QPARC CHALLENGE 2022

Simplices in Hilbert Space

“NISQy Business”

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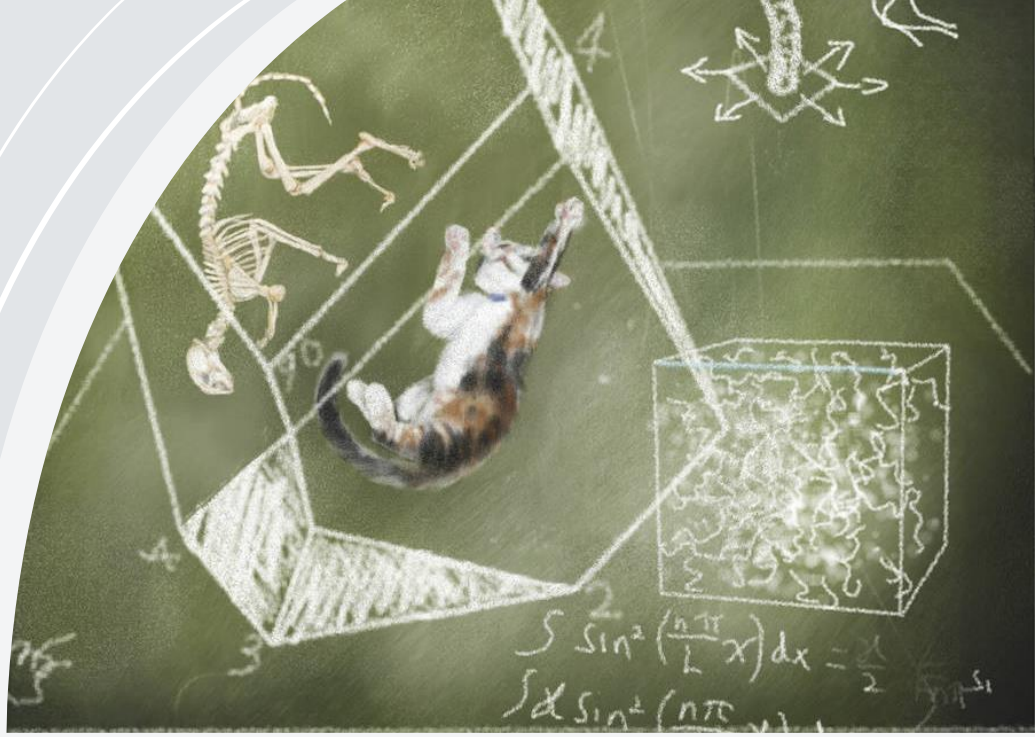
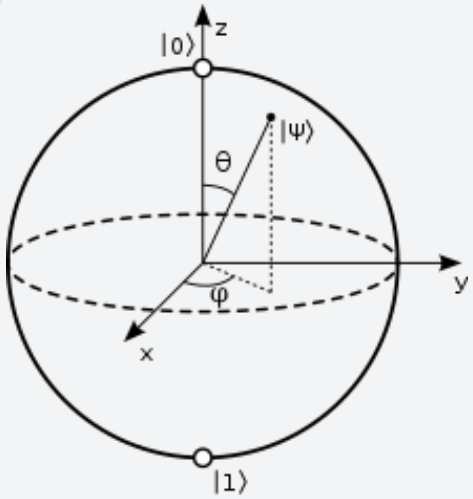


Introduction

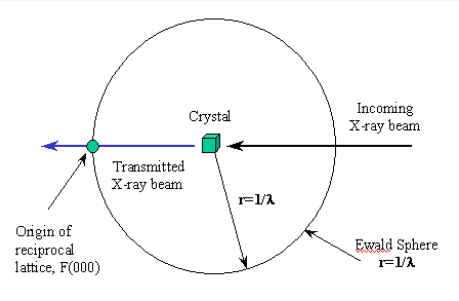
In this expository piece, this project compares several algorithms such as:

- BFGS Algoritihm to solve non linear optimisation problems acting on mapping STO-3G, a gaussian quadrature used in pySCF to partially diagonalize 2nd order hessian matrices and Partial diagonalization in the iterative Davidson method for B3LYP used in commercial VASP DFT GGA+U calculations

