System-adapted Quantum Chemistry with Tequila

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Acknowledgement

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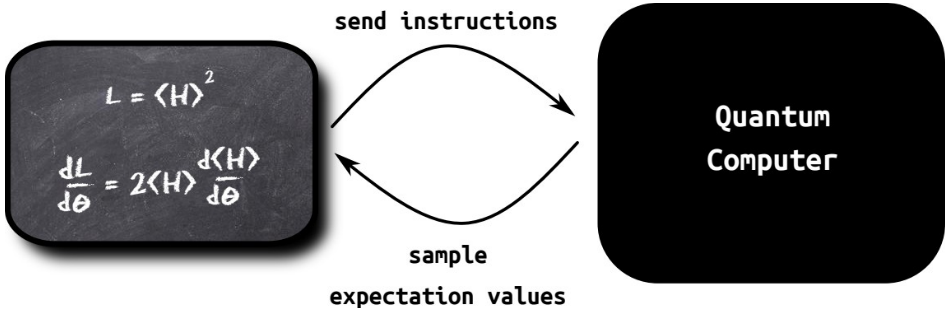
Quantum Chemistry on Quantum Computers



Generators: Hermitian Operators

$$G_{abkl} = i(a_a^\dagger a_i a_b^\dagger a_j - h.c.)$$

Circuits from unitaries

$$U(\theta) = e^{-i\frac{\theta}{2}G}$$

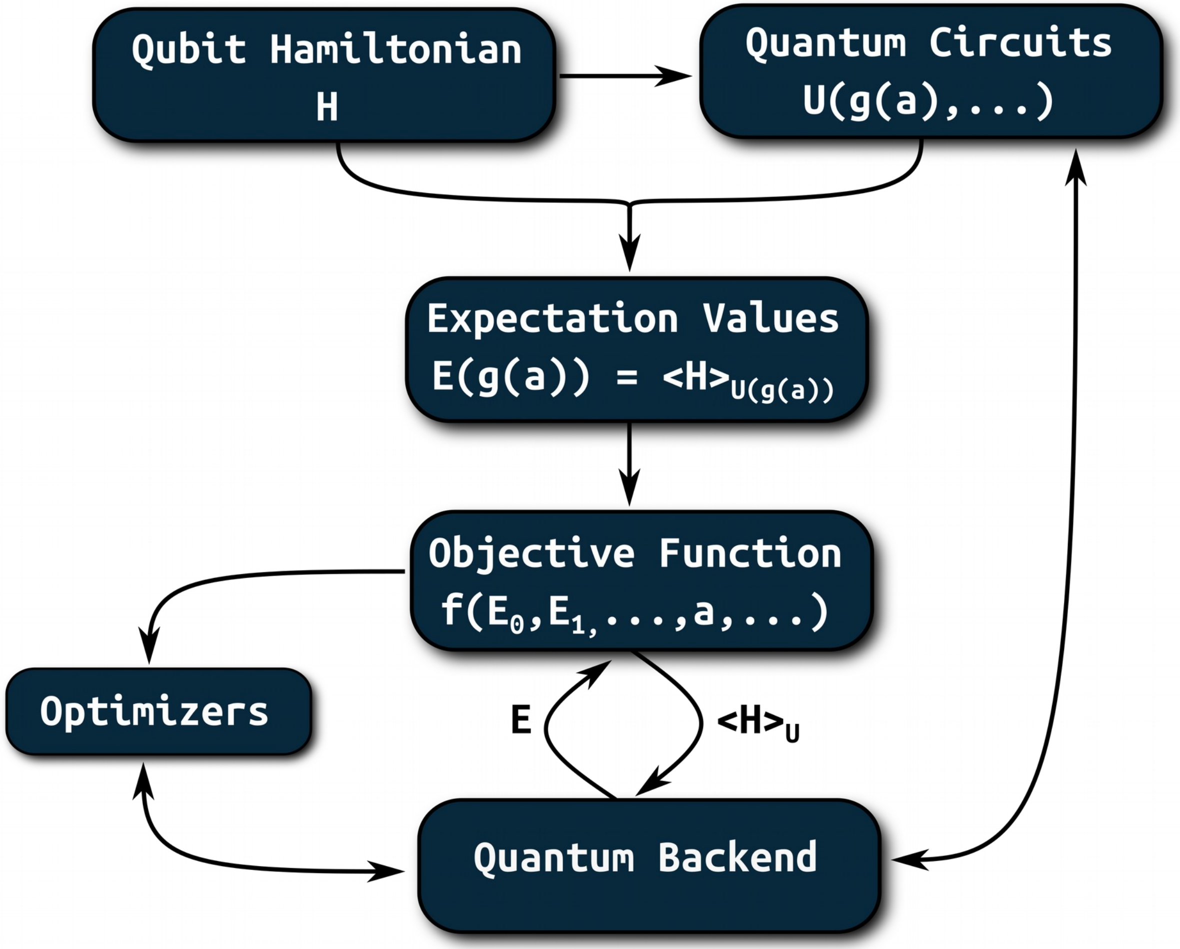
Fermionic operators are mapped to paulistrings

