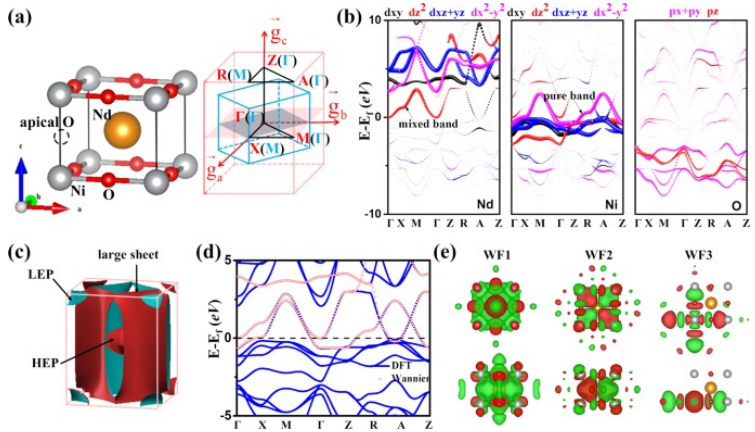
Fermionic Gaussian Approx.
- ~ exp(M) quasipoly(N)

lattice model | single-site mean-field theory | cluster mean-field theory

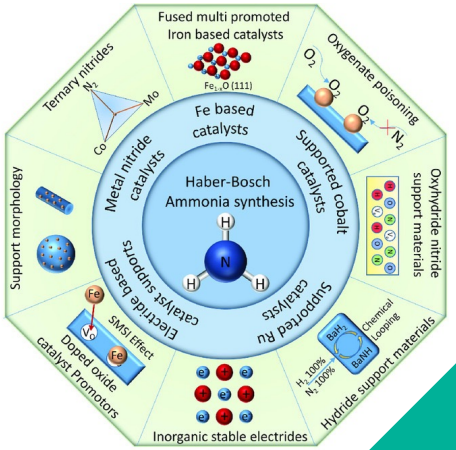


(Cluster DMFT: Spatial Correlations)

Potential Applications
High-T Superconductivity



(Heterogenous) Catalysis
(e.g., Green Ammonia)



Technical Overview

Workflow

Input: $\mu_{\alpha\beta}$, $U_{\alpha\beta\gamma\delta}$, $V_{i\alpha}$, ϵ_{ij}

↓

Construct H_F (OpenFermion)

↓ J-W | B-K, etc.

Construct H_Q (OpenFermion/Qulacs)

↓

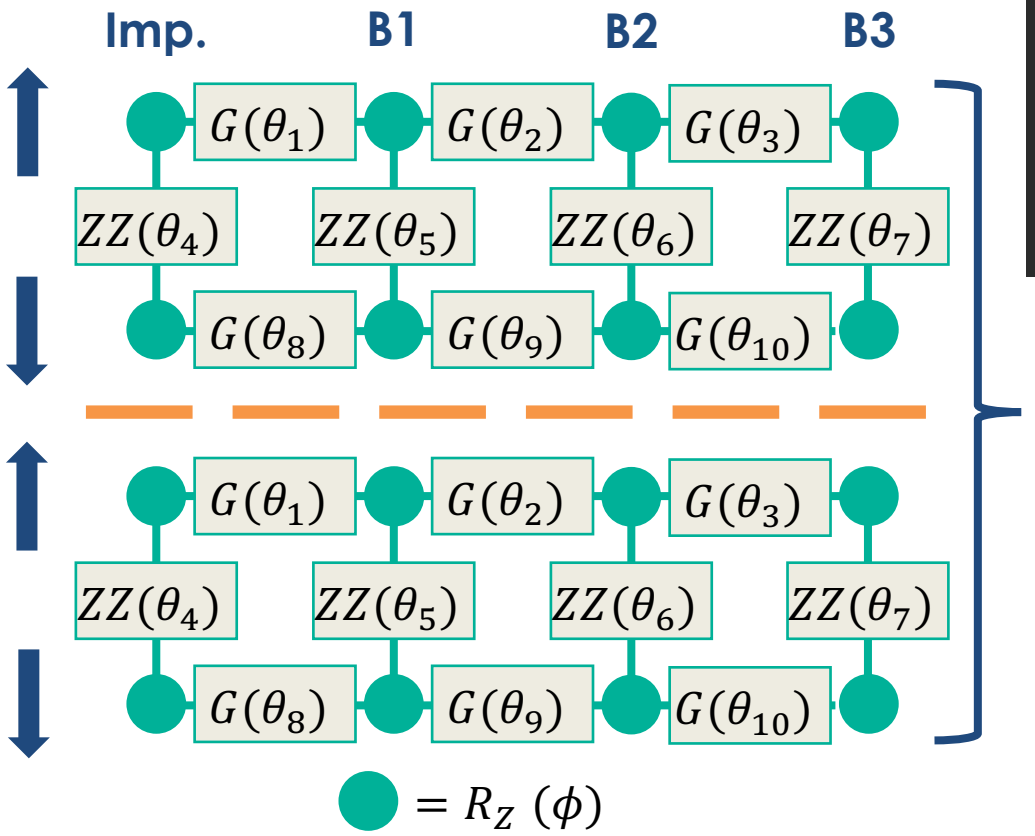
ED (OF) | VQE (Qiskit/Qul.)

1P Green's Function

Hybrid* SP/HV Ansatz**

Hamiltonian Symmetries: charge, spin, time-reversal

(20 CZs per tile-layer)



Preliminary Performance

```
        Z-spin eigenvalue: 0
        Init. Occ. Inds: [0, 1, 3, 5]
        GS Energy: -14.458763069397431
        GS Energy Diff: 0.002414026970855687
         message: Optimization terminated successfully.
success: True
 status: 1
    fun: -14.458763069397431
      x: [ 2.114e+00 -2.104e-01 ...  1.095e+00  1.363e+00]
   nfev: 6950
  maxcv: 0.0
        GS Charge, Spin Check: 4.0 0.0
```

```
Exact GS Charge, Spin: 4.000 0.000
-14.461177096368349
```

Resource Estimates

1 impurity, 2 bath sites
= 6 qubits
d = 2 layers
(7 x 2) x 2 = 28 CZ gates
~100 energy evaluations
~10 tensor factor bases
~1,000 shots per basis
~10Hz => 27.7 hrs

* Frankansatz, **Shoutout to David O-A. and Ben H.