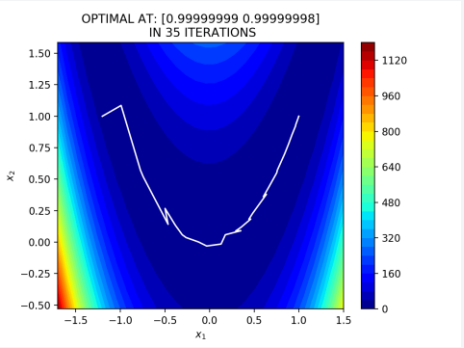
- VQE ansatz circuit topology is hypothesized to have analogues to quantum errors



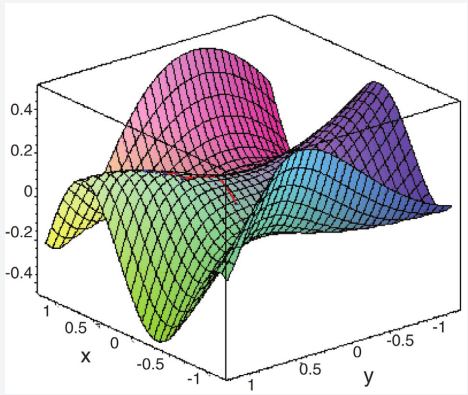
Bloch Sphere



Ewald sphere



STO-3G Quadrature

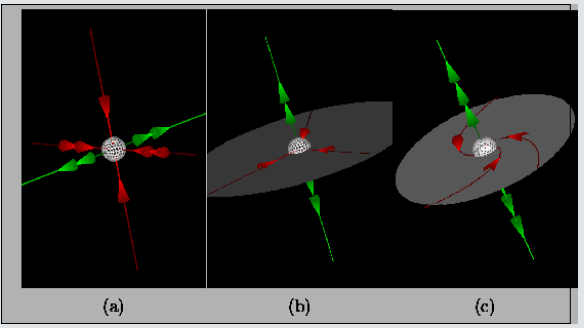


GGA+U

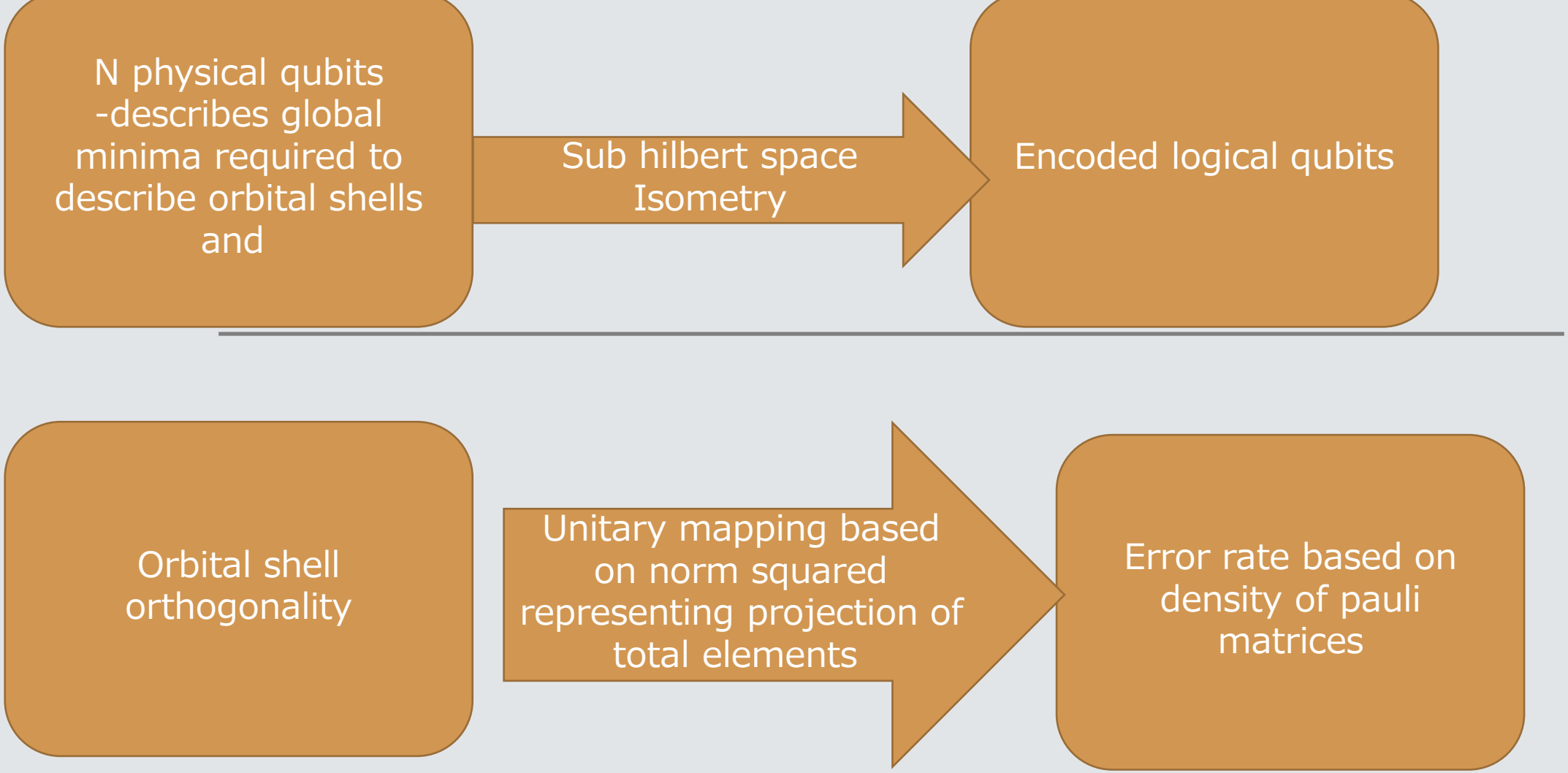
Project Motivations

- For a given Hilbert space, we can find there to be a norm which, provided a sufficiently adequate quantum circuit with which to calculate exact ground state energies of a provided quantum molecule yield a set of quantum errors providing a target.
- https://ionq.com/posts/june-24-2021-hello-many-worlds

e^{kbt}(Physical Qubits can be represented as Source and logical qubits from encoding as target in Hilbert space. A mapping between them can be made.