$$a_k^\dagger = 1^{\otimes k-1}\sigma_k^- \sigma_Z^{\otimes n-k}$$

Variational optimization

$$\min_\theta \left(\langle H \rangle_{U_\theta}\right) \equiv \min_\theta \left(\langle 0| U^\dagger(\theta) H U(\theta) |0\rangle\right)$$

Tequila



The Meta-Variational Quantum Eigensolver (Meta-VQE): Learning energy profiles of parameterized Hamiltonians for quantum simulation

Alba Cervera-Lierta,[1,2] Jakob S. Kottmann,[1,2] and Alán Aspuru-Guzik[1,2,3,4]

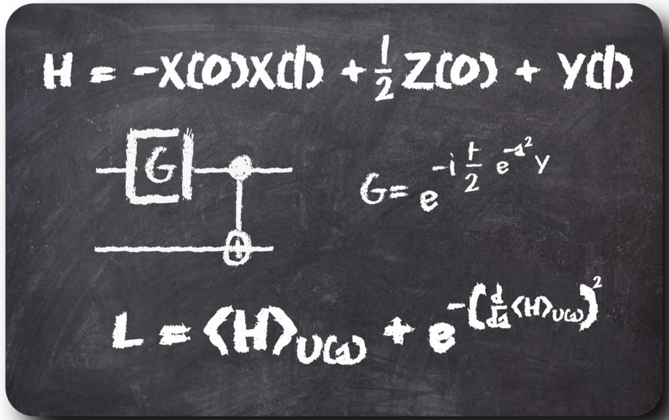
Quantum Computer-Aided design of Quantum Optics Hardware

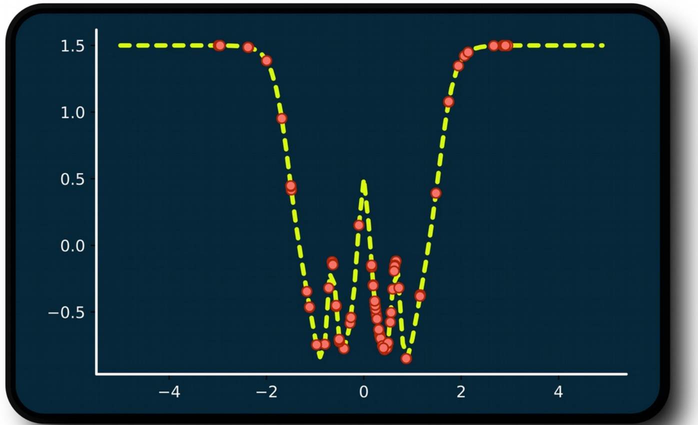
Jakob S. Kottmann,[1,2] Mario Krenn,[1,2,3] Thi Ha Kyaw,[1,2] Sumner Alperin-Lea,[1,2] and Alán Aspuru-Guzik[1,2,3,4]

Reducing qubit requirements while maintaining numerical precision for the Variational Quantum Eigensolver: A Basis-Set-Free Approach

Jakob S. Kottmann,[1,2,*] Philipp Schleich,[3] Teresa Tamayo-Mendoza,[4,1,2] and Alán Aspuru-Guzik[1,2,5,6,†]

