Quantum Machine Learning for Complex Chemical Systems

Sabre Kais
Department of Chemistry and Physics
Purdue University
http://www.chem.purdue.edu/kais

Outline

- **Introduction:** Brief introduction to our research in the field of **quantum information and quantum computing for complex chemical systems**.
- **QML Model:** Quantum machine learning and the **Restricted Boltzmann Machine (RBM);**

  Quantum algorithm that can filter any energy eigenstate of the system;

  Quantum circuit; implement our algorithm on quantum simulators and actual **IBM-Q**

Applications: **Electronic Structure of Molecules:** Simple molecules such as H_2, LiH, and H_2O

Electronic Structure Calculations of 2D Materials: Hexagonal Boron Nitride and Graphene

Molybdenum Disulfide MoS_2 and Tungsten disulfide WS_2

- **Finite Size Scaling and Quantum Phase Transitions:** Quantum Rabi Model

  (Two-level system interacting with an optical field)

- **Future Work:** QML for open quantum dynamics, quantum state tomography, quantum thermodynamics, quantum optimization to solve advanced inverse design problems for science and engineering applications and implementations on quantum devices with reduction of the algorithm cost.

Our Research in the Field of Quantum Information and Quantum Computing

Zheng Huang
2002-2007

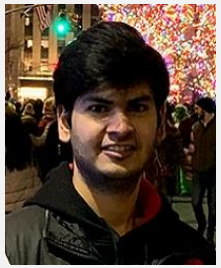
- Entanglement and Chemical Reactions
- Quantum Coherence in Complex Chemical Systems
- Electronic Structure Calculations of Molecules and Materials
- Dimensional Scaling, Finite Size Scaling and Quantum Phase Transitions
- Data Analytics and Quantum Machine Learning
- Open Quantum Dynamics and quantum encryption protocols
- Quantum Games for Quantum Education (Quantum tic-tac-toe)

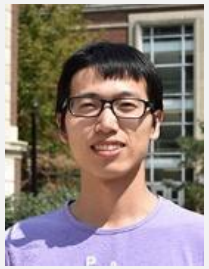
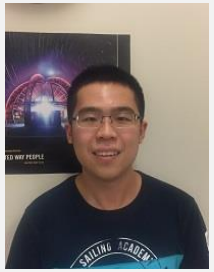
http://www.chem.purdue.edu/kais

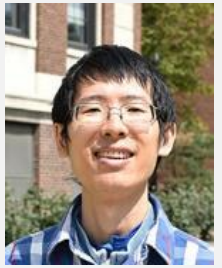
https://arxiv.org/search/?searchtype=author&query=Sabre+Kais

Quantum Information and Computation for Complex Systems

Chemistry, Physics, Computer Science, Electrical and Computer Engineering










https://www.chem.purdue.edu/kais/

DEPARTMENT OF ENERGY · UNITED STATES OF AMERICA ·

NSF

PURDUE UNIVERSITY
Discovery Park
BIRCK NANOTECHNOLOGY CENTER

QUANTUM[SM]
SCIENCE
CENTER

AFOSR

Electronic Structure on a Quantum Computer

Gate Model

Adiabatic Model

Quantum Machine Learning

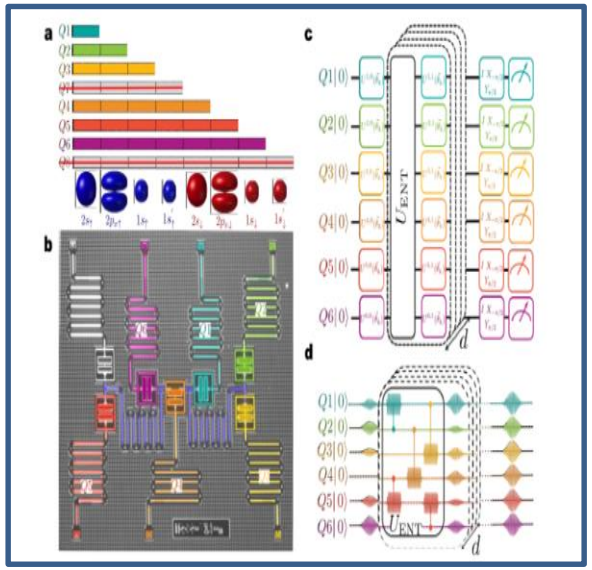
Phase Estimation

…

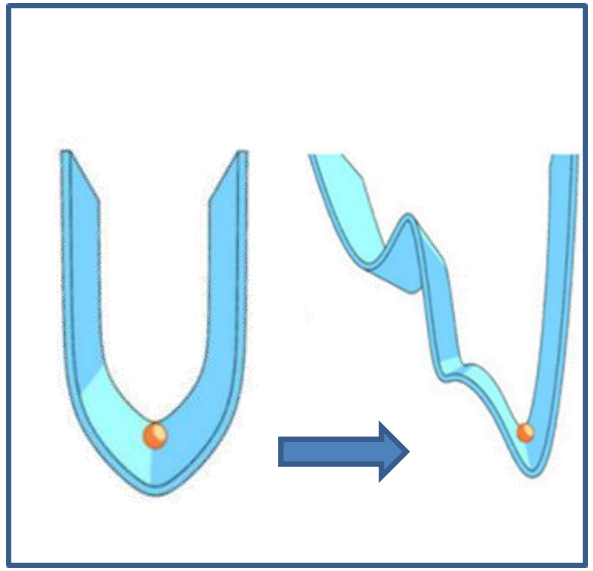
Direct Methods

…

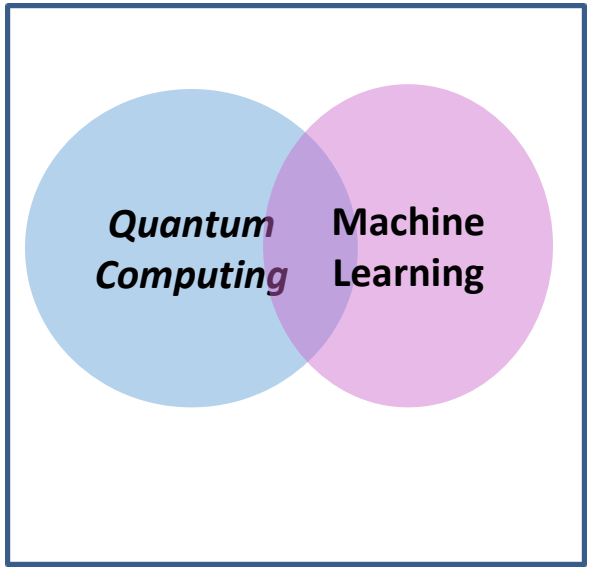
Hybrid Algorithms



Qubit and Qudit Space



Ising Type Hamiltonian

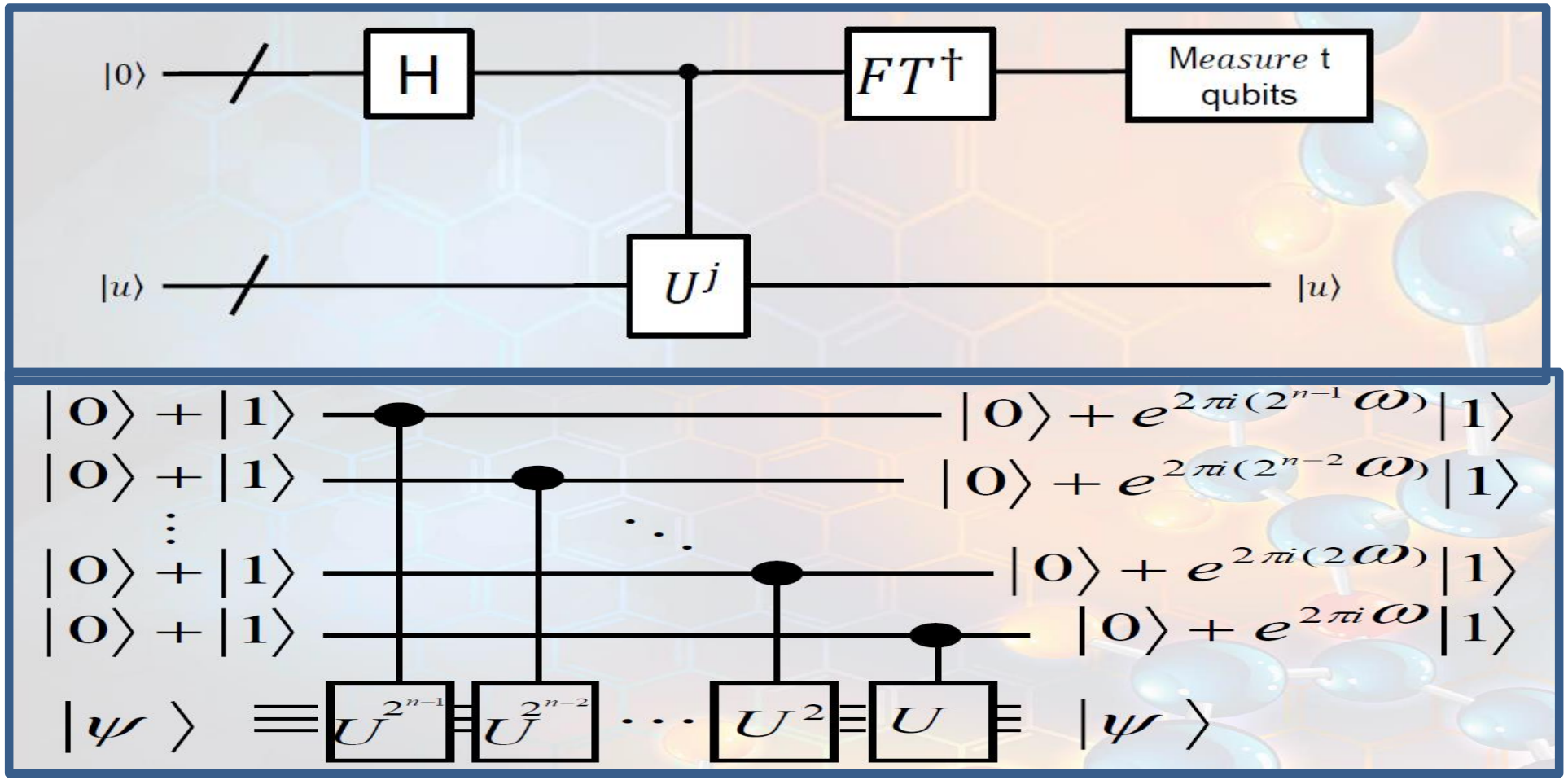


Restricted Boltzmann Machine

Quantum Phase Estimation Algorithm

Is a quantum algorithm to estimate the phase (or eigenvalue) of an eigenvector of a unitary operator.

$$U = e^{-iEt} = e^{2\pi i\varphi}$$



Initially introduced by Alexei Kitaev in 1995 and **Seth Lloyd**, **Phys. Rev. Lett. 83, 5162 (1999)**

Quantum Phase Estimation Algorithm

Simulated quantum computation of molecular energies A Aspuru-Guzik, AD Dutoi, PJ Love, M Head-Gordon, Science 309 (5741), 1704-1707 (2005)

Phys. Chem. Chem. Phys. 10, 5388–5393 (2008)

PAPER www.rsc.org/pccp | Physical Chemistry Chemical Physics

Quantum algorithm for obtaining the energy spectrum of molecular systems

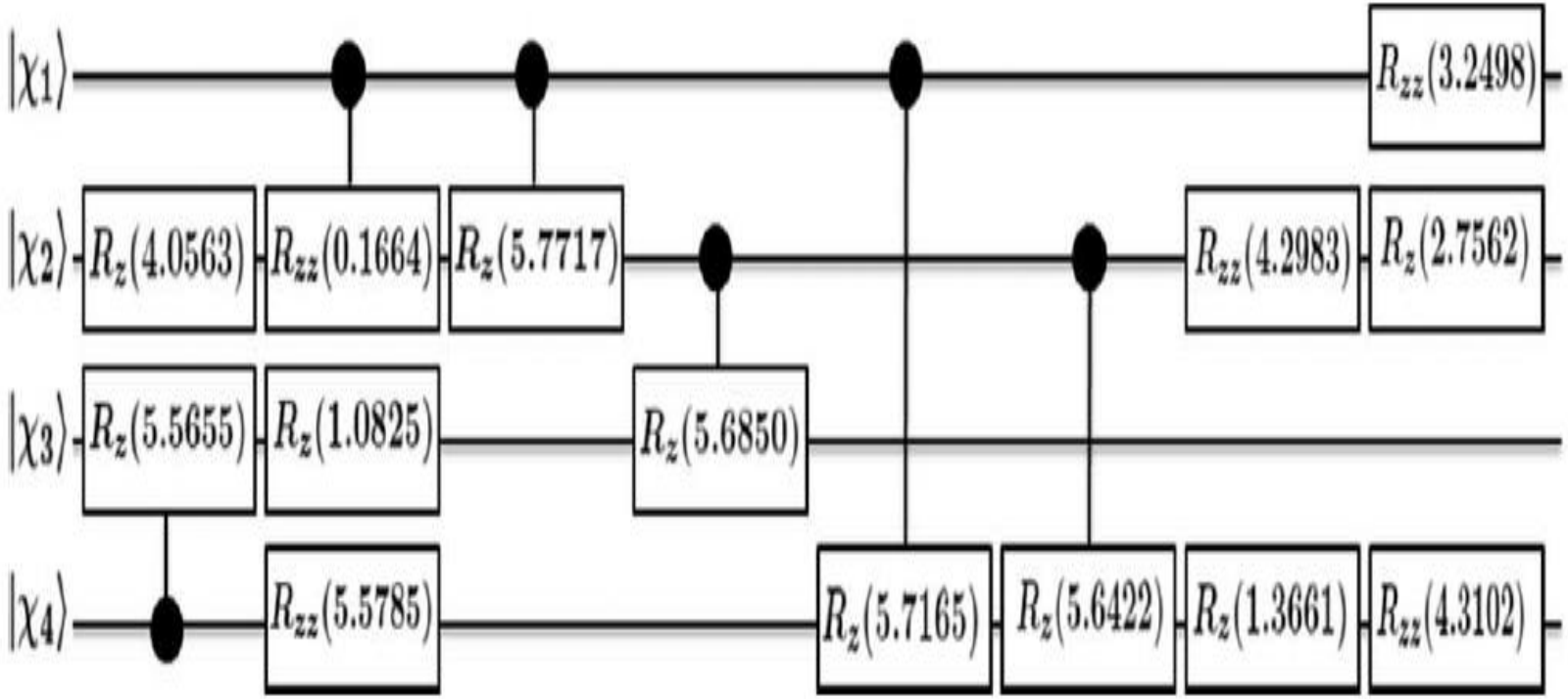
Hefeng Wang,[a] Sabre Kais,*[a] Alán Aspuru-Guzik[b] and Mark R. Hoffmann[c]

Ph.D. 2004-2008; Now: School of Physics at Xi'an Jiaotong University, China

We have presented a quantum algorithm to obtain the energy spectrum of molecular systems based on the multiconfigurational self-consistent field (MCSCF) wave function. We demonstrated that such an algorithm can be used to obtain the energy spectrum of the water molecule.

Quantum Classical Hybrid Algorithm (2011)

The circuit design for the unitary propagator for the Hydrogen Molecule, H2



Anmer Daskin

Dept. of Computer Engineering, Istanbul Medeniyet University, Turkey

THE JOURNAL OF CHEMICAL PHYSICS 134, 144112 (2011)

“ Decomposition of unitary matrices for finding quantum circuits: Application to molecular Hamiltonians”

Anmer Daskin and Sabre Kais

Quantum Classical Hybrid Algorithm (2011)

$$f(U_a, U_t) = \sum_{i=1}^{2^n} \sum_{j=1}^{2^n} |U_{t(ij)} - U_{a(ij)}|$$

$$U = e^{-iH}$$

Decomposition of a given unitary matrix

in terms of quantum gates

$$\begin{pmatrix} \alpha_{11} & \alpha_{12} & . & . & . & \alpha_{1n} \\ \alpha_{21} & \alpha_{22} & . & . & . & \alpha_{2n} \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ \alpha_{n1} & \alpha_{n2} & . & . & . & \alpha_{nn} \end{pmatrix} \equiv G_1 \otimes G_2 \otimes G_3 \otimes \ldots \otimes G_{m-1} \otimes G_m$$

Unitary Matrix

Quantum Gates
(I,X,Y,Z,CNOT, CZ, Rx, Ry, Rz …)

THE JOURNAL OF CHEMICAL PHYSICS 137, 234112 (2012)

Universal programmable quantum circuit schemes to emulate an operator

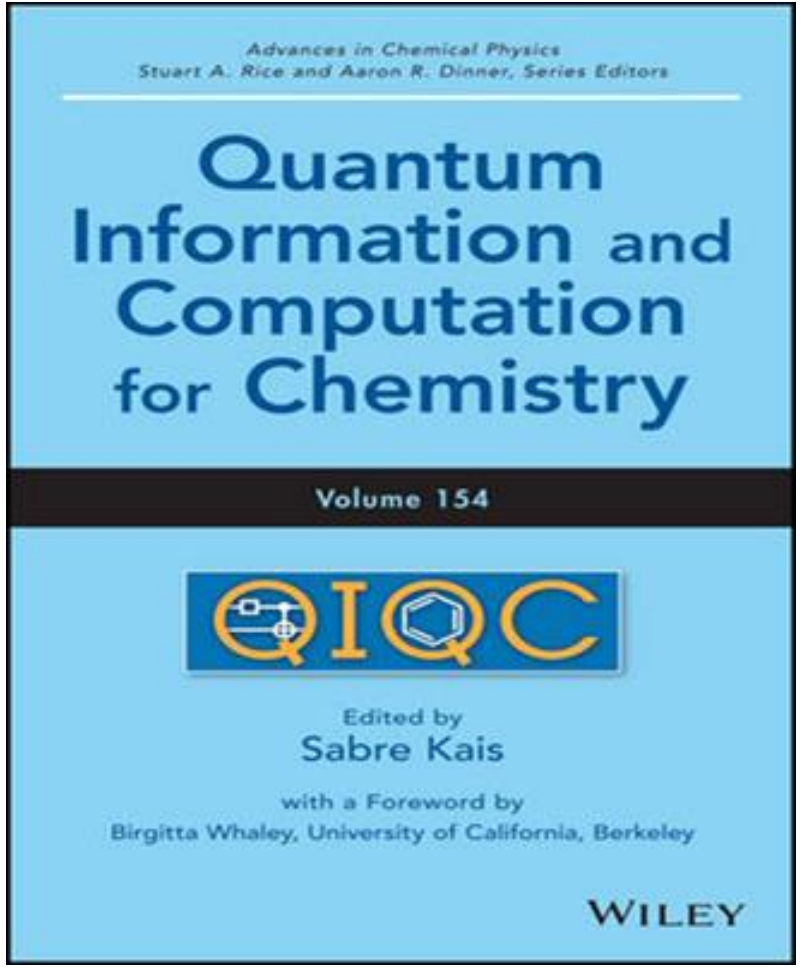
Anmer Daskin,[1] Ananth Grama,[1] Giorgos Kollias,[1] and Sabre Kais[2,3,a)]

References in the Field Before 2014

Advances in Chemical Physics, Vol 154 (2014)

17 Chapters Covering different Aspects of the field

QIS For Chemical systems



NSF-CCI Center (2010-2013)

Quantum Information for Quantum Chemistry

Ken Brown (Duke) ; Peter Love (Tufts); Sabre Kais (Purdue)
Daniel Lidar (USC) and Alan Aspuru-Guzik (Toronto)

https://www.chem.purdue.edu/kais/nsf-cci/index.html

Recent Review Articles:

Yudong Cao
Ph.D 2012 – 2016
Zapata Computing, Inc.