There also exists a total number of simplices generated from logical qubits which can be measured in the form of errors aggregated from noisy qubits. This projection creates a sub Hilbert space in group U. This wedge product space also creates a metrizable distance [[*n*,*k*,*d*]] --> ⌋(*d*−1)/2⌊ for QBP(Supremum) and e^kbt(Infininum).



For a given partial diagonalization, there exists an eigenmanifold describing saddle points, when there is no commutable orbital (on H) interaction or a gaussian norm representing unitary matrices

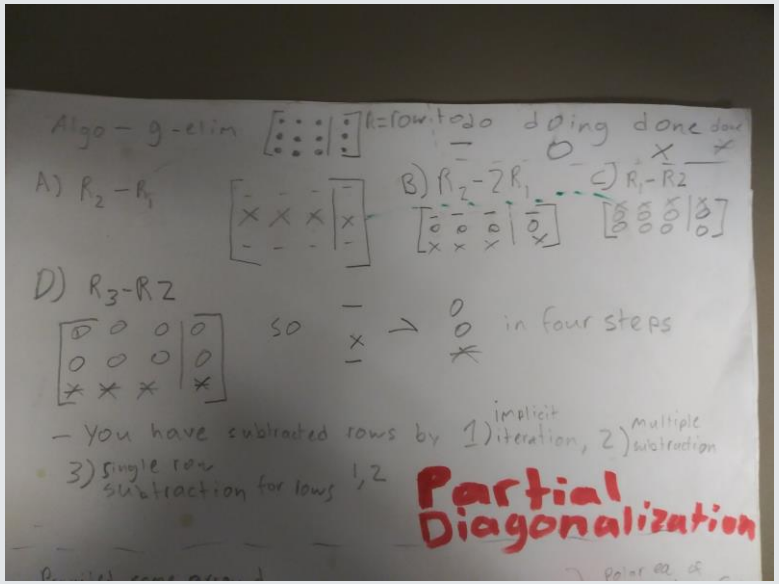

N physical qubits
-describes global minima required to describe orbital shells and
Sub hilbert space Isometry
Encoded logical qubits
Orbital shell orthogonality
Unitary mapping based on norm squared representing projection of total elements
Error rate based on density of pauli matrices