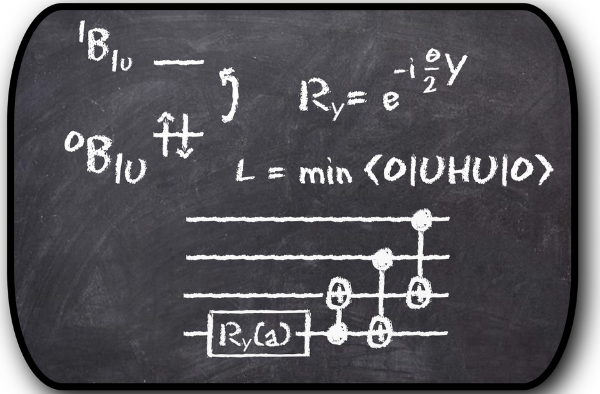
Tequila

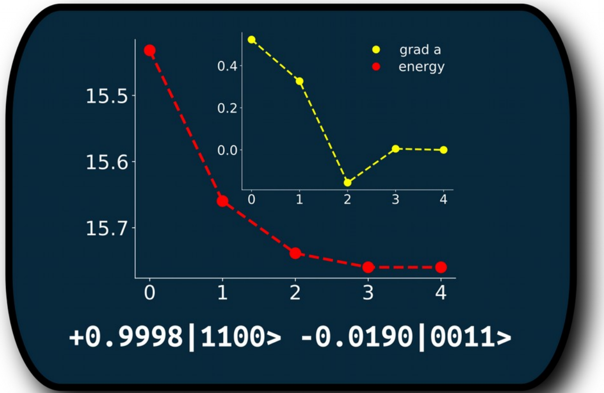





```
a = tq.Variable("a")
U = tq.gates.Ry(angle=(-a**2).apply(tq.numpy.exp)*pi, target=0)
U += tq.gates.X(target=1, control=0)
H = tq.QubitHamiltonian.from_string("-1.0*X(0)X(1)+0.5Z(0)+Y(1)")
E = tq.ExpectationValue(H=H, U=U)
dE = tq.grad(E, "a")
objective = E + (-dE**2).apply(tq.numpy.exp)
result = tq.minimize(method="phoenics", objective=objective)
```

Tequila





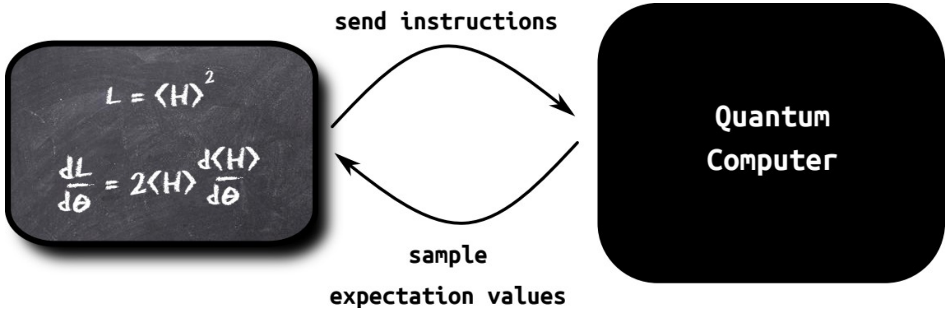

```python
active = {"b1u": [0, 1]}
mol = tq.chemistry.Molecule("beh2.xyz", "6-31g", active)
H = mol.make_hamiltonian()
U = tq.gates.Ry("a", 0)
U += tq.gates.CNOT(0, 1) + tq.gates.CNOT(0, 2)
U += tq.gates.CNOT(1, 3) + tq.gates.X([2, 3])
expv = tq.ExpectationValue(U, H)
result = tq.optimizer_scipy.minimize(expv, "bfgs")
wfn = tq.simulate(U, variables=result.angles)
```

Quantum Chemistry on Quantum Computers

Generators: Hermitian Operators

$$G_{abkl} = i(a_a^\dagger a_i a_b^\dagger a_j - h.c.)$$

```
mol.make_excitation_generator([(a,i),(b,j)])
```