1. Y. Cao et al, “Quantum chemistry in the age of quantum computing,” Chemical Reviews 119, 19, 10856 (2019).

2. S. McArdle et al., “Quantum computational chemistry,” Reviews of Modern Physics 92, 1, 015003 (2020).

3. B. Bauer et al., “Quantum algorithms for quantum chemistry and quantum materials science,” Chemical Reviews 120, 22, 12685 (2020)

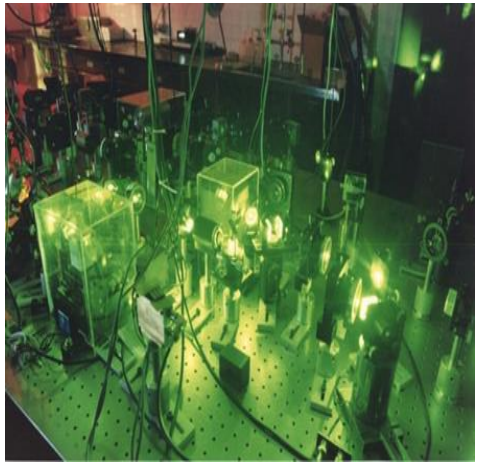
• • • • • •

Summary

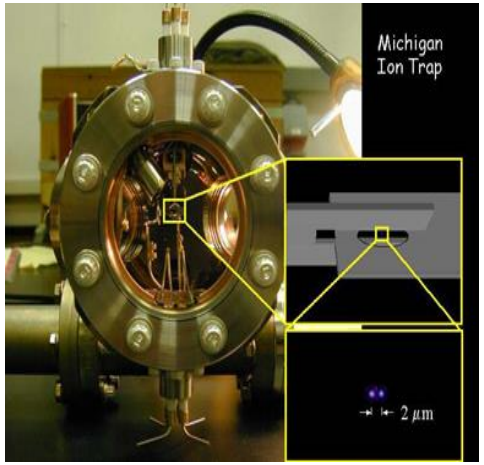
We have theoretical and experimental results for

Simple Molecules: H_2, H_2O, LiH, BeH_2, He_2,… H_{12}
(2-12 qubits)

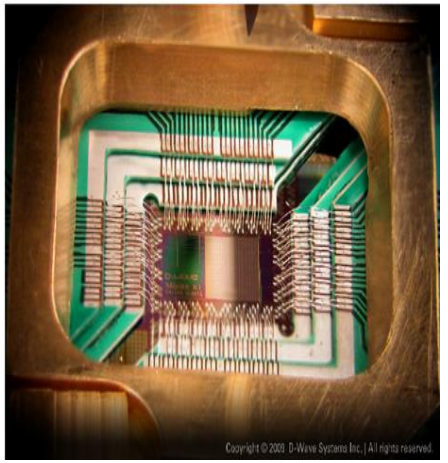
NMR



Optical



Trapped Ions



Superconducting

What is Next?

Challenges: Hardware

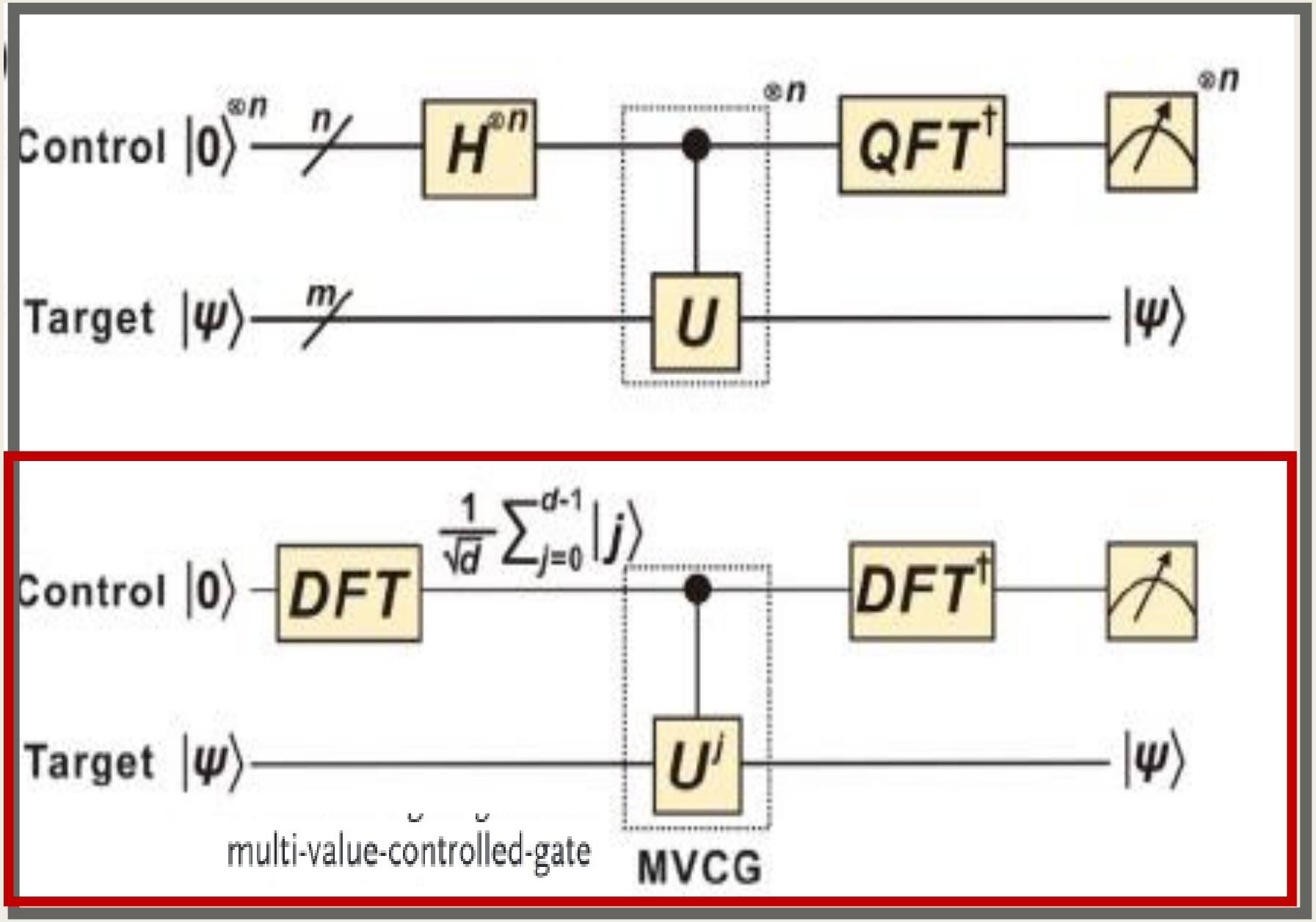
- **Quantum Volume:** Circuit **width** (# qubits); circuit **depth** (# quantum gates) and architecture of the device (**connectivity** of the qubits)
- **quantum error corrections** (**Fault-Tolerant Quantum Computer**)

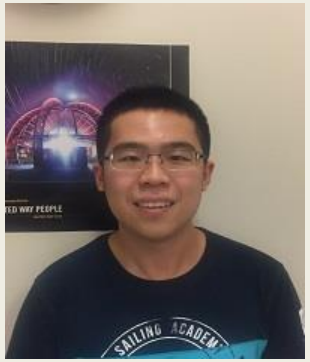
Hardware improvements alone is not enough!

We need to design efficient programmable quantum circuits for molecular Hamiltonians

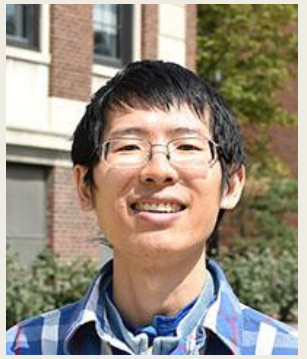
- **Quantum Classical Hybrid Algorithms**
- **Adiabatic Quantum Algorithms**
- **Quantum Machine Learning Algorithms**
- **Developing Algorithms in Qudit-Space**
- **Programmable Quantum Simulator**

Phase Estimation with Qudits





Yuchen Wang

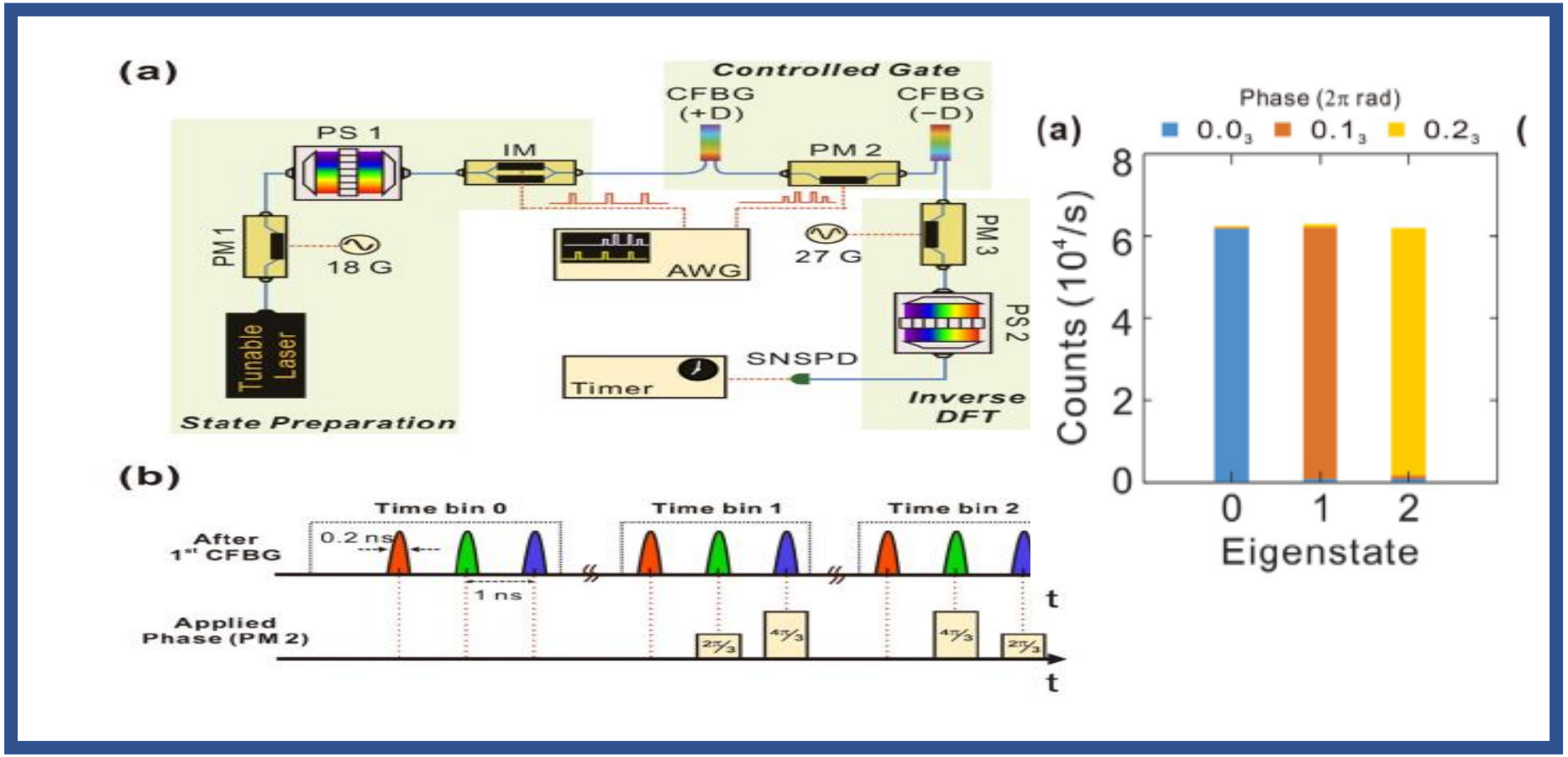


Zixuan Hu

ADVANCED QUANTUM TECHNOLOGIES
www.advquantumtech.com

Quantum Phase Estimation with Time-Frequency Qudits in a Single Photon

Hsuan-Hao Lu, Zixuan Hu, Mohammed Saleh Alshaykh, Alexandria Jeanine Moore, Yuchen Wang, Poolad Imany, Andrew Marc Weiner, and Sabre Kais**



Andrew M. Weiner
ECE, Purdue

***Adv. Quantum Technology* 1900074 (2019)**

Qudit Quantum Gates

The Z gate and X gate are generalized to d-dimension

$$X = \begin{pmatrix} 0 & 0 & \cdots & 0 & 1 \\ 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 \end{pmatrix} \quad Z = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & \omega & 0 & \cdots & 0 \\ 0 & 0 & \omega^2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & 0 \\ 0 & 0 & 0 & \cdots & \omega^{d-1} \end{pmatrix}, \qquad \omega = e^{2\pi i/d}$$

$$Z \mid j\rangle = e^{\frac{2\pi i}{d}\cdot j} \mid j\rangle \quad X \mid j\rangle = \mid j+1\rangle \quad \text{where } j = 0,1,2,\cdots,d-1.$$

$$\frac{1}{\sqrt{d}} \begin{pmatrix} 1 & 1 & 1 & 1 & \cdots & 1 \\ 1 & \omega_d & \omega_d^2 & \omega_d^3 & \cdots & \omega_d^{d-1} \\ 1 & \omega_d^2 & \omega_d^4 & \omega_d^6 & \cdots & \omega_d^{2(d-1)} \\ 1 & \omega_d^3 & \omega_d^6 & \omega_d^9 & \cdots & \omega_d^{3(d-1)} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \omega_d^{d-1} & \omega_d^{2(d-1)} & \omega_d^{3(d-1)} & \cdots & \omega_d^{(d-1)(d-1)} \end{pmatrix}$$

Qudit Fourier Transform

$$\mid +\rangle = \sum_{i=0}^{d-1} \mid i\rangle.$$

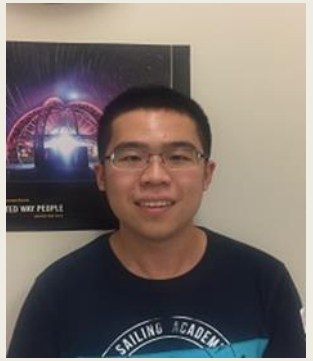
$$QFT \mid j\rangle = Z^j \mid +\rangle.$$

Review Article

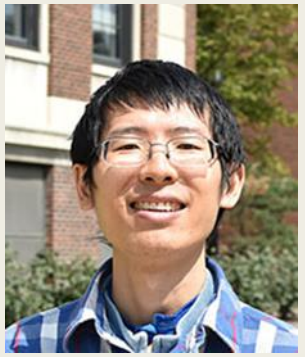
"Qudits and High-Dimensional Quantum Computing"

Y. Wang, Z. Hu; Barry Sanders, Sabre Kais,

Frontiers in Physics (2020)



Yuchen Wang



Zixuan Hu

Barry Sanders

THE JOURNAL OF PHYSICAL CHEMISTRY B

Article

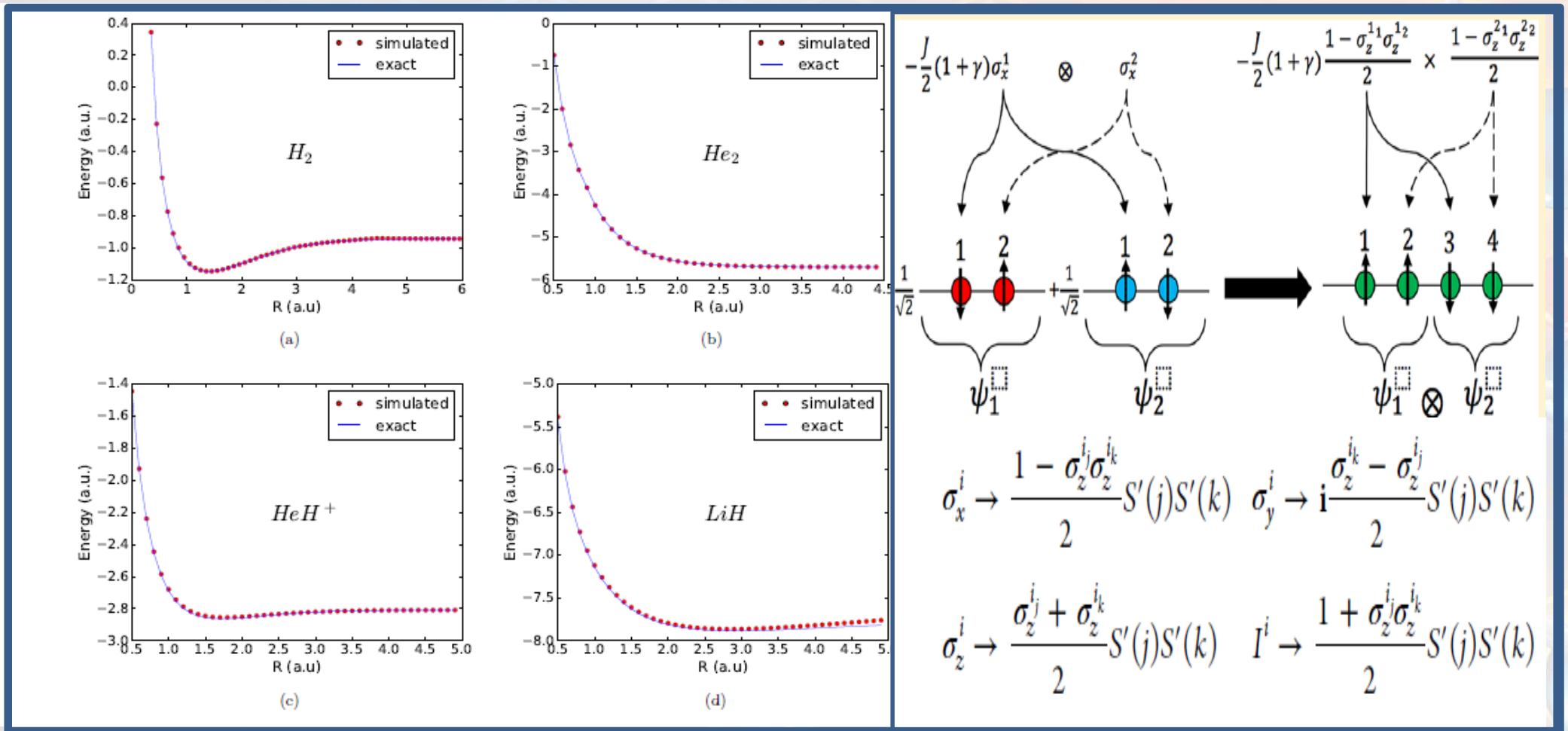
pubs.acs.org/JPCB

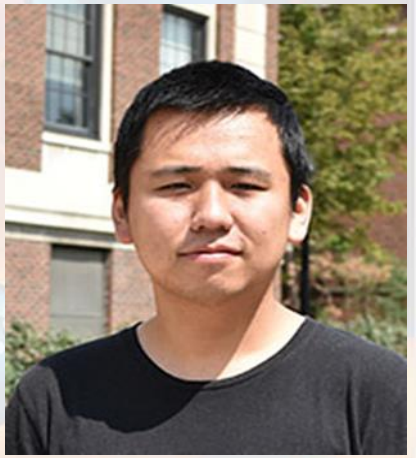
J. Phys. Chem. B 2018, 122, 3384−3395

Electronic Structure Calculations and the Ising Hamiltonian

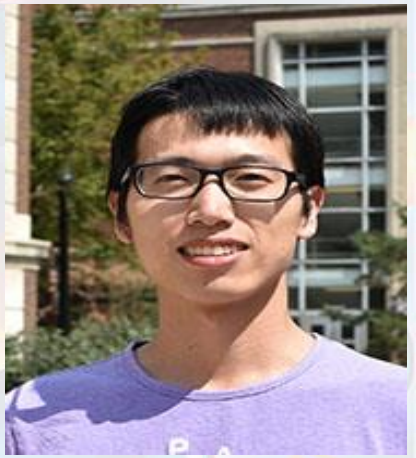
Rongxin Xia,[†] Teng Bian,[†] and Sabre Kais*[,†,‡,§]

$$H_p = \sum_{i}^{N} h_i \sigma_i^z + \sum_{j>i}^{N} J_{ij} \sigma_i^z \sigma_j^z$$