Comparing Davidson method with BGFS

```
 ethr =  1.00E-06,  avg # of iterations =  8.0

    total cpu time spent up to now is      21.2 secs

    total energy              =    -44.29902159 Ry
    estimated scf accuracy    <      0.02648278 Ry

    iteration #  2     ecut=    80.00 Ry     beta= 0.70
    Davidson diagonalization with overlap

---- Real-time Memory Report at c_bands before calling an iterative solver
         72 MiB given to the printing process from OS
          0 MiB allocation reported by mallinfo(arena+hblkhd)
       1069 MiB available memory on the node where the printing process lives
```

Hessian 2nd order representation

$$H_x = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} \\ \frac{\partial^2 f}{\partial x_1 x_2} & \frac{\partial^2 f}{\partial x_2^2} \end{bmatrix}$$



Background information

- HO2 -> J·W(H) -> finish off logic chart in lateX
- Electrons are our physical qubits
- For each electron H[Insert diagram here] which represents
- Hermition Operator – we take $H = -H$

Issues

Some issues we can across:

https://github.com/TenninYan/quantum-circuits/blob/master/error_mitigation/error_mitigation_exp_example.py

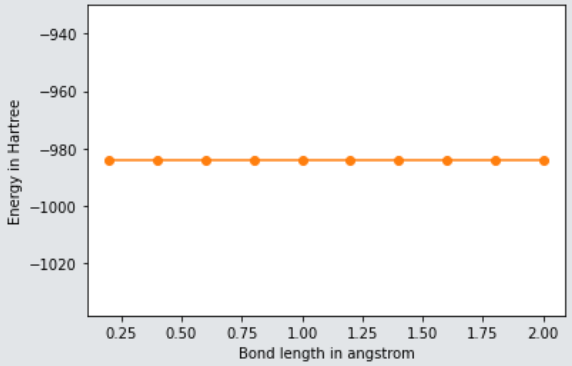
Qamuy's Jobpb2.py, We are not given the error rates from the backend. The protobuffer allowing the qamuy api () to reference the backend of a given target provider for error (Hadamard, Cnot) has ambiguity. We solved this by using the ionq target provider from Azure.

Titanium Oxide didn’t converge.

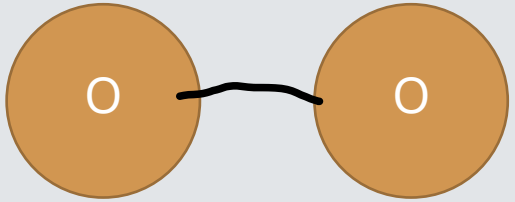
In google collab(qulacs/openfermion standalone), H20 did not converge. This is likely due to an issue Tennin also brought up https://github.com/qulacs/qulacs/issues/79

Meaningful Calculations

"Interestingly, their calculations suggested that the TiO2 molecule is linear in the excited states." [1]



LUMO of titanium dioxide from Hamiltonian



6b2 orbital for TiO2

Conclusion

Each orbital shell represents a non linear dynamic for

The frequency of the error rate remains an open ended problem for VQE

Bibliography

[0]Cao, C., Hu, J., Zhang, W., Xu, X., Chen, D., Yu, F., Li, J., Hu, H., Lv, D. and Yung, M., 2022. *Towards a Larger Molecular Simulation on the Quantum Computer: Up to 28 Qubits Systems Accelerated by Point Group Symmetry*. [online] arXiv.org. Available at: <https://arxiv.org/abs/2109.02110> [Accessed 22 May 2022].

[1] [Wu, H. and Wang, L., 1997. Electronic structure of titanium oxide clusters: TiOy (y = 1−3) and (TiO2)n (n = 1−4). The Journal of Chemical Physics, 107(20), pp.8221-8228(8225).]

Thank you for your time