Circuits from unitaries

$$U(\theta) = e^{-i\frac{\theta}{2}G}$$

```
tq.gates.Trotterized(G,"a", 1)
```

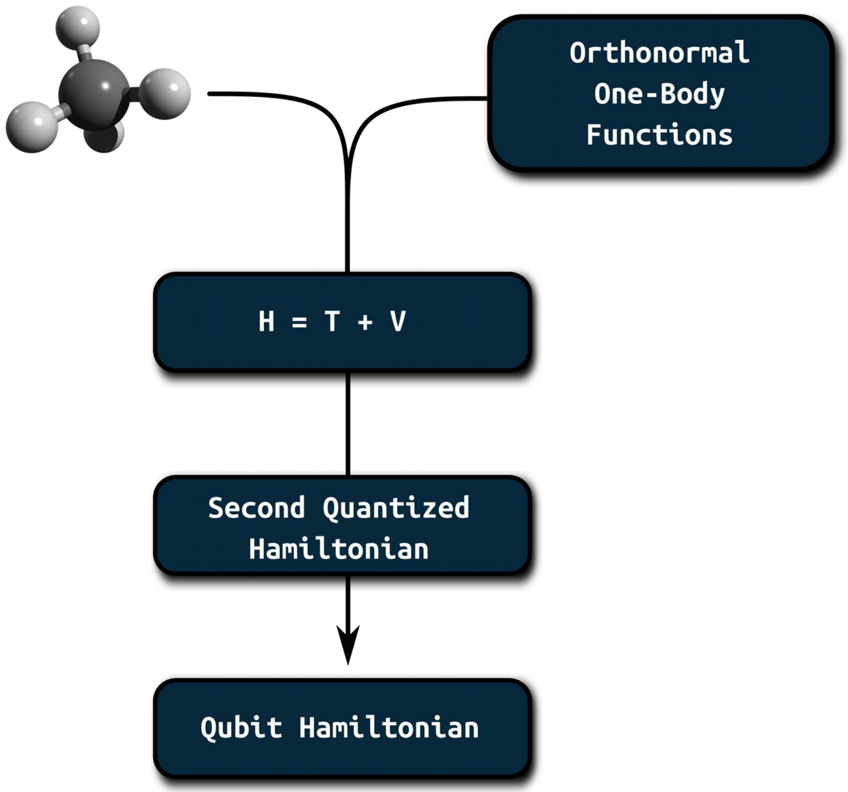
Fermionic operators are mapped to paulistrings

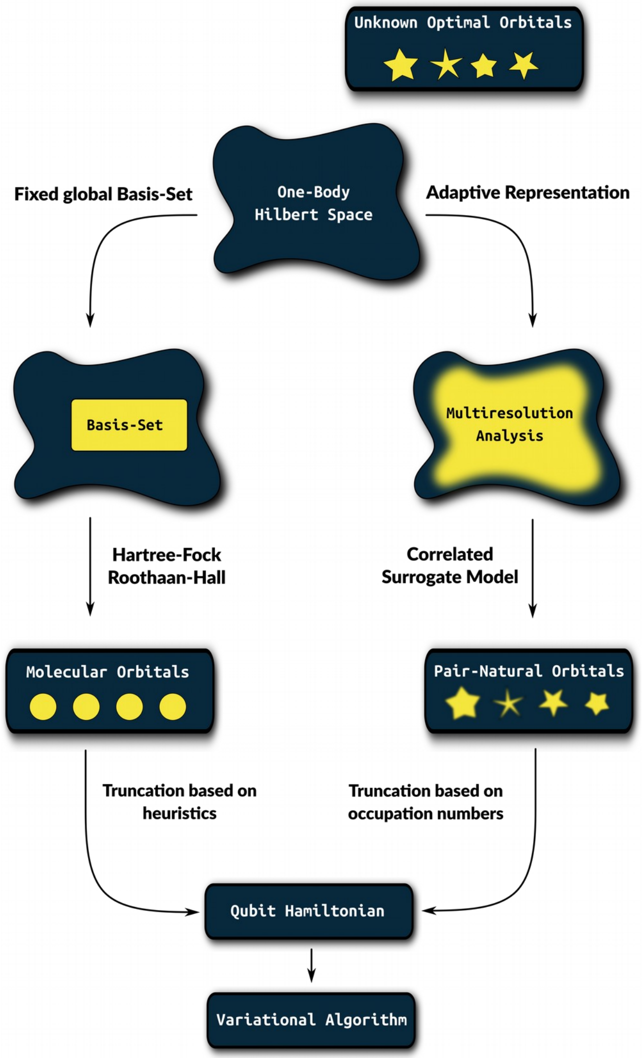
$$a_k^\dagger = 1^{\otimes k-1} \sigma_k^- \sigma_Z^{\otimes n-k}$$