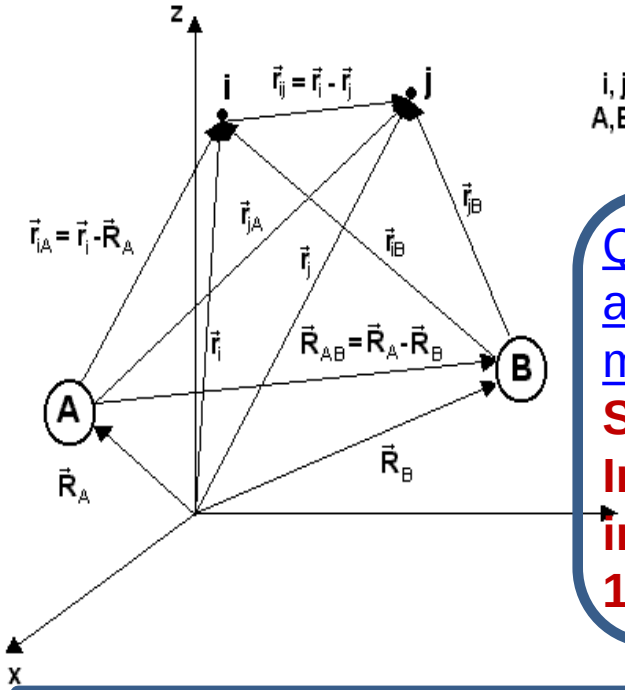
Rongxin Xia



Teng Bian

Quantum Criticality and Phase Transitions

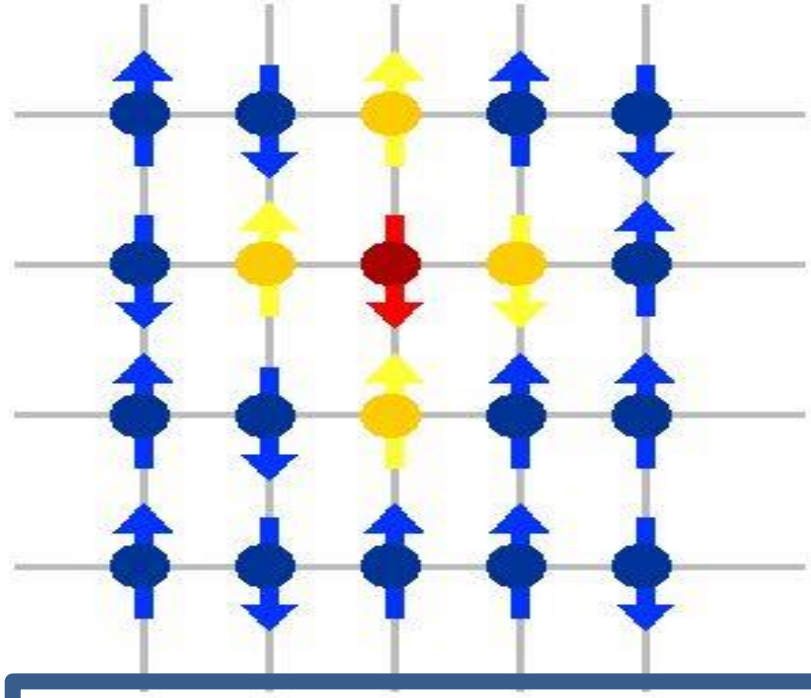
Electronic Structure
Quantum Mechanics



i, j ≡ electrons (N)
A,B ≡ nuclei (M)

[Quantum critical phenomena and stability of atomic and molecular ions](#)
S Kais, P Serra
International Reviews in Physical Chemistry
19, 97 (2000)

Ising Model
Statistical Mechanics



Phase Transitions

Symmetry Breaking

Quantum Machine-Learning

REVIEW

14 september 2017 | VOL 549 | NA T U RE |

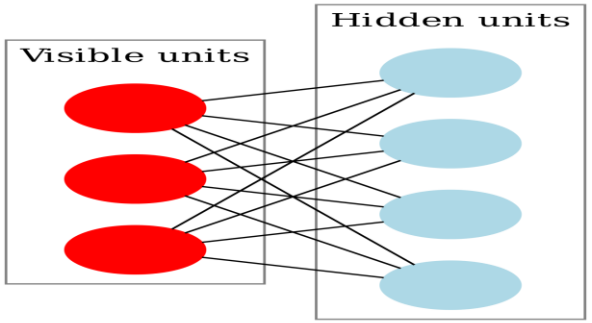
doi:10.1038/nature23474

Quantum machine learning

Jacob Biamonte[1,2], Peter Wittek[3], Nicola Pancotti[4], Patrick Rebentrost[5], Nathan Wiebe[6] & Seth Lloyd[7]

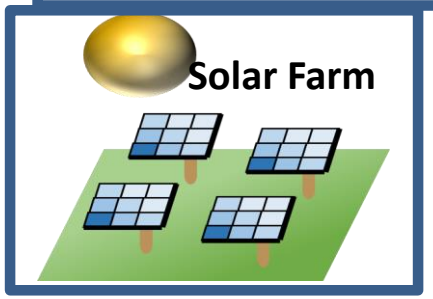
Quantum Principal Component Analysis (PCA), Quantum Support Vector Machines (QSVM), Quantum Reinforcement Learning, quantum supervised and unsupervised learning, kernel design for Gaussian processes, Gaussian process regression , quantum classifier or a plethora of linear algebra routines like HHL, QSVD, qBLAS

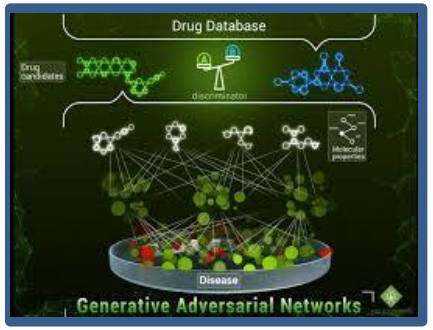
Deep Learning and Artificial Neural Network
"Restricted Boltzmann Machine (RBM)"

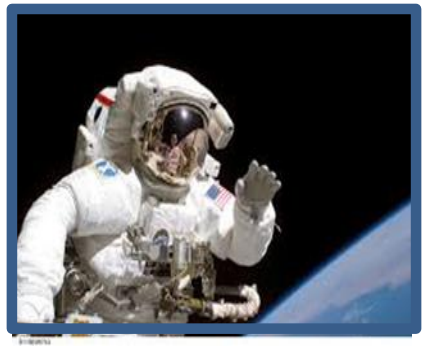


Machine Learning

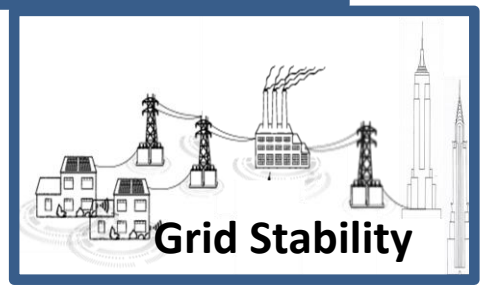
A branch of **artificial intelligence**, concerned with the design and development of algorithms that allow computers to evolve behaviors based on empirical data.



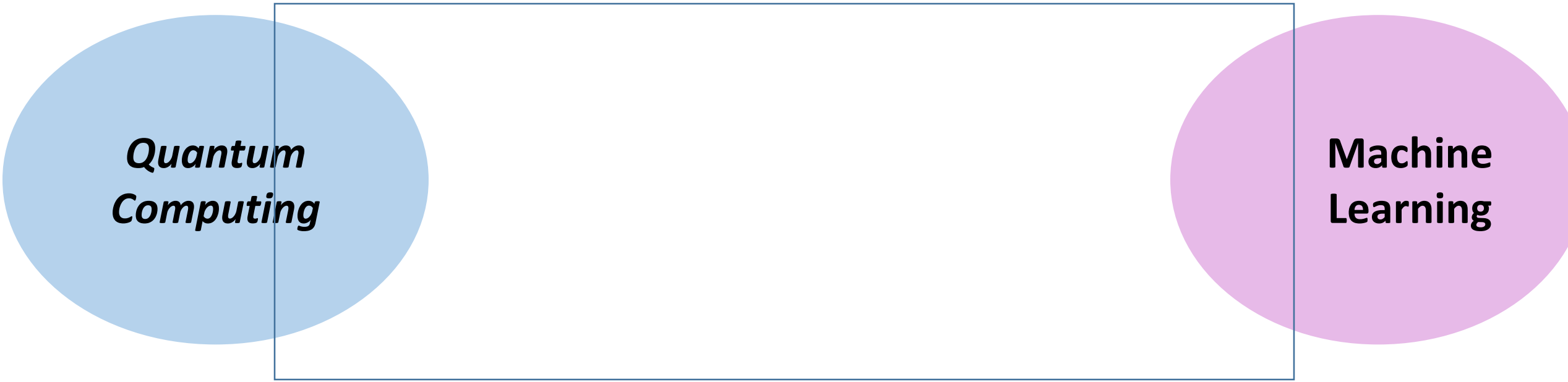




Self-driving meal machines at Purdue University



Quantum Machine Learning

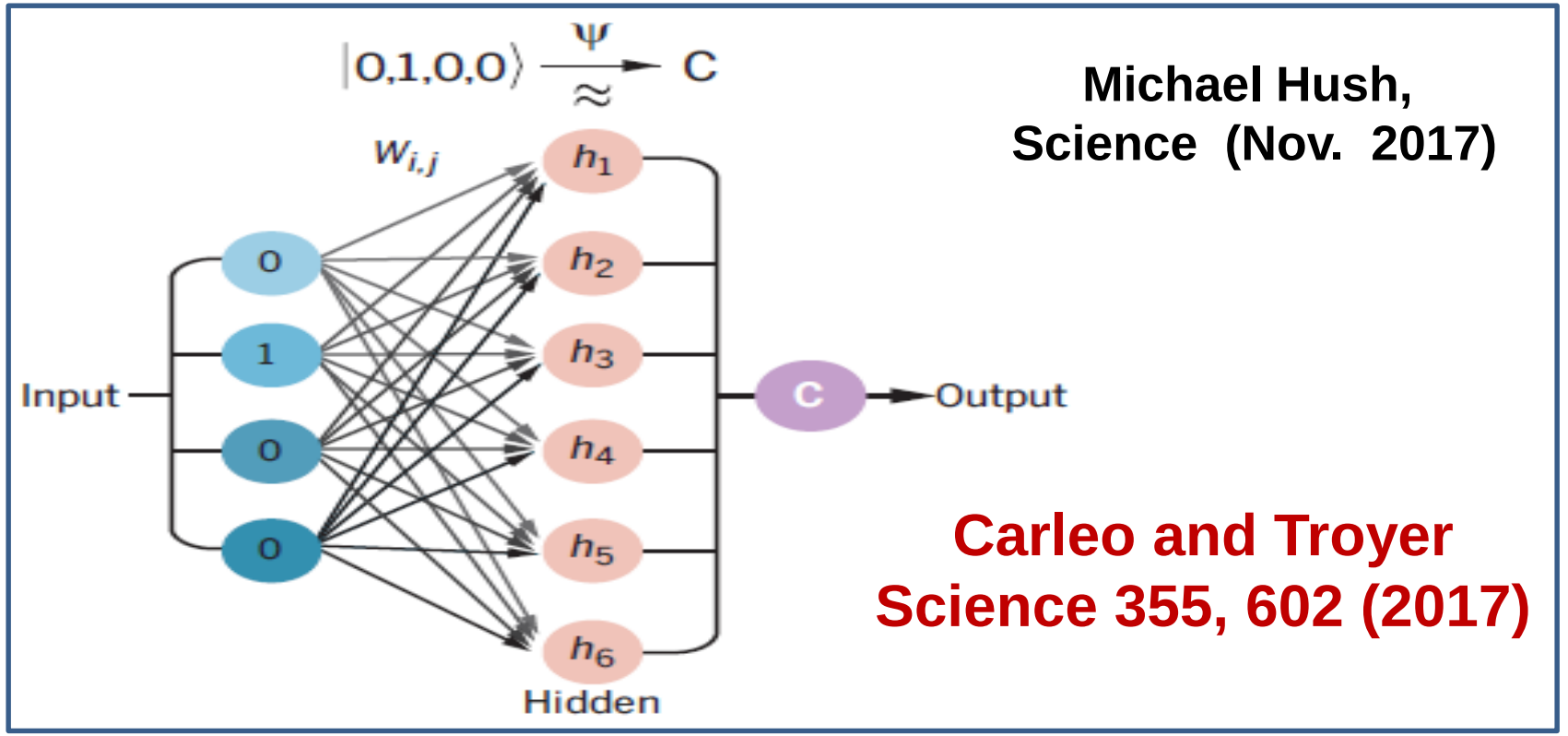


Developing game-changing quantum algorithms to perform machine learning tasks on large-scale scientific datasets for various industrial and technological applications

Quantum many-body problem and artificial neural networks

Challenge: Describing the nontrivial correlations encoded in the exponential complexity of the many-body wave function

However, wave functions representing many physical many-body systems can be characterized by an amount of information much smaller than the maximum capacity of the corresponding Hilbert space



RESEARCH ARTICLE

MANY-BODY PHYSICS

Solving the quantum many-body problem with artificial neural networks

Giuseppe Carleo[1]* and Matthias Troyer[1,2]

Science 355, 602 (2017)

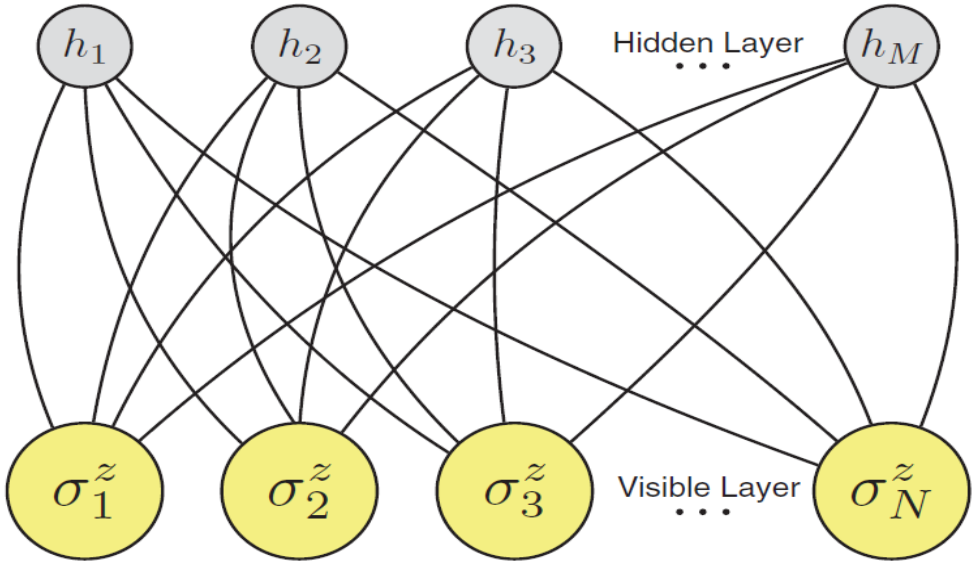


Fig. 1. Artificial neural network encoding a many-body quantum state of *N* spins. A restricted Boltzmann machine architecture that features a set of *N* visible artificial neurons (yellow dots) and a set of *M* hidden neurons (gray dots) is shown. For each value of the many-body spin configuration $\mathcal{S} = (\sigma_1^z, \sigma_2^z, \ldots, \sigma_N^z)$, the artificial neural network computes the value of the wave function $\Psi(S)$.

$$\Psi_M(\mathcal{S};\mathcal{W}) = \sum_{\{h_i\}} e^{\sum_j a_j\sigma_j^z + \sum_i b_i h_i + \sum_{ij} W_{ij} h_i \sigma_j^z}$$

Transverse-field Ising (TFI) Model

$$\mathcal{H}_{\mathrm{TFI}} = -h\sum_i \sigma_i^x - \sum_{ij}\sigma_i^z\sigma_j^z$$

Antiferromagnetic Heisenberg (AFH) model

$$\mathcal{H}_{\mathrm{AFH}} = \sum_{ij} \sigma_i^x\sigma_j^x + \sigma_i^y\sigma_j^y + \sigma_i^z\sigma_j^z$$

Restricted Boltzmann Machine (RBM)

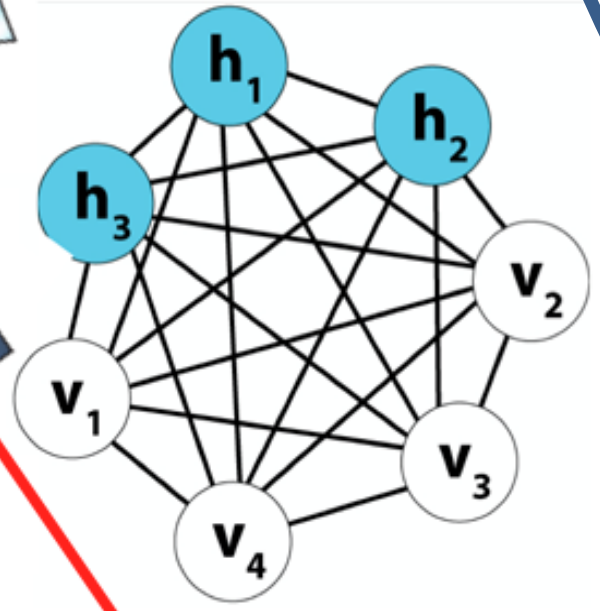
Statistical Physics

BOLTZMANN LAW

$$p \sim e^{-E/kT}$$

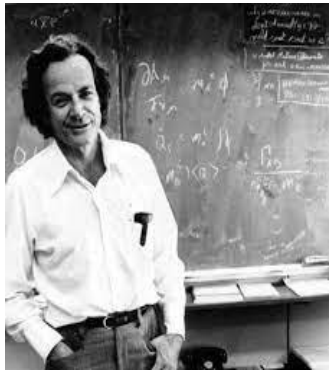
QUANTUM CIRCUITS

BOLTZMANN MACHINES



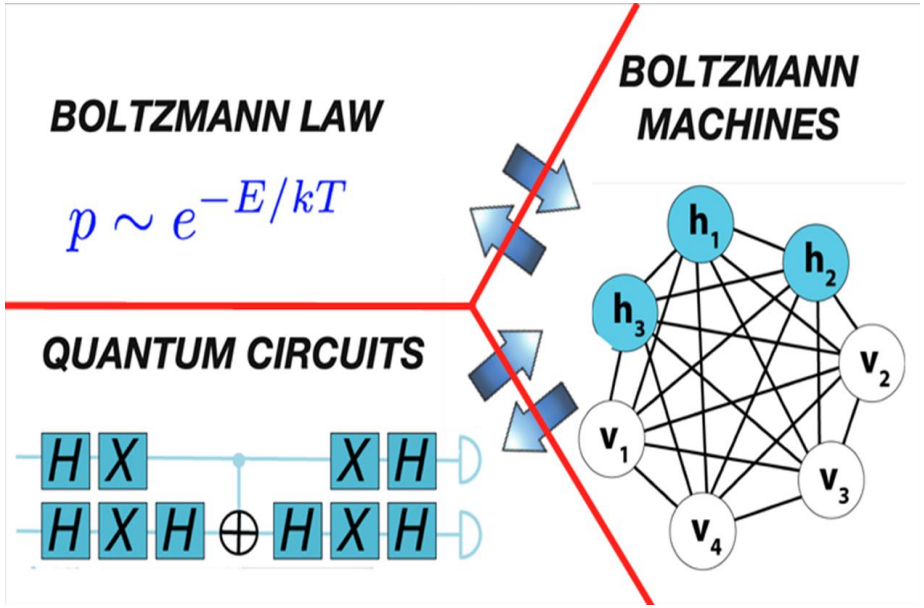
Neural Network

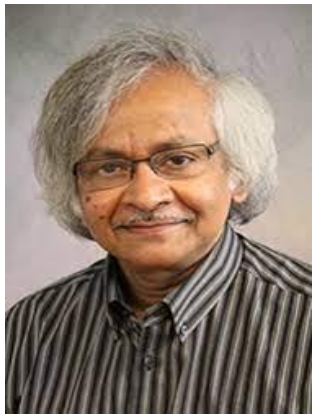
Quantum Computing



John Hopfield

Boltzmann Law: Physics to Computers





Supriyo Datta, ECE Purdue

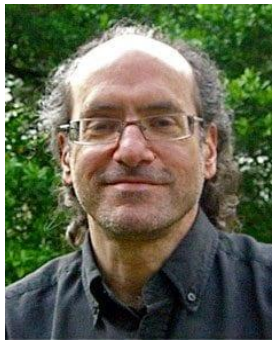
Restricted Boltzmann Machine(RBM)

RBMs were first introduced more than two decades ago (Smolensky, 1987)

Smolensky, P. Information processing in dynamical systems: Foundations of harmony theory. Parallel Distributed Processing: Volume 1: Foundations, pp. 194–281. MIT Press, Cambridge, 1987.

They have recently been used as constituents of "deep belief network" learning systems (Hinton et al., 2006)

"A fast learning algorithm for deep belief nets. Neural Computation, 18(7):1527–1554, 2006.



Paul Smolensky

Johns Hopkins

Geoffrey Hinton

Toronto

OBJECTIVE

DEFINITION OF THE PROBLEM

For an arbitrary d-dimensional system characterized by its self-adjoint Hamiltonian operator $\hat{H} \in \mathbb{C}^{d\times d}$ we want to access the eigenstates $\psi(\vec{X})$ of $\hat{H}$ and its corresponding eigen-energies and other properties.

This is a very general problem that encompasses almost all of traditional quantum chemistry

OUR APPROACH

- We shall construct a neural-network to learn the required state of the system
- We shall construct a quantum-circuit to train the network
- We shall implement the machine on a quantum computer

Restricted Boltzmann Machine (RBM)

BACKBONE OF THE TALK

nature COMMUNICATIONS

***Nature Comm*. 9, 4195 (2018)**

ARTICLE

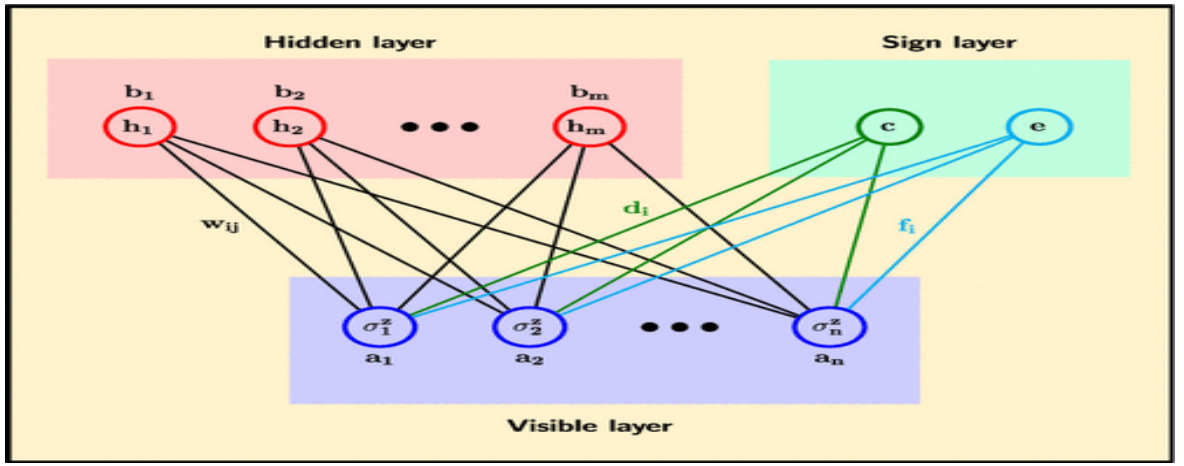
DOI: 10.1038/s41467-018-06598-z OPEN

Quantum machine learning for electronic structure calculations

Rongxin Xia[1] & Sabre Kais[1,2,3]

Implementation of Quantum Machine Learning for Electronic Structure Calculations of Periodic Systems on Quantum Computing Devices

S.H Sureshbabu, M. Sajjan, S. Oh and S. Kais



Journal of Chemical Information and Modeling

61, 6, 2667–2674 (2021)

Quantum Machine-Learning for Eigenstate Filtration in Two-Dimensional Materials

Manas Sajjan, Shree Hari Sureshbabu, Sabre Kais

arXiv:2105.09488 **(2021)**

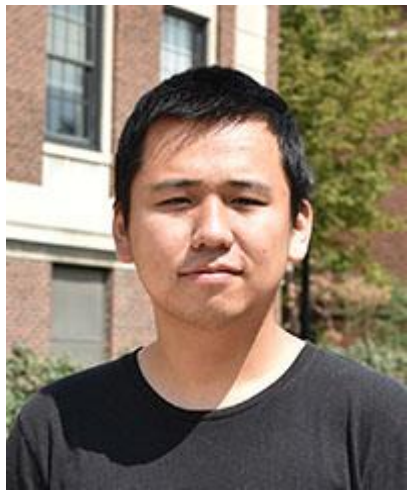
Herein we demonstrate a quantum algorithm that can filter any energy eigenstate of the system based on either symmetry properties or on a predefined choice of the user. We implement our algorithm for two-dimensional materials on actual IBM-Q quantum devices.

Model: Restricted Boltzmann Machine

Goal: Quantum Machine Learning for Material Design


Manas Sajjan


Shree Hari Sureshbabu


Rongxin Xia


Junxu Li


Raja Selvarajan


Sangchul Oh

What to Expect: Our Main Contributions

1. Will construct a three-layered RBM that will be trained to learn any arbitrary state of the system.

2. RMB will be implemented on a quantum device, by designing a quantum circuit with quadratic resource requirements (circuit width, circuit depth, parameter count)

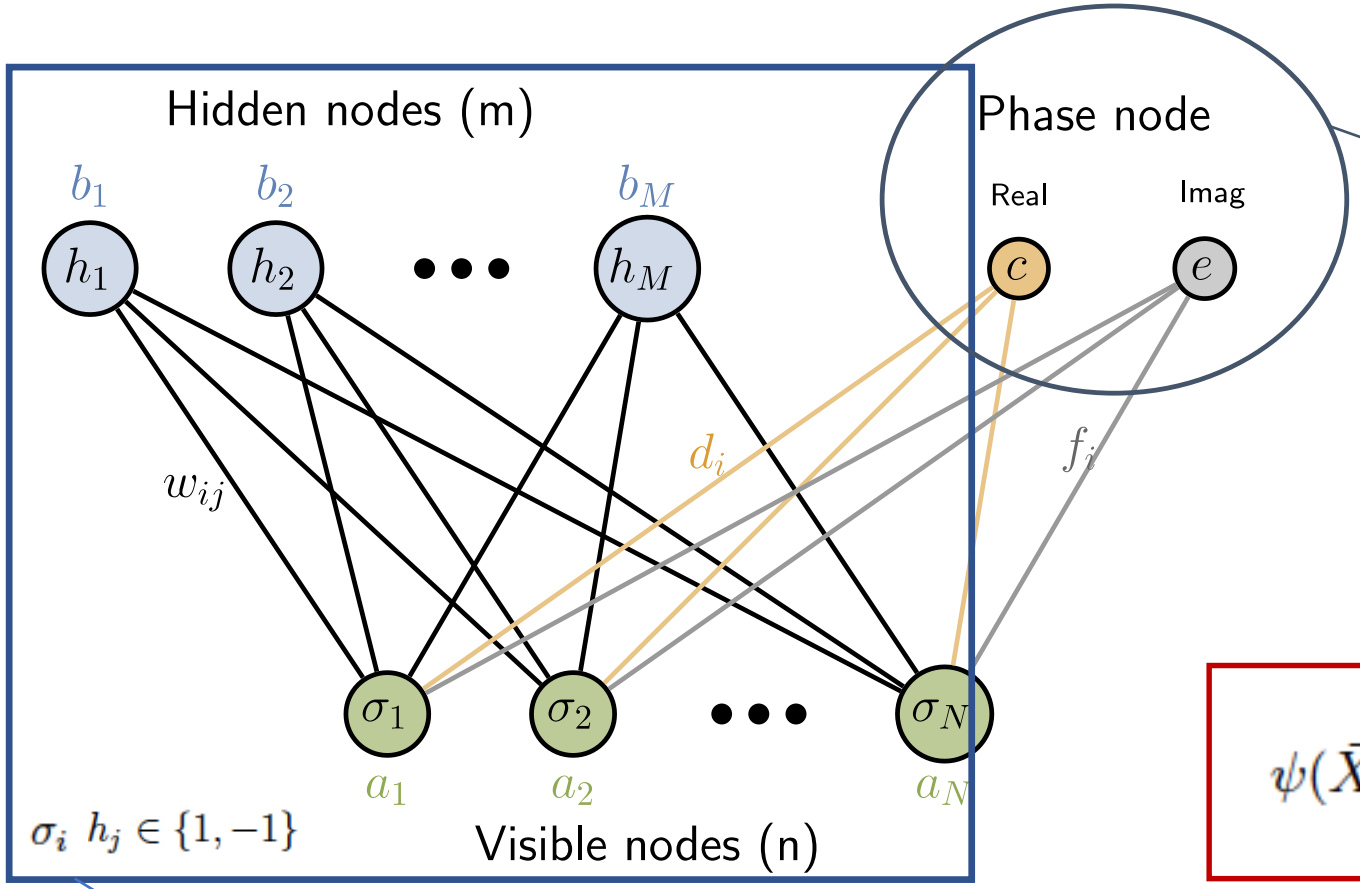
3. Will derive a generic lower bound for the successful sampling of the quantum circuit in the algorithm in terms of the parameters of the network.

4. Will apply our algorithm on important 2D materials like graphene and monolayer transition metal di-chalcogenides (TMDCs):Molybdenum disulfide MoS_2 and Tungsten disulfide WS_2

5. All numerical experiments will be implemented on quantum simulator (Qiskit) and also on actual NISQ devices using the quantum processors at IBM.

We will show that the performance of our algorithm is in excellent agreement with the exact value in each case

NETWORK ARCHITECTURE (RESTRICTED BOLTZMANN MACHINE ANSATZ)



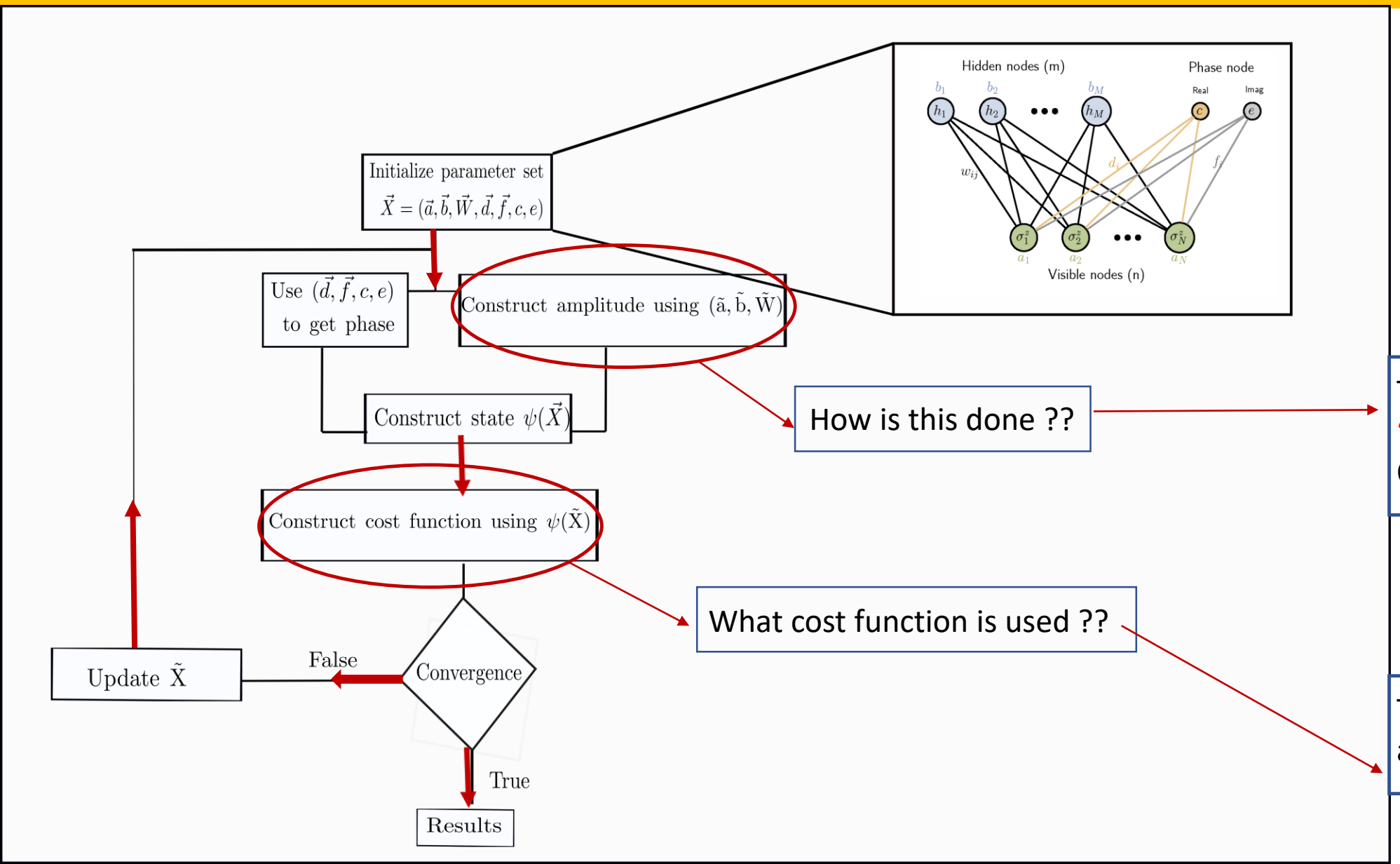
$$s(\vec{d}, \vec{f}, c, e, \vec{\sigma}) = \tanh\left[(c + \sum_i d_i\sigma_i) + i(e + \sum_i f_i\sigma_i)\right]$$

$$\psi(\vec{X}) = \sum_{\sigma} \sqrt{\tilde{p}(\vec{a}, \vec{b}, \vec{W}, \vec{\sigma})}\, s(\vec{d}, \vec{f}, c, e, \vec{\sigma}) |\sigma_1\sigma_2 ... \sigma_n\rangle$$

$$P(\vec{a}, \vec{b}, \vec{W}, \vec{\sigma}, \vec{h}) = \frac{e^{\sum_i a_i\sigma_i + \sum_j b_j h_j + \sum_{ij} w_{ij}\sigma_i h_j}}{\sum_{\{\sigma h\}} e^{\sum_i a_i\sigma_i + \sum_j b_j h_j + \sum_{ij} w_{ij}\sigma_i h_j}}$$

$$\tilde{p}(\vec{a}, \vec{b}, \vec{W}, \vec{\sigma}) = \sum_h P(\vec{a}, \vec{b}, \vec{W}, \vec{\sigma}, \vec{h})$$

ALGORITHM – A BROAD OVERVIEW



How is this done ??

This will bring the "quantum" in Quantum Machine Learning

What cost function is used ??