Variational optimization

$$\min_\theta \left(\langle H \rangle_{U_\theta} \right) \equiv \min_\theta \left(\langle 0 | U^\dagger(\theta) H U(\theta) | 0 \rangle \right)$$

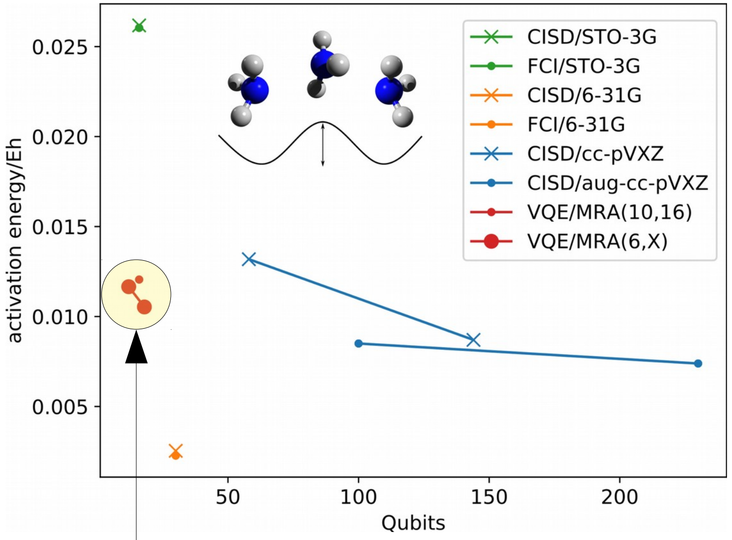
A Basis-Set-Free VQE

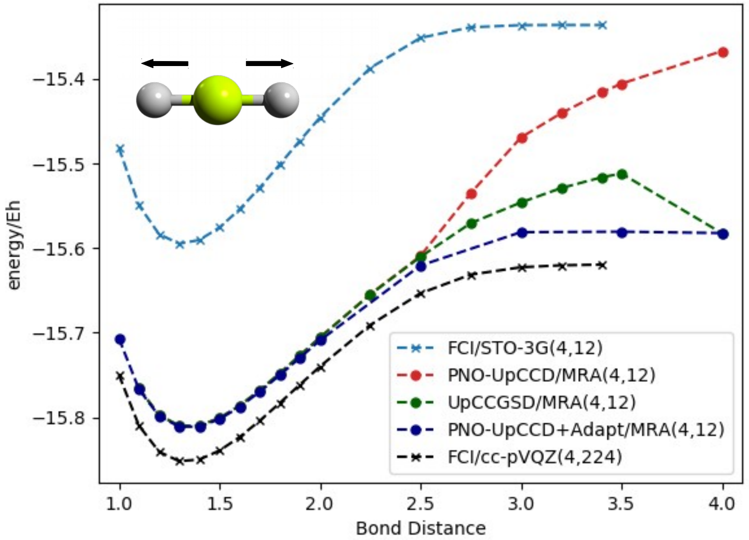




A Basis-Set-Free VQE

System	Metric	Qubits/MRA	Qubits/GBS	More
He	MAX	**4**	4-10	Fig. 3
Be	MAX	**10**	10-18	Fig. 3
H_2	NPE	**4**	20-56	Figs. 5, 4
H_2	NPE	**8**	20-56	Figs. 5, 4
H_2	NPE	**20**	56-120	Figs. 5, 4
H_2	MAX	**4**	8	Figs. 5, 4
H_2	MAX	**8**	20-56	Figs. 5, 4
H_2	MAX	**20**	56	Figs. 5, 4
LiH	NPE	**12**	20-38	Figs. 5, 4
LiH	NPE	**20**	38	Figs. 5, 4
LiH	MAX	**12**	20-38	Figs. 5, 4
LiH	MAX	**20**	170-288	Figs. 5, 4
BH	NPE	**12-20**	38-88	Figs. 5, 4
BH	MAX	**12-20**	38-88	Figs. 5, 4
NH_3	ΔE	**12-18**	58-100	Fig. 2





Circuit Sizes (in UCC operators):