To be described later on a case by case basis

QUANTUM CIRCUIT FOR CONSTRUCTING THE AMPLITUDE

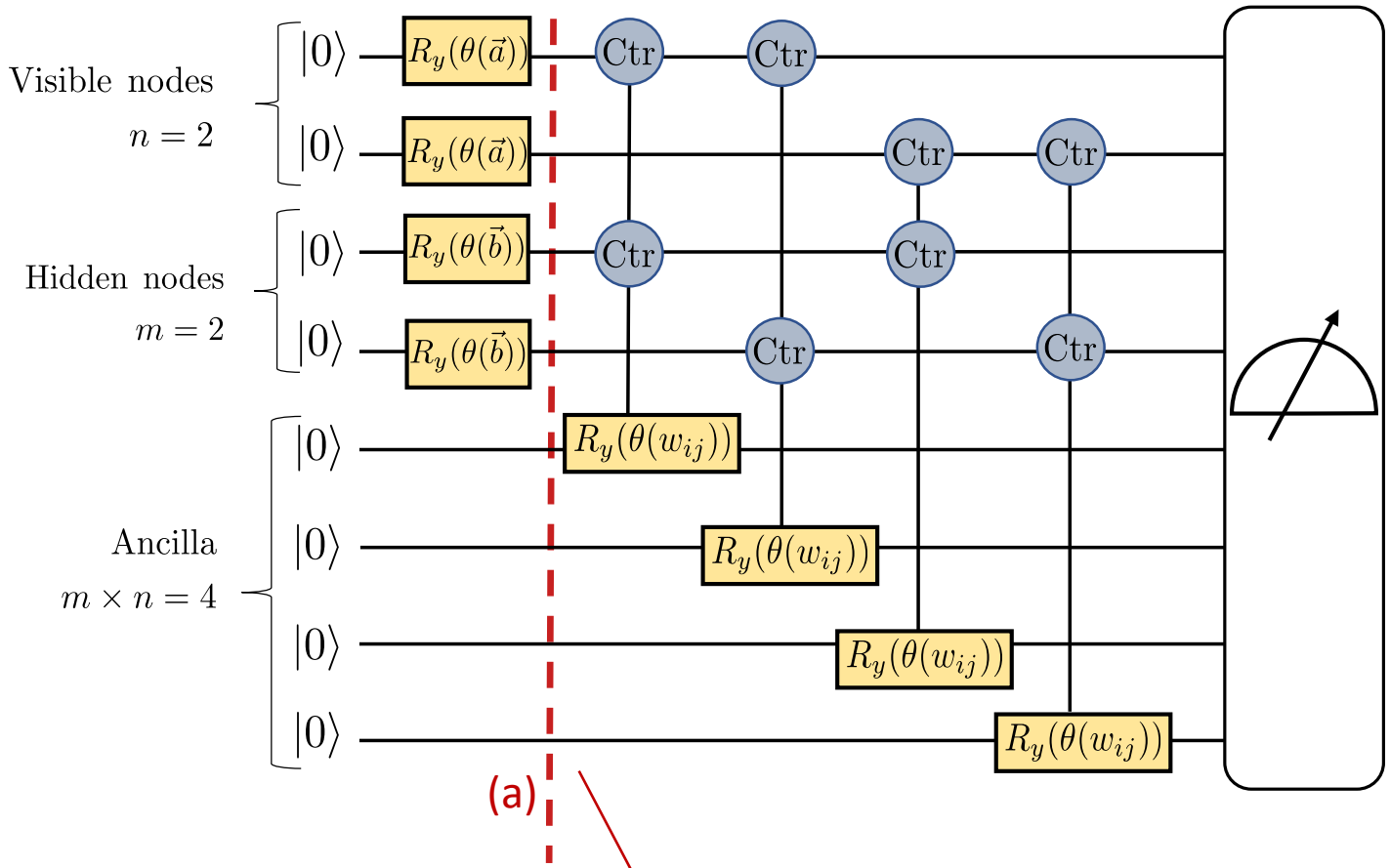
We shall describe a circuit to construct in the second step of the algorithm as described in the previous slides. We shall hereafter adopt the following notation:

Notations to be used

- Each neuron in visible node is mapped to one qubit in the circuit. For n visible neurons we have n visible qubits
- Each neuron in the hidden nodes is mapped to one qubit in the circuit. For m hidden neurons we have m qubits
- Additionally, we shall use (n*m) ancillary qubits too
- The states of visible qubits shall be denoted by $|\ldots\rangle_v$ and that hidden qubits shall be denoted by $|\ldots\rangle_h$. Note that $|0\rangle_v$ corresponds to $\sigma_i = -1$ and $|0\rangle_h$ corresponds to $h_j = -1$.
- The state of ancilla will be denoted by $|\ldots\rangle_a$
- The combined state of all qubits will be denoted by $|\psi_{v,h,a}\rangle$

$$Q(\vec{a},\vec{b},\vec{W},\vec{\sigma},\vec{h}) = \frac{e^{\frac{1}{k}(\sum_i a_i\sigma_i+\sum_j b_j h_j+\sum_{ij} w_{ij}\sigma_i h_j)}}{\sum_{\{\sigma h\}} e^{\frac{1}{k}(\sum_i a_i\sigma_i+\sum_j b_j h_j+\sum_{ij} w_{ij}\sigma_i h_j)}}$$

CONSTRUCTION OF AMPLITUDE USING QUANTUM CIRCUIT



$$R_y(\theta(\vec{a})) = \begin{bmatrix} \sqrt{\frac{e^{-a_i/k}}{e^{-a_i/k}+e^{a_i/k}}} & \sqrt{\frac{e^{a_i/k}}{e^{-a_i/k}+e^{a_i/k}}} \\ \sqrt{\frac{e^{a_i/k}}{e^{-a_i/k}+e^{a_i/k}}} & \sqrt{\frac{e^{-a_i/k}}{e^{-a_i/k}+e^{a_i/k}}} \end{bmatrix}$$

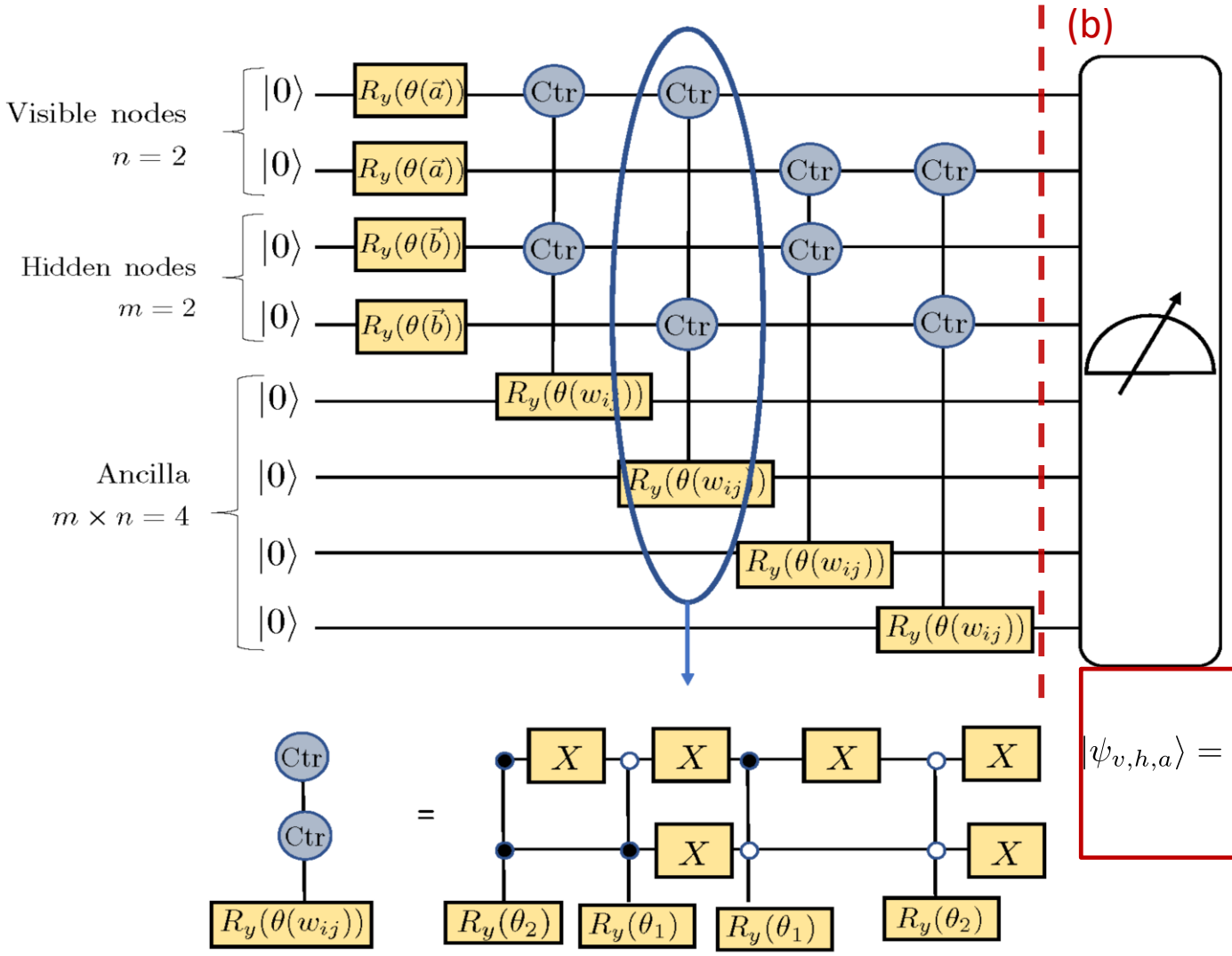
$$R_y(\theta(\vec{b})) = \begin{bmatrix} \sqrt{\frac{e^{-b_j/k}}{e^{-b_j/k}+e^{b_j/k}}} & \sqrt{\frac{e^{b_j/k}}{e^{-b_j/k}+e^{b_j/k}}} \\ \sqrt{\frac{e^{b_j/k}}{e^{-b_j/k}+e^{b_j/k}}} & \sqrt{\frac{e^{-b_j/k}}{e^{-b_j/k}+e^{b_j/k}}} \end{bmatrix}$$

State at (a)

$$|\psi_{v,h,a}\rangle = \sum_{(\vec{\sigma},\vec{h})} \sqrt{O(\vec{\sigma},\vec{h},\vec{a},\vec{b})}|\vec{\sigma}\vec{h}\rangle_{vh} \otimes |0\rangle_a$$

$$O(\vec{\sigma},\vec{h},\vec{a},\vec{b}) = \frac{e^{\frac{\sum_i a_i\sigma_i + \sum_j b_j h_j}{k}}}{\sum_{\vec{\sigma}\vec{h}} \frac{e^{\sum_i a_i\sigma_i + \sum_j b_j h_j}}{k}}$$

CONSTRUCTION OF AMPLITUDE USING QUANTUM CIRCUIT



$$CCR_y(\theta_2(\vec{W}))|11\rangle_{vh}|0\rangle_a = \sqrt{\frac{e^{W_{ij}/k}}{e^{|W_{ij}|/k}}}|11\rangle_{vh}|1\rangle_a + \sqrt{1 - \frac{e^{W_{ij}/k}}{e^{|W_{ij}|/k}}}|11\rangle_{vh}|0\rangle_a$$

$$CCR_y(\theta_2(\vec{W}))|00\rangle_{vh}|0\rangle_a = \sqrt{\frac{e^{W_{ij}/k}}{e^{|W_{ij}|/k}}}|00\rangle_{vh}|1\rangle_a + \sqrt{1 - \frac{e^{W_{ij}/k}}{e^{|W_{ij}|/k}}}|00\rangle_{vh}|0\rangle_a$$

$$CCR_y(\theta_1(\vec{W}))|10\rangle_{vh}|0\rangle_a = \sqrt{\frac{e^{-W_{ij}/k}}{e^{|W_{ij}|/k}}}|10\rangle_{vh}|1\rangle_a + \sqrt{1 - \frac{e^{-W_{ij}/k}}{e^{|W_{ij}|/k}}}|10\rangle_{vh}|0\rangle_a$$

$$CCR_y(\theta_1(\vec{W}))|01\rangle_{vh}|0\rangle_a = \sqrt{\frac{e^{-W_{ij}/k}}{e^{|W_{ij}|/k}}}|01\rangle_{vh}|1\rangle_a + \sqrt{1 - \frac{e^{-W_{ij}/k}}{e^{|W_{ij}|/k}}}|01\rangle_{vh}|0\rangle_a$$

State at (b)

$$|\psi_{v,h,a}\rangle = \sum_{(\vec{\sigma},\vec{h})} \sqrt{O(\vec{\sigma},\vec{h},\vec{a},\vec{b})}|\vec{\sigma}\vec{h}\rangle_{vh} \otimes \sqrt{(1-\eta(\vec{W},\vec{\sigma},\vec{h})}|0\rangle_a + \sqrt{\eta(\vec{W},\vec{\sigma},\vec{h})}|1\rangle_a$$

$$\eta(\vec{W},\vec{\sigma},\vec{h}) = \frac{e^{\frac{1}{k}(\sum_{i,j} w_{ij}\sigma_i h_j)}}{e^{\frac{1}{k}\sum_{i,j}|w_{ij}|}}$$

CONSTRUCTION OF AMPLITUDE USING QUANTUM CIRCUIT

$$|\psi_{v,h,a}\rangle = \sum_{(\vec{\sigma},\vec{h})} \sqrt{O(\vec{\sigma},\vec{h},\vec{a},\vec{b})}|\vec{\sigma}\vec{h}\rangle_{vh} \otimes \sqrt{(1-\eta(\vec{W},\vec{\sigma},\vec{h})}|0\rangle_a + \sqrt{\eta(\vec{W},\vec{\sigma},\vec{h})}|1\rangle_a)$$

$$O(\vec{\sigma},\vec{h},\vec{a},\vec{b}) = \frac{e^{\frac{\sum_i a_i\sigma_i + \sum_j b_j h_j}{k}}}{\sum_{\vec{\sigma}\vec{h}} e^{\frac{\sum_i a_i\sigma_i + \sum_j b_j h_j}{k}}} \qquad \eta(\vec{W},\vec{\sigma},\vec{h}) = \frac{e^{\frac{1}{k}(\sum_{i,j} w_{ij}\sigma_i h_j)}}{e^{\frac{1}{k}\sum_{i,j}|w_{ij}|}}$$

We make projective measurements on above state and post-select all measurement results wherein ancillas $|\vec{1}\rangle_a$ are in W . We call such events successful sampling.

Lower bound on Probability of successful sampling and choice of k-parameter

$$P_{success} = P(\vec{1}_a) = \sum_{\vec{\sigma},\vec{h}} \frac{e^{\frac{1}{k}(\sum_i a_i\sigma_i + \sum_j b_j h_j)}}{\sum_{\sigma,h} e^{\frac{1}{k}(\sum_i a_i\sigma_i + \sum_j b_j h_j)}} \times \frac{e^{\frac{1}{k}(\sum_{i,j} w_{ij}\sigma_i h_j)}}{e^{\frac{1}{k}\sum_{i,j}|w_{ij}|}}$$

$$P_{success} \geq \frac{e^{\frac{1}{k}(\sum_{i,j} w_{ij}\tanh(a_i/k)\tanh(b_j/k)}}{e^{\frac{1}{k}\sum_{i,j}|w_{ij}|}}$$

$\tanh(a_i/k) \to \pm 1, \tanh(b_j/k) \to \pm 1$

$$\frac{1}{e^{\frac{2}{k}(\sum_{ij}|w_{ij}|)}}$$

$$k = \max(\sum_{ij}\frac{|w_{ij}|}{2}, 1)$$

$\tanh(a_i/k) \to (a_i/k), \tanh(b_j/k) \to (b_j/k)$

$|a_i| \leq a_0 \ \forall \ i$ and $|b_j| \leq b_0 \ \forall \ j$

$$\frac{1}{e^{(\frac{1}{k}+\frac{a_0 b_0}{k^3})(\sum_{i,j}|w_{ij}|}}$$

Manas Sajjan and Shree Hari Sureshbabu and Sabre Kais. Quantum Machine-Learning for Eigenstate Filtration in Two-Dimensional Materials, **2021**,2105.09488,arXiv

RESOURCE REQUIREMENTS AND IMPLEMENTATION DETAILS

- **The number of qubits required for all our systems :**
  - 2 qubits to represent the visible nodes (n)
  - 2 qubits to represent the hidden nodes (m)
  - 4 ancilla qubits (n+m)
- **The number of quantum gates** required to sample the Gibb's distribution are:
  - 4 single qubit Rotation gates (R_y) (n+m)
  - 4 Controlled-Controlled Rotation gates ($C - C - R_y$) (n×m).
  - 24 Bit-flip (X) gates (6 × n×m).

Number of iterations= 30000 for **quantum simulator** and in batches of **500 for IBM-Q devices**

We run simulations on the classical computer and on the following platforms

- **The IBM-Q** is an online platform that offers IBM's quantum processors via the cloud. The algorithm is tested on 27 qubit quantum processors from IBM (IBM-Sydney and IBM-Toronto)
- ***Qiskit quantum simulator especially the qasm backend***

RESOURCE REQUIREMENTS: Quantum Advantage

- **Classical RBM:**

Classically, constructing such a full RBM distribution will require tracking amplitudes from a **2^(m+n)** dimensional state space and hence has exponential resource requirements in preparation.

Long, P. M.; Servedio, R. A. Restricted Boltzmann Machines are hard to approximately evaluate or simulate. ICML 2010 - Proceedings, 27th International Conference on Machine Learning 2010, 703–710.

proved that a polynomial time algorithm for classically simulating or constructing a full RBM distribution is not only absent now but is unlikely to exist even in future as long as the polynomial hierarchy remains uncollapsed.

- **Current RBM quantum circuit:**

The quantum circuit in our algorithm uses **m+n+m×n** qubits only for constructing the state indicating an **O(m × n)** scaling in qubit resource which if expressed in terms of hidden node density α = m/n is **O(α n^2)**

CHOICE OF COST FUNCTION

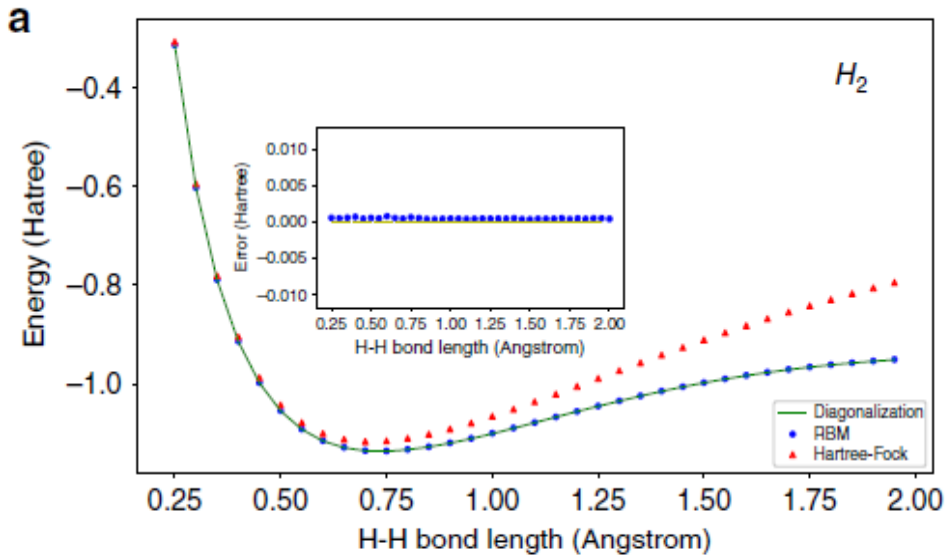
We want valence band/ground state of each of the systems to be studied. We can use the RBM ansatz constructed from the circuit and variationally minimize

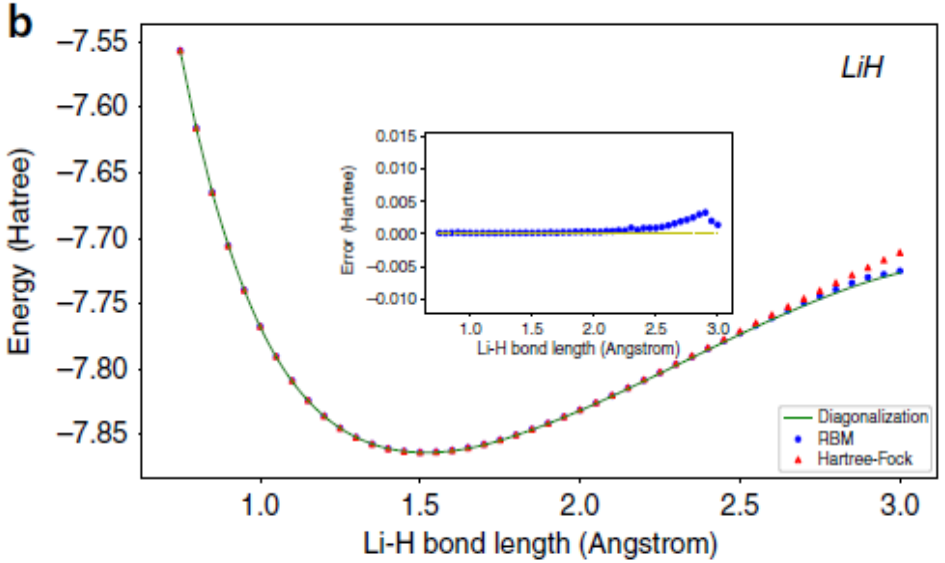
$$\langle \psi(\vec{X}) | H | \psi(\vec{X}) \rangle$$

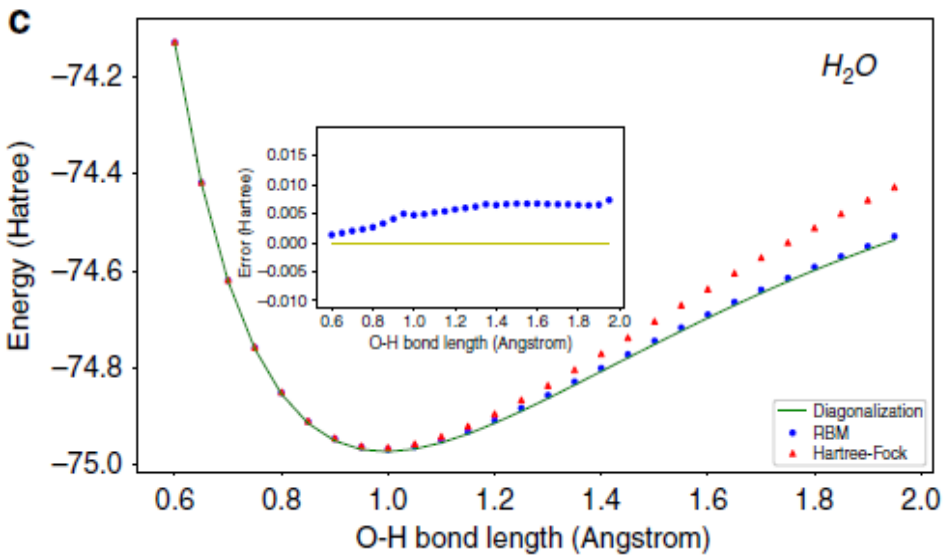
Cost function

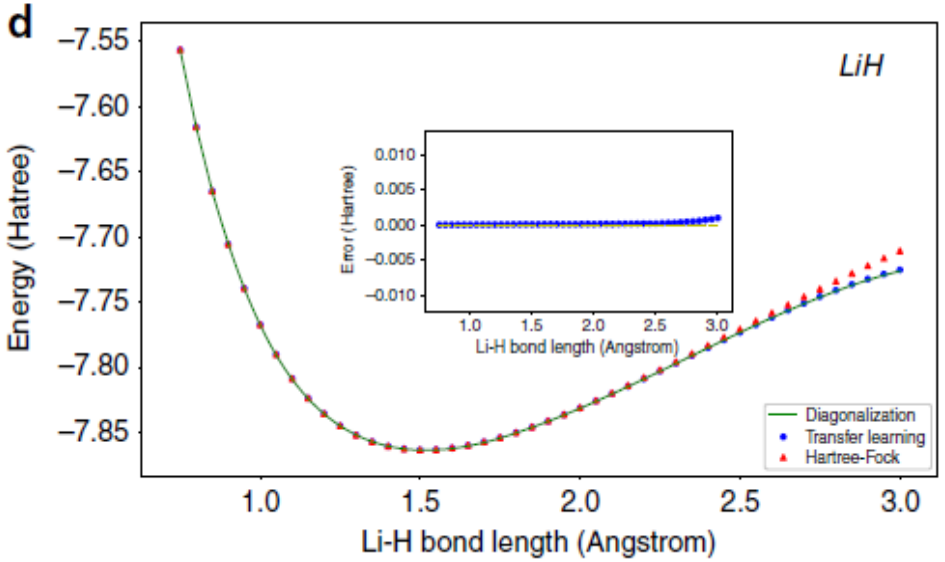
Good old variational theorem for ground state !

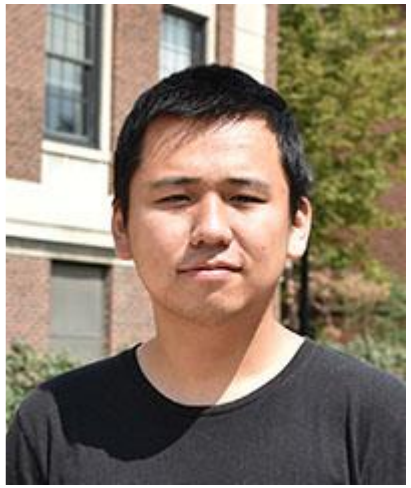
Results









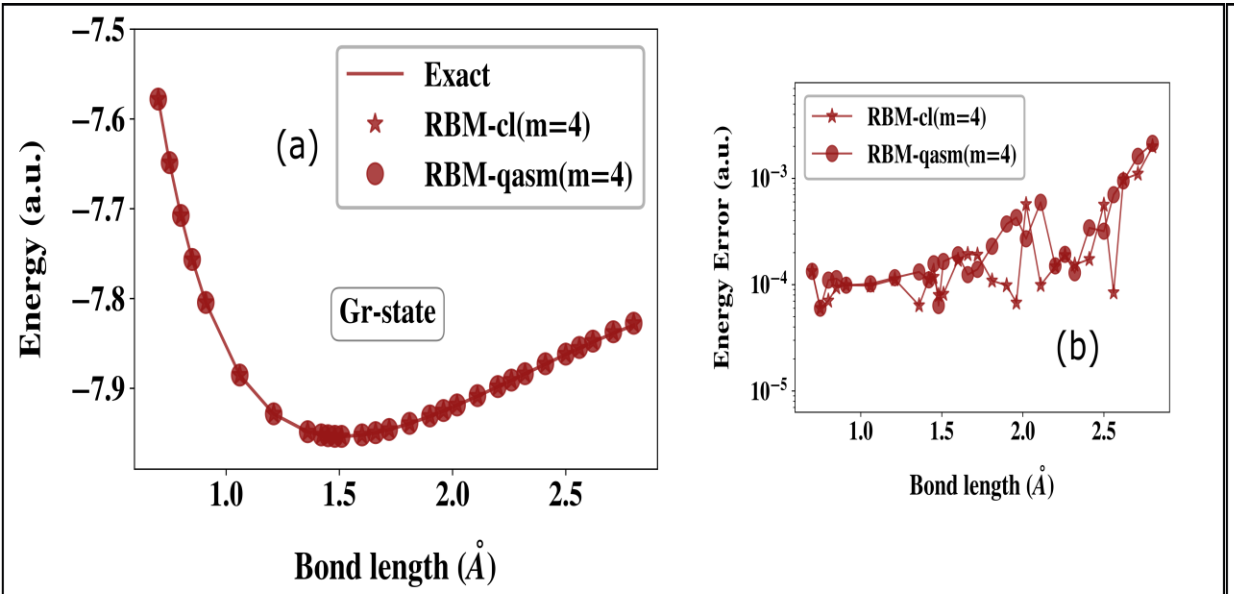


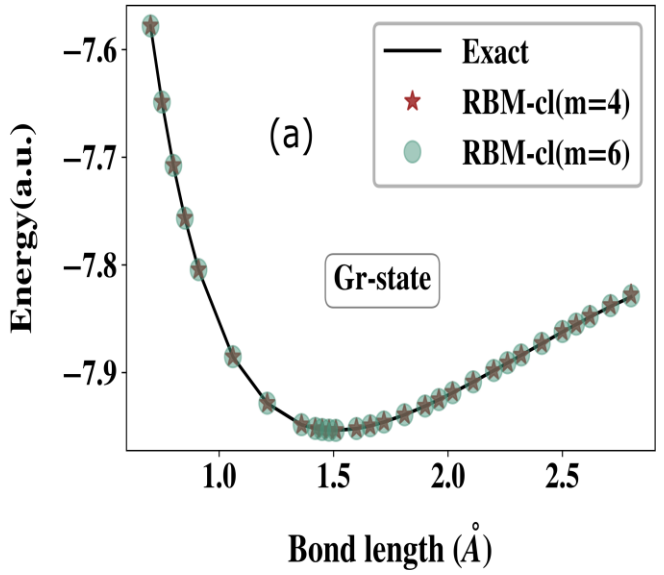
Rongxin Xia

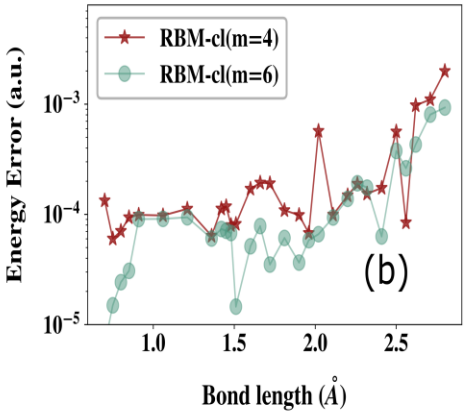
The results of H_2 (n = 4, m =8, iterations=10,000), LiH (n = 4, m = 8, iterations=40,000) and H_2O (n = 6, m = 6, iterations=40,000)

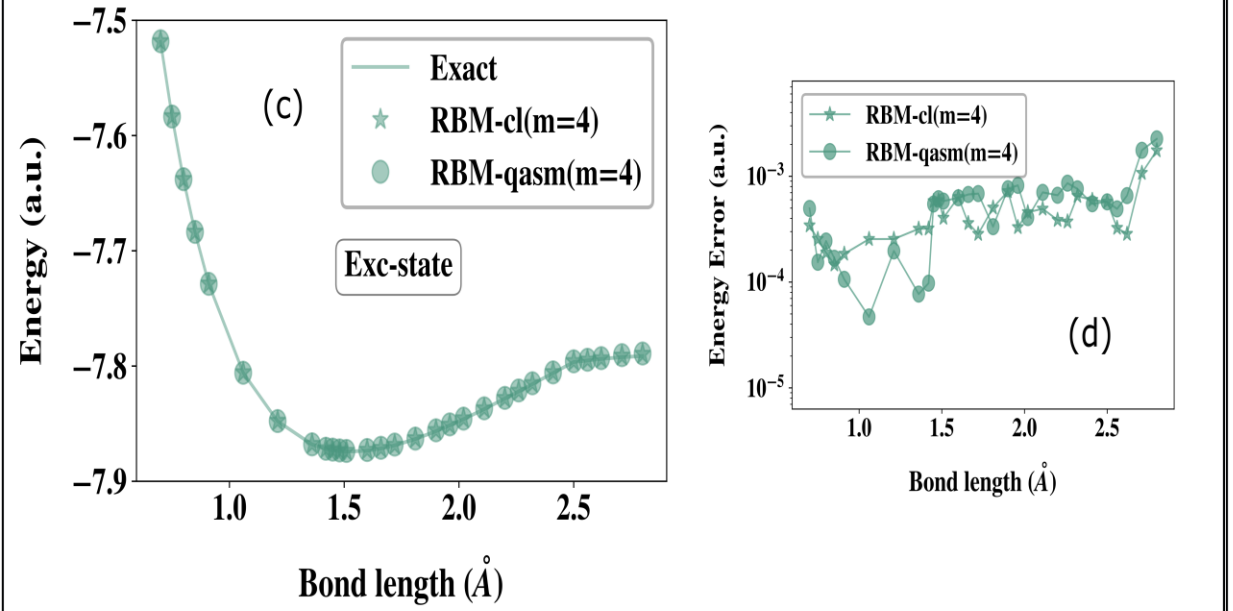
Nature Comm. 9, 4195 (2018)

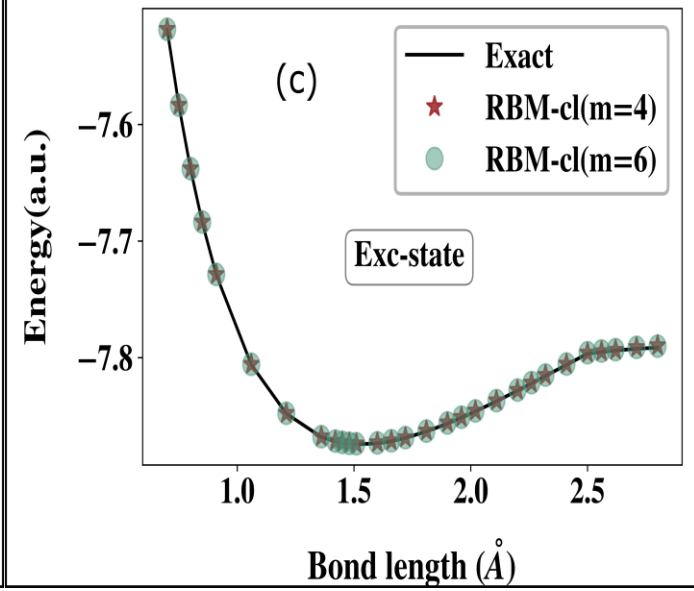
LiH Molecule (Change of Density = m/n)

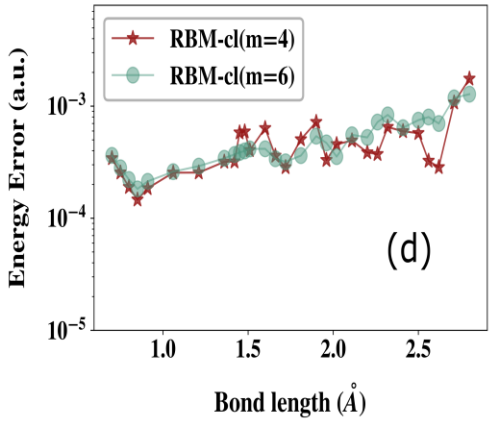












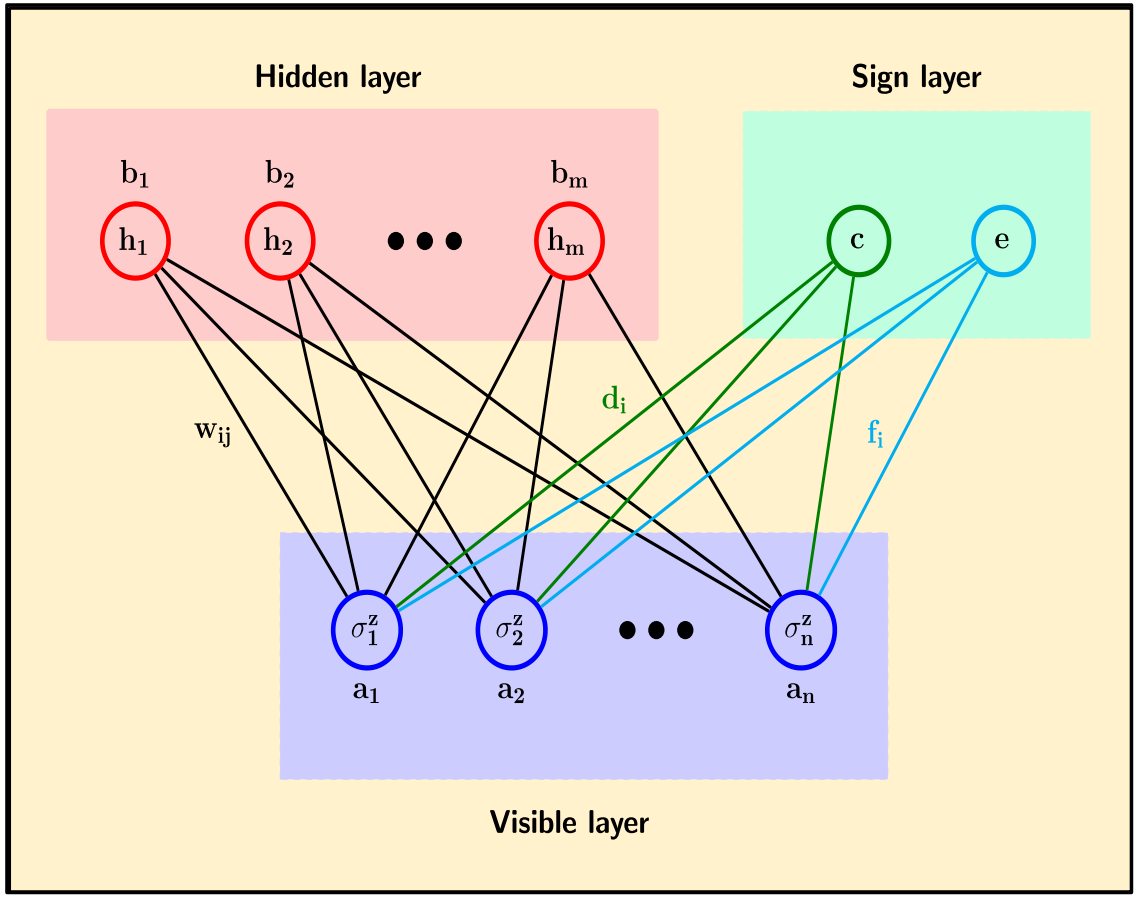
Methodology

- **The wavefunction can be expressed as:**

$$|\phi\rangle = \sum_x \sqrt{P(x)}\, s(x)|x\rangle$$

$$P(\mathbf{x}) = \frac{\sum_{\{h\}} e^{\sum_i a_i \sigma_i^z + \sum_j b_j h_j + \sum_{ij} w_{ij} \sigma_i^z h_j}}{\sum_{x'} \sum_{\{h\}} e^{\sum_i a_i \sigma_i^z + \sum_j b_j h_j + \sum_{ij} w_{ij} \sigma_i^z h_j}}$$

$$s(x) = tanh\left(\left(c + \sum_i d_i\, \sigma_i^z\right) + i\left(e + \sum_i f_i\, \sigma_i^z\right)\right)$$



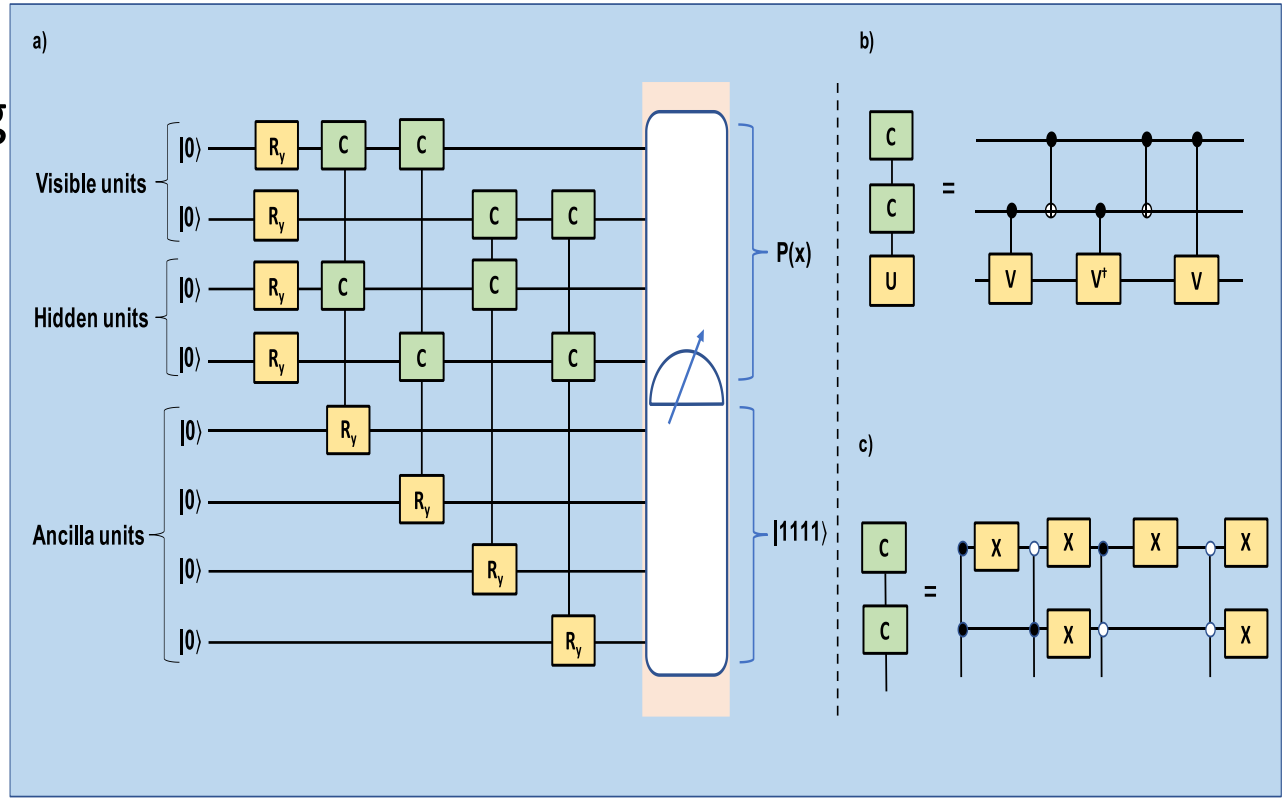
- **Given Hamiltonian H and a trial state $|\phi\rangle = \sum_x \phi(\mathbf{x})\,|x\rangle$** we compute the expectation value:

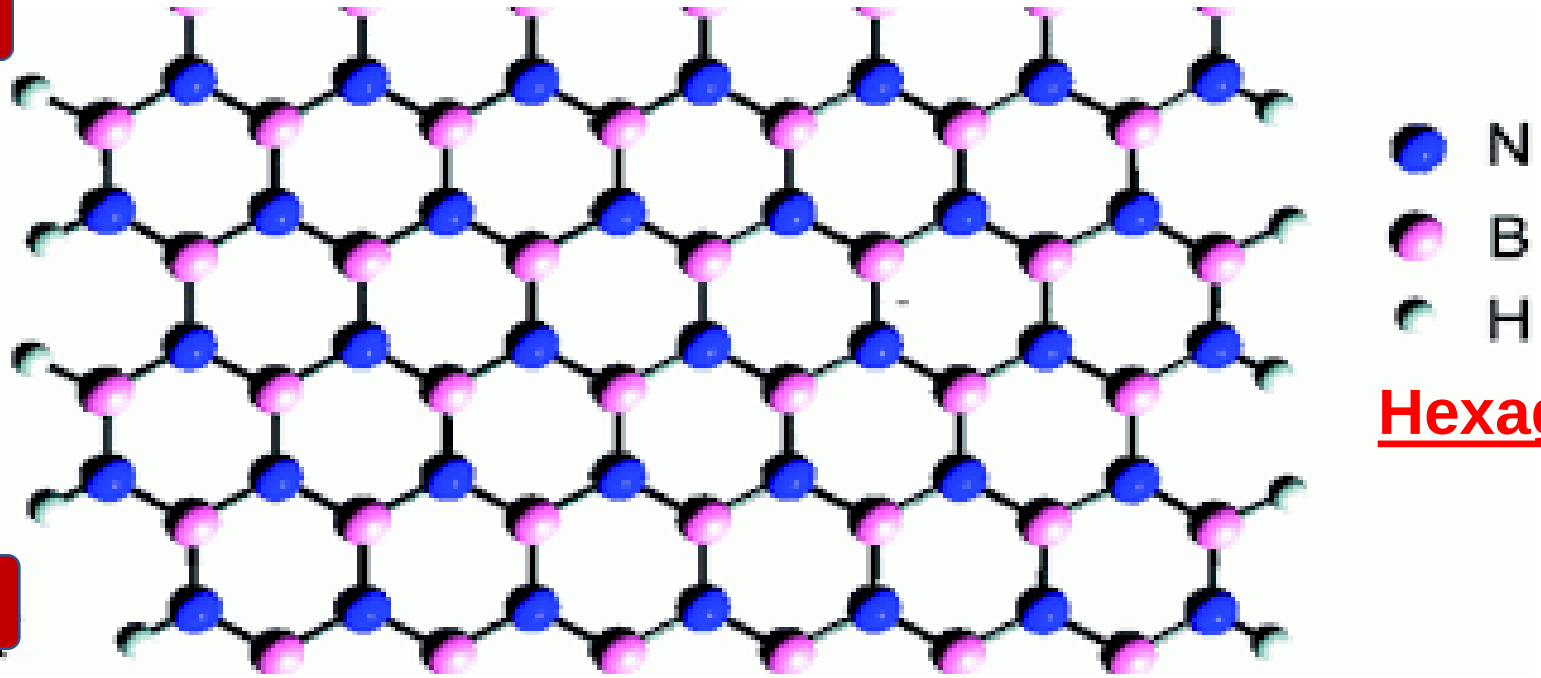
$$\langle H \rangle = \frac{\langle \phi | H | \phi \rangle}{\langle \phi | \phi \rangle}$$

Kanno, Shu, and Tomofumi Tada. "Many-body calculations for periodic materials via restricted Boltzmann machine-based VQE." *Quantum Science and Technology* 6, no. 2 (2021): 025015.

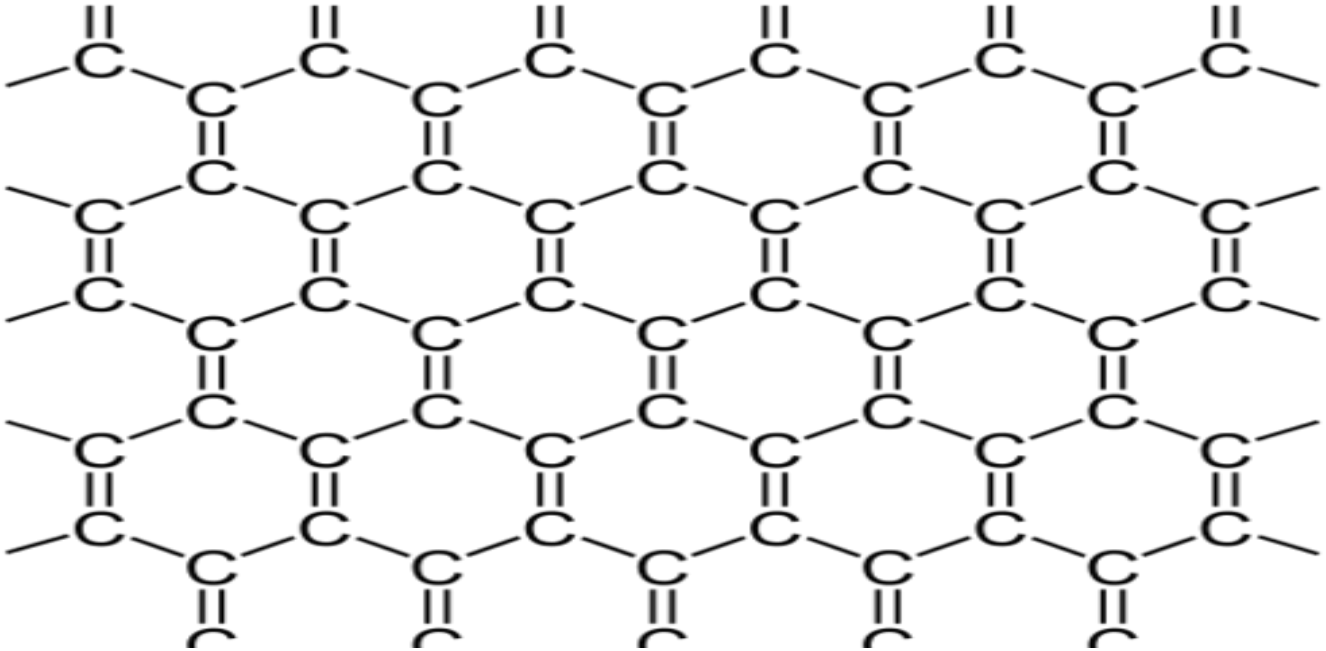
Quantum algorithm to sample Gibbs distribution

- **This algorithm is based on** sequential applications of controlled-rotation operations, which tries to calculate a distribution P(x) with an ancilla qubit showing whether the sampling for P(x) is successful
- **The quantum circuit mainly consists of two types of operations:**
  - A one-qubit operation, R_y, that corresponds to a rotational operation whose angle is determined by the bias parameters a_i(visible) and b_j(hidden)
  - A three-qubit operation, C-C-R_y, that is a controlled-controlled-rotation whose angle is determined by the connection parameter w_{ij}





Hexagonal-Boron Nitride (h-BN)

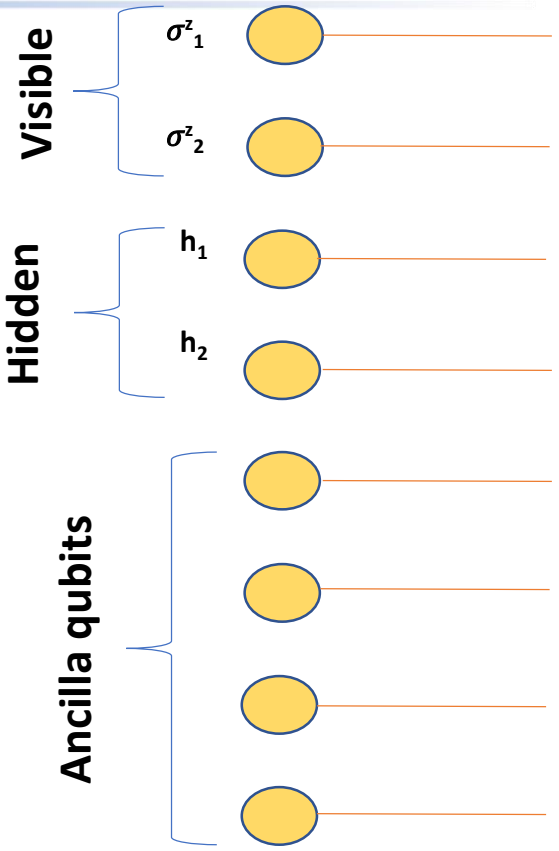


Graphene

Implementation on the IBM-Q machine

- **The IBM-Q** is an online platform that offers IBM's quantum processors via the cloud. Programming the circuit is done through the open-source quantum computing software development framework called *Qiskit.*
- ***Qiskit*** is made up of four elements that each work together to enable quantum computing and these elements are: *Terra, Aer, Ignis*, and *Aqua*.
- The algorithm is tested on 27 qubit quantum processors from IBM.
- **The number of qubits required:**
  - 2 qubits to represent the visible nodes (n)
  - 2 qubits to represent the hidden nodes (m)
  - 4 ancilla qubits (n+m)
- **The number of quantum gates** required to sample the Gibb's distribution are:
  - 4 single qubit Rotation gates (R_y) (n+m)
  - 4 Controlled-Controlled Rotation gates ($C - C - R_y$) (n×m).
  - 24 Bit-flip (X) gates (6 × n×m).

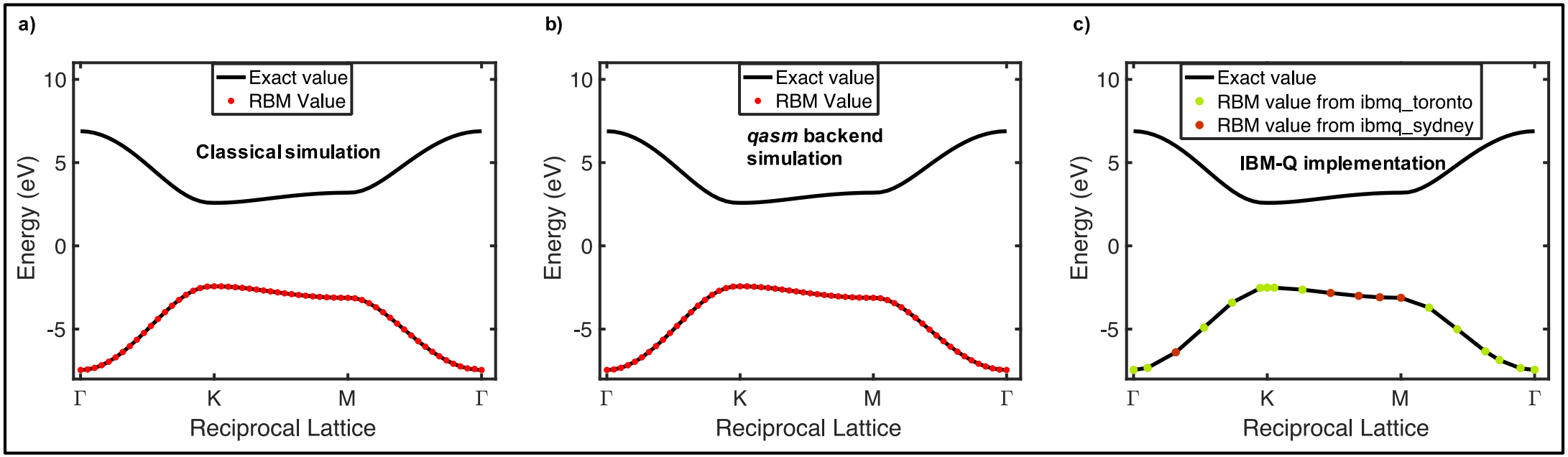
Number of iterations= 30000 for **IBM-qasm** and about **500 for IBM-Q**



Shree Hari Sureshbabu

Results

Implementation on IBM-Q to obtain electronic structure of hexagonal Boron Nitride (h-BN)

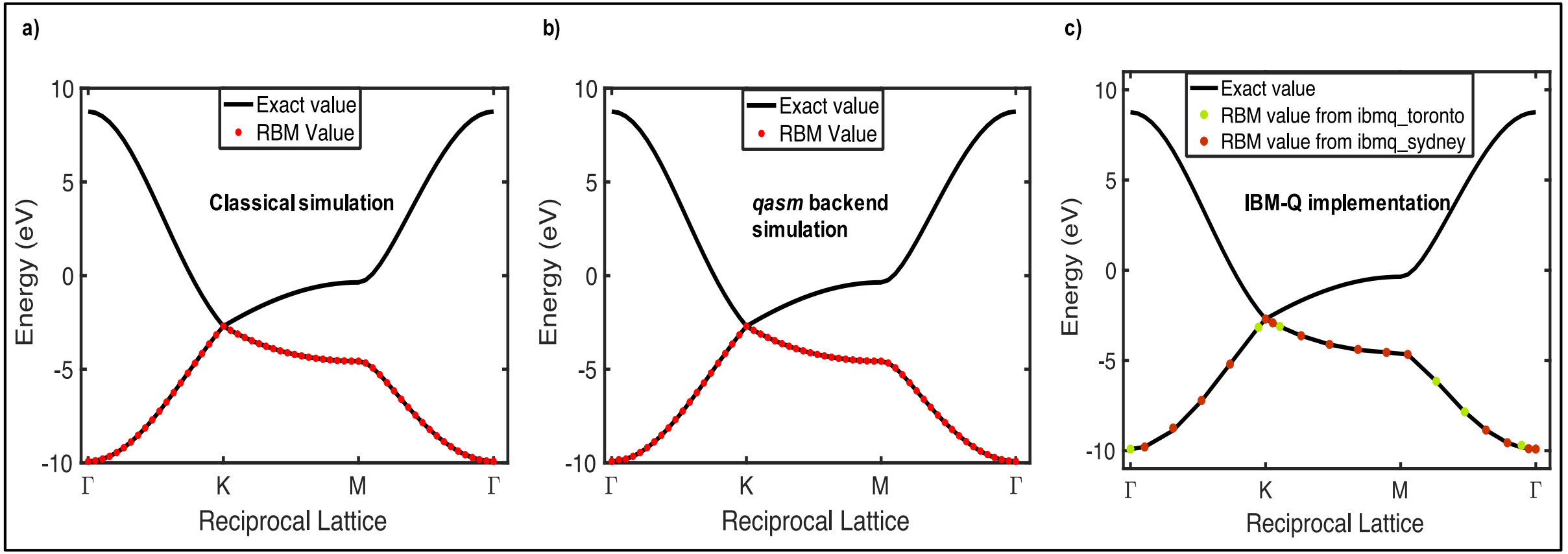


Band structures of h-BN calculated using (a) classical simulation with transfer learning (red marker). The solid black curve stands for the exact diagonalization of the tight-binding Hamiltonian. (b) Qiskit qasm backend combined with the transfer learning method (red marker). (c) The implementation the RBM sampling circuit on *ibmq toronto* (green) and *ibmq sydney* (red).

Journal of Chemical Information and Modeling **61, 6, 2667–2674 (2021)**

Results

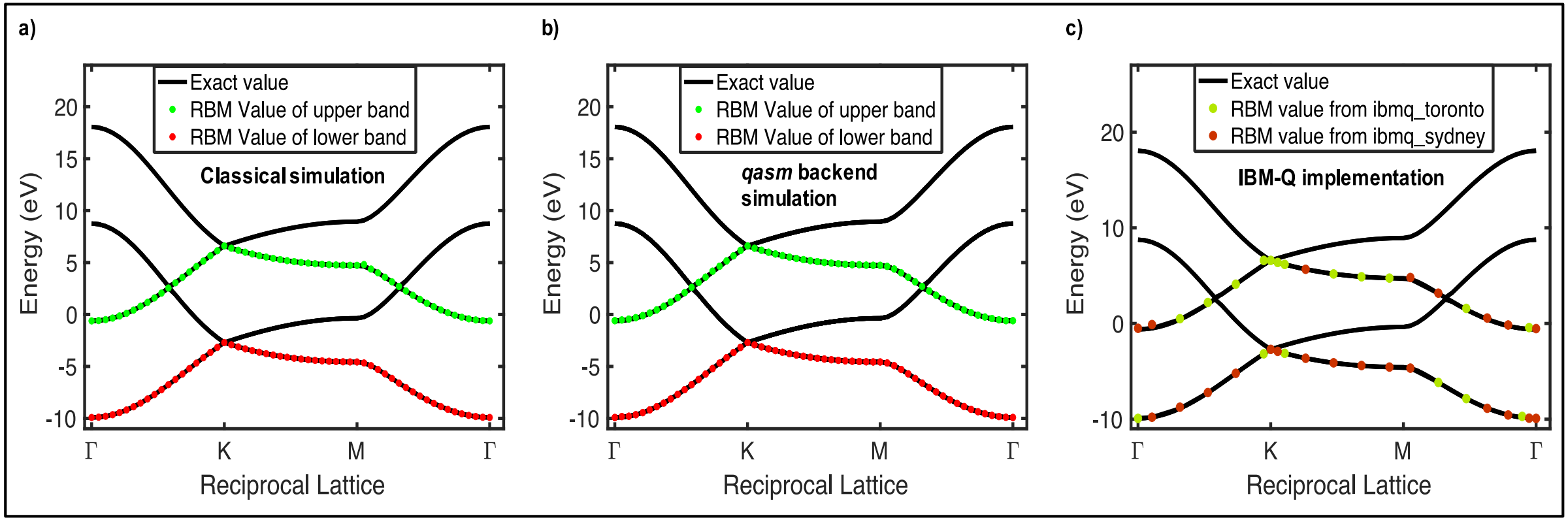
Implementation on IBM-Q to obtain electronic structure of Graphene (Hubbard U = 0 eV)



Band structures of graphene with U=0 eV calculated using (a) classical simulation with transfer learning (red marker). The solid black curve stands for the exact diagonalization of the tight-binding Hamiltonian. (b) Qiskit qasm backend combined with the transfer learning method (red marker). (c) The implementation the RBM sampling circuit on *ibmq toronto* (green) and *ibmq sydney* (red).

Results

Implementation on IBM-Q to obtain electronic structure of Graphene (Hubbard U = 9.3 eV)



Band structures of graphene with U=9.3 eV calculated using (a) classical simulation with transfer learning (red marker). The solid black curve stands for the exact diagonalization of the tight-binding Hamiltonian. (b) Qiskit qasm backend combined with the transfer learning method (red marker). (c) The implementation the RBM sampling circuit on *ibmq toronto* (green) and *ibmq sydney* (red).

Sureshbabu, Shree Hari, Manas Sajjan, Sangchul Oh, and Sabre Kais. "Implementation of Quantum Machine Learning for Electronic Structure Calculations of Periodic Systems on Quantum Computing Devices." J. Chemical Information and Modeling 61, 2667 (2021)

PROBLEM TO BE STUDIED

DEFINITION OF THE PROBLEM

We want to perform a constrained minimization problem as follows wherein we minimize the energy of the system among all choices of states that an eigenstates of some operator

$$\min_{\forall \psi \in S} \langle H \rangle_{\psi}$$

$$\mathrm{S} = \{|\psi\rangle \mid \hat{\mathrm{O}}|\psi\rangle = \omega|\psi\rangle, |\psi\rangle \in \mathbb{C}^{\mathrm{d}}\}$$

Why is this important ?

- We can target arbitrary eigenstate based on symmetry operators that commutes with H.

For ex we may want the minimum energy state with a certain fixed spin angular momentum.

CHOICE OF COST FUNCTION

Cost function

$$F(|\psi\rangle, \hat{H}, \hat{O}, \lambda) = \langle\psi|\hat{H}|\psi\rangle + \lambda\langle\psi|(\hat{O} - \omega)^2|\psi\rangle$$

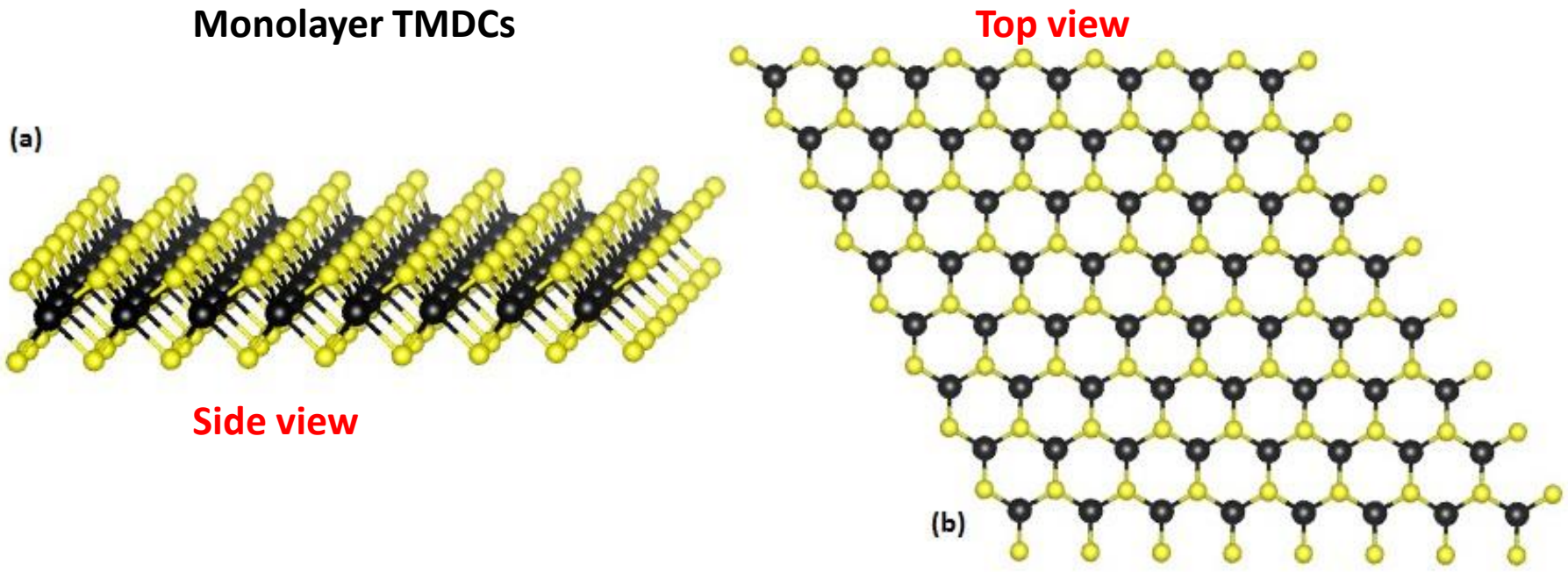
Intuitive explanation is that the second term is the variance of operator O and is non-negative. Since we penalize the variance with a high penalty parameter , so only way the cost function is minimized is if the
State has zero-variance with operator O or is an eigenstate of O

Manas Sajjan and Shree Hari Sureshbabu and Sabre Kais. Quantum Machine-Learning for Eigenstate Filtration in Two-Dimensional Materials, **2021**,2105.09488,arXiv

Excited states

- We variationally compute the excited states too by using orthogonality restriction on the ground states.

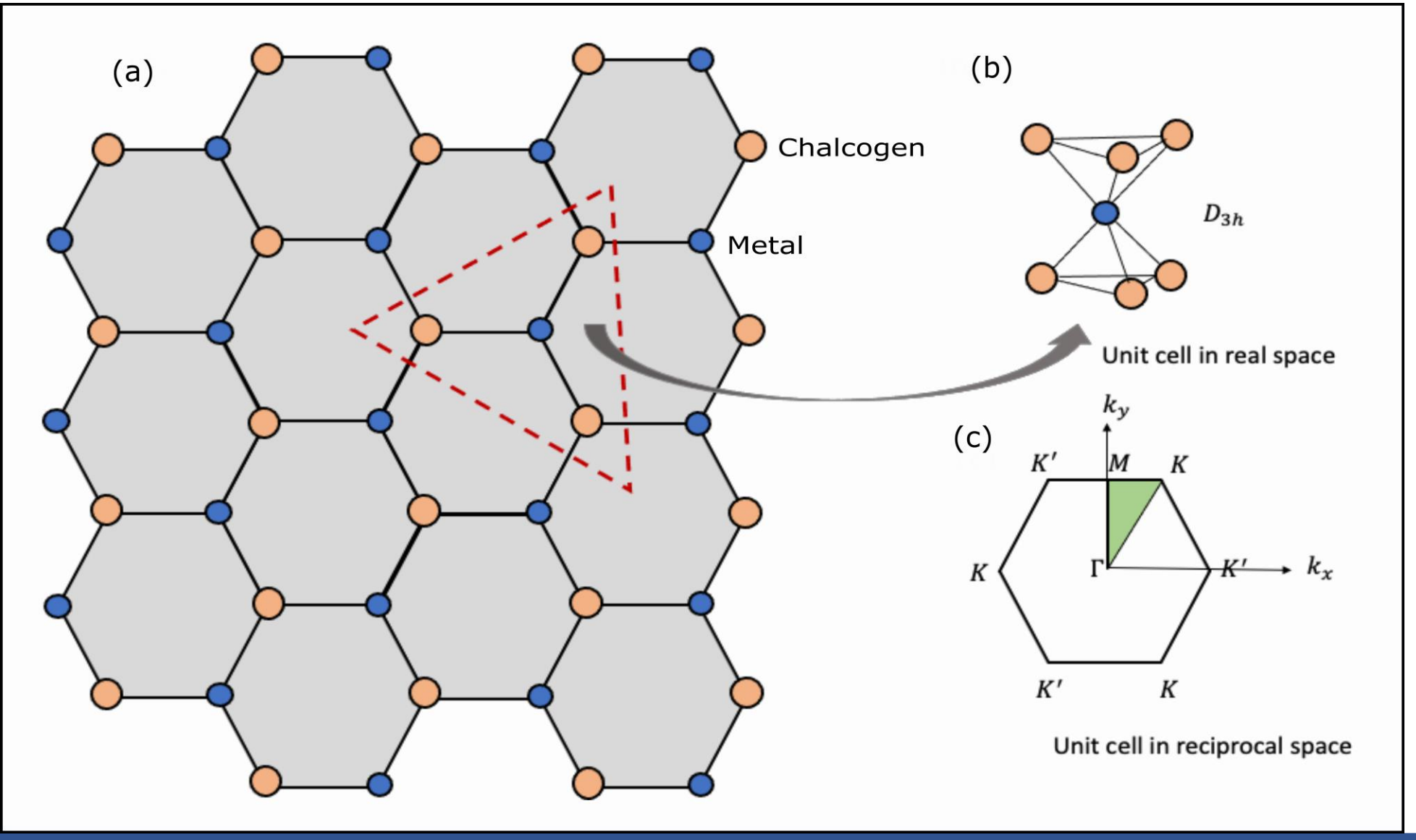
- We have applied the results to TMDCs (Transition –metal dichalcogenides)



Manas Sajjan

Molybdenum disulfide MoS_2 Tungsten disulfide WS_2

The top view of the TMDC monolayer: MoS_2 and WS_2



The orange atoms are a chalcogen (S) The blue atoms are the metal centre (Mo, W)

(k_x, k_y) $\Gamma = (0,0), K = (\frac{4\pi}{3a_0}, 0), M = (\frac{\pi}{a_0}, \frac{\pi}{\sqrt{3}a_0})$ where a_0 is the metal-chalcogen bond length.

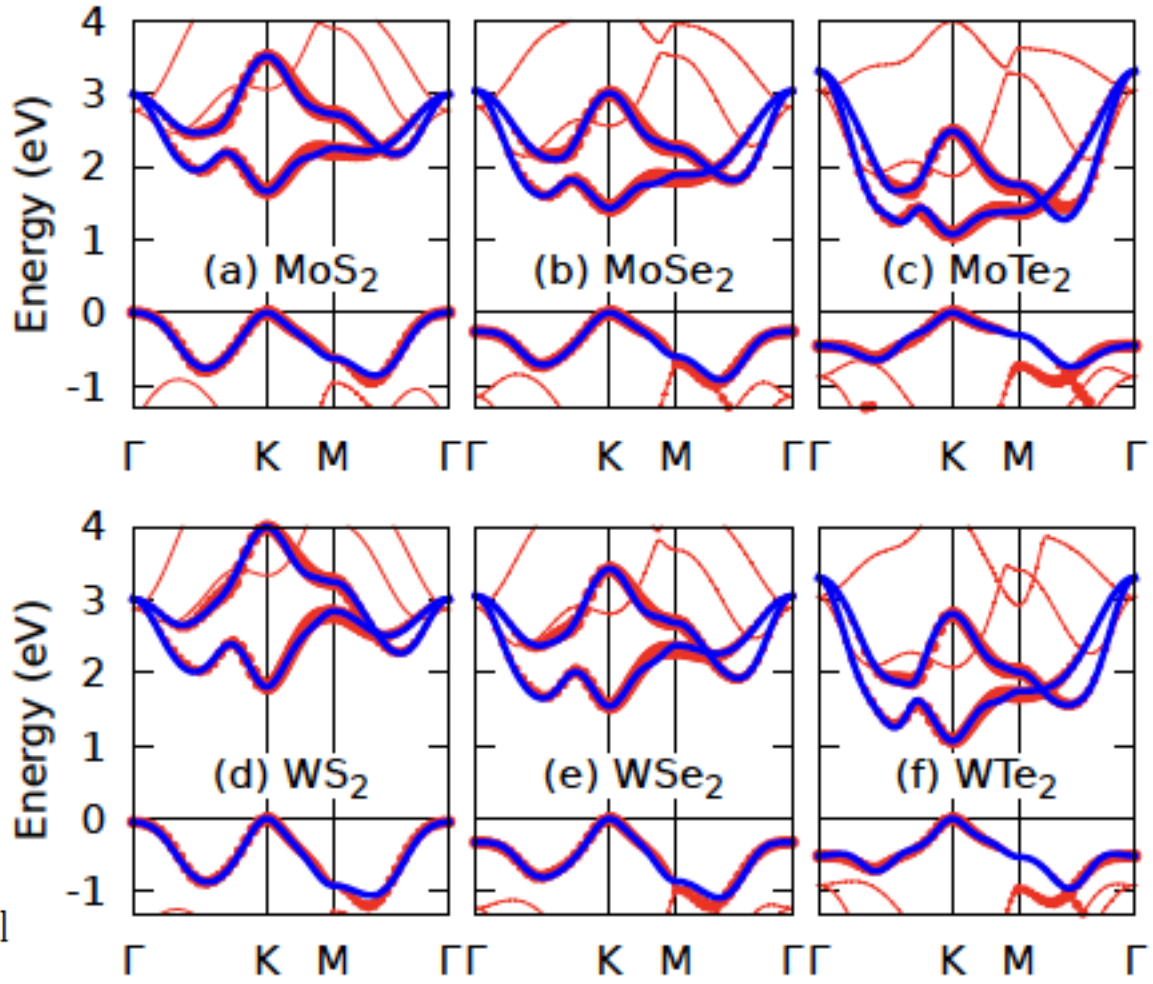
HAMILTONIAN BEING USED

A three-band tight-binding Hamiltonian involving the following orbitals of the transition metal. This Tight-binding is very accurate in energy across the entire BZ as lack of chalcogen orbitals is somewhat compensated using third-nearest neighbor interaction

$$|0\rangle = d_{z^2}$$

$$|1\rangle = d_{xy}$$

$$|2\rangle = d_{x^2-y^2}$$



Liu, G. B.; Shan, W. Y.; Yao, Y.; Yao, W.; Xiao, D. Three-band tight-binding model for monolayers of group-VIB transition metal dichalcogenides. Physical Review B - Condensed Matter and Materials Physics **2013**, 88, 1–11.

CHOICE OF OPERATOR TO FILTER EXCITED STATES

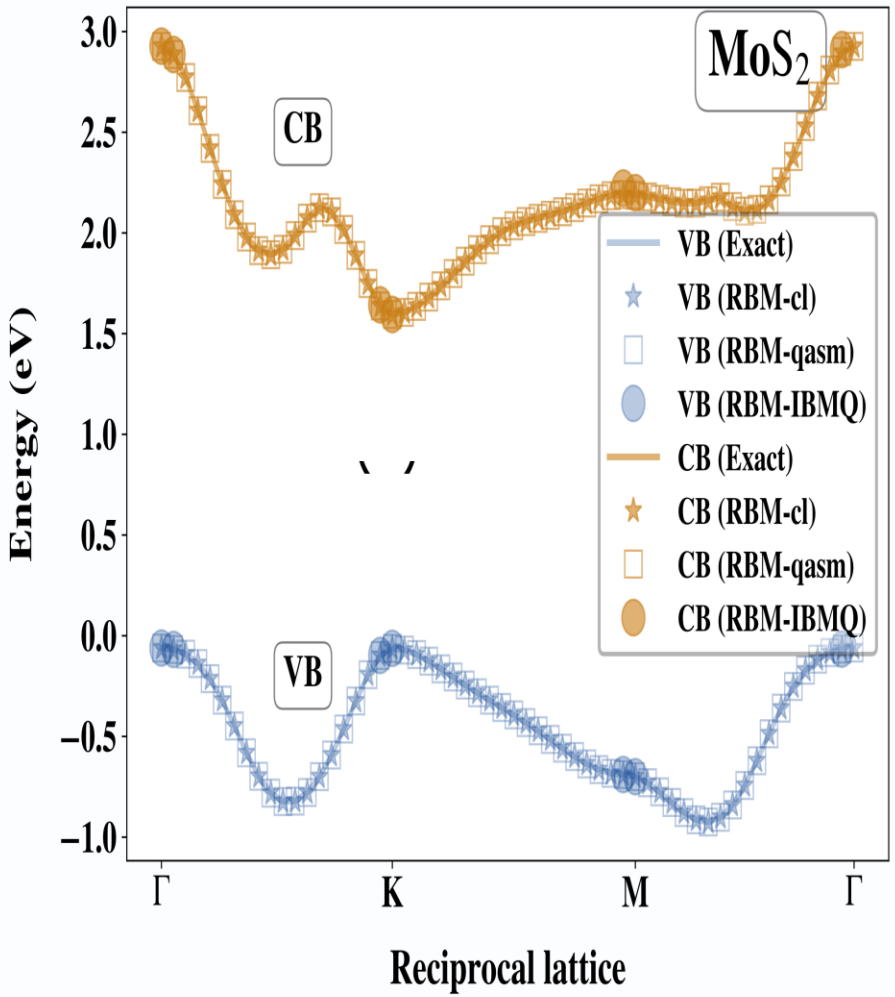
$$\hat{O} = |g\rangle\langle g|$$

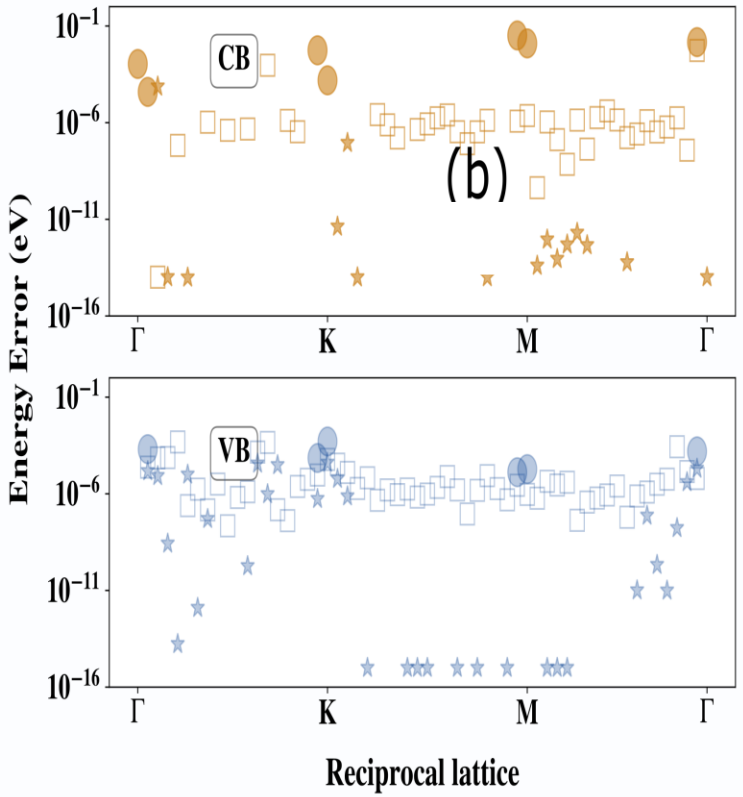
$$\omega = 0$$

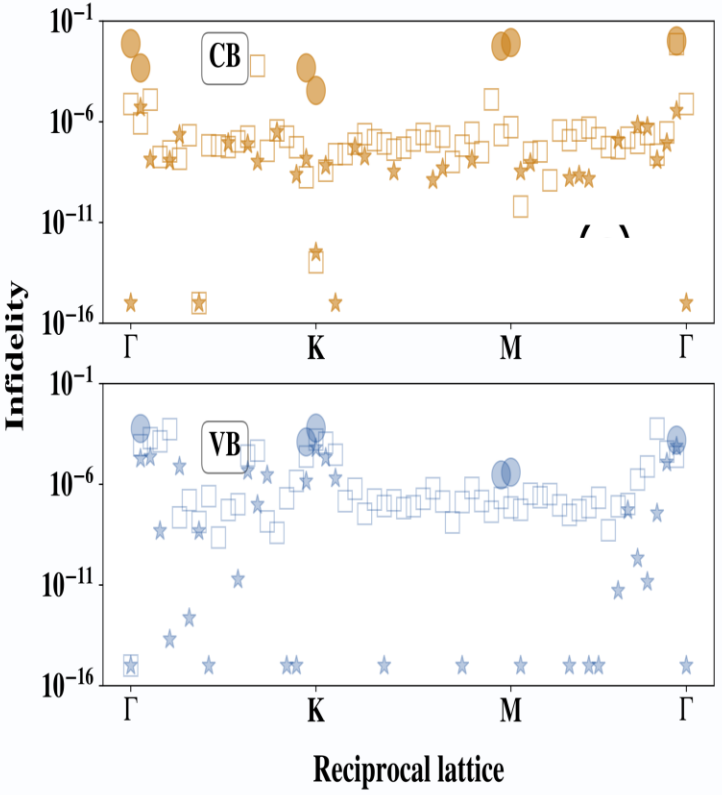
$$\lambda \geq ||\mathrm{H}||_2$$

Formally equivalent to deflation as all projection operators are idempotent