PNO-UpCCD: 4

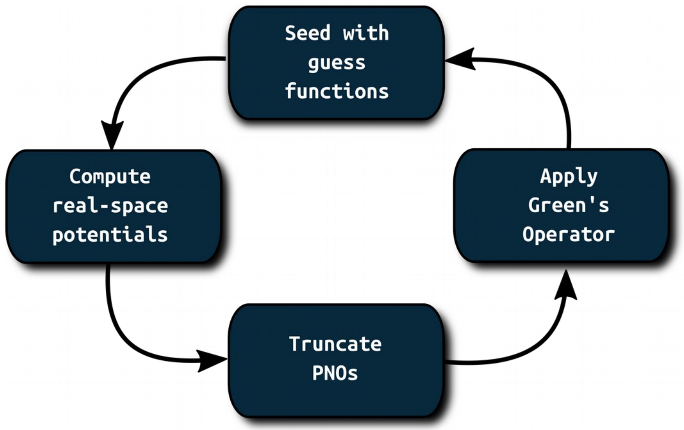
+Adapt : 20 – 100

UpCCGSD : 45

JSK et. al. ArXiv:2008.02819; Adapt: Grimsley et. al. Nat. Comm. 2019; UpCCGSD: Lee et. al. JCTC 2019

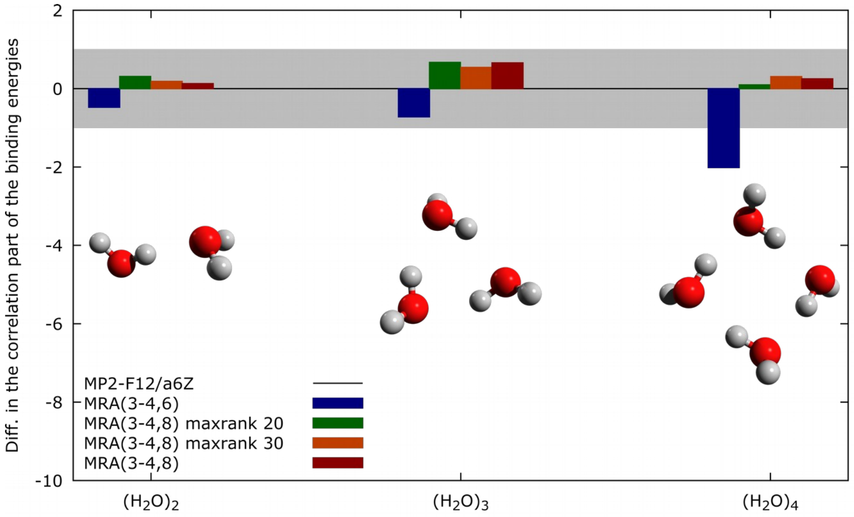
Directly Determined MRA-PNOs

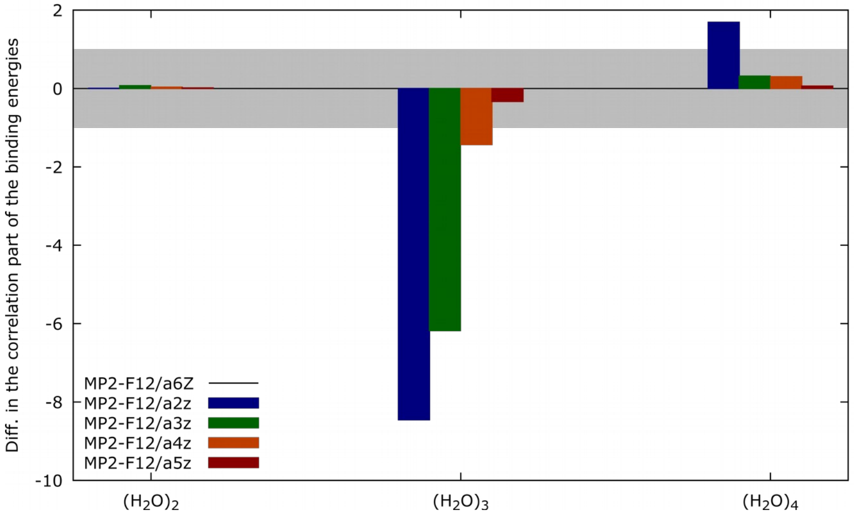
Adaptive and basis-set-free approach



$$\left(\frac{\Delta^2}{2} + V\right)|\Psi\rangle = E\,|\Psi\rangle$$

$$\Psi(r) = -2\int \mathrm{d}r'\, G_E(r,r')V(r')\,\Psi(r')$$



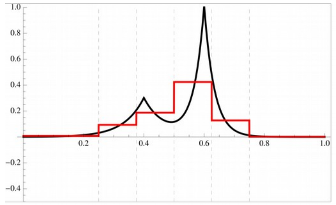


github.com/m-a-d-n-e-s-s/madness

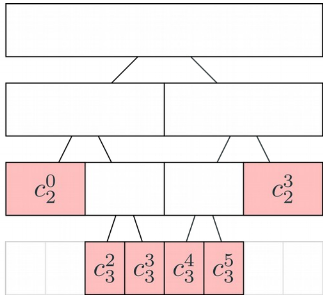
JSK, F. A. Bischoff, E. F. Valeev. J. Chem. Phys. 152, 074105; https://doi.org/10.1063/1.5141880

Recap: Basis-Set-Free Quantum Chemistry

Multiresolution Analysis (MRA)



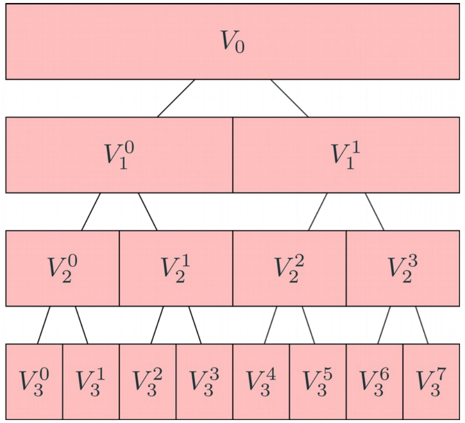
$$|f\rangle = \sum_{nl} c_n^l |\varphi_n^l\rangle$$

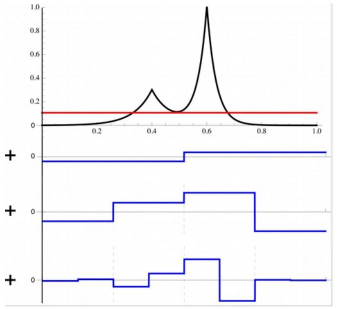


$$V_0 \subset V_1 \subset V_2 \subset \cdots \subset \mathbf{L}^2$$

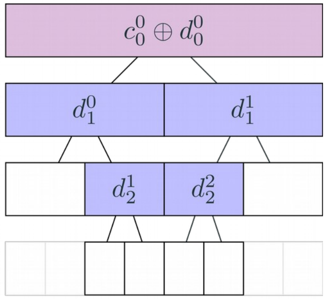
$$V_n = \bigoplus_{l=0}^{l=2^n-1} V_n^l$$

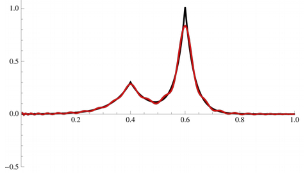
$$V_{n+1} = V_n \oplus W_n$$

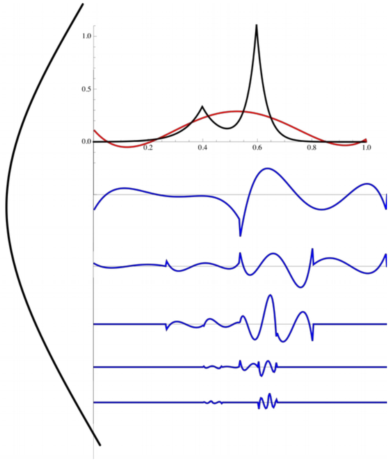


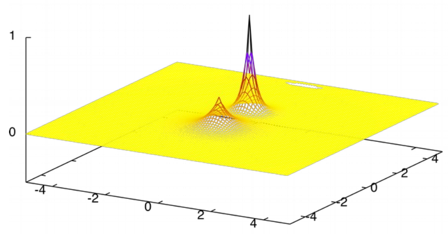


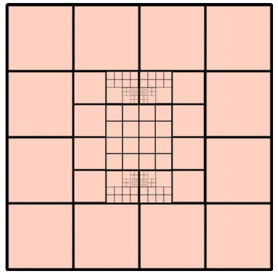
$$|f\rangle = c_0|\varphi_0\rangle + \sum_{nl} d_n^l |\psi_n^l\rangle$$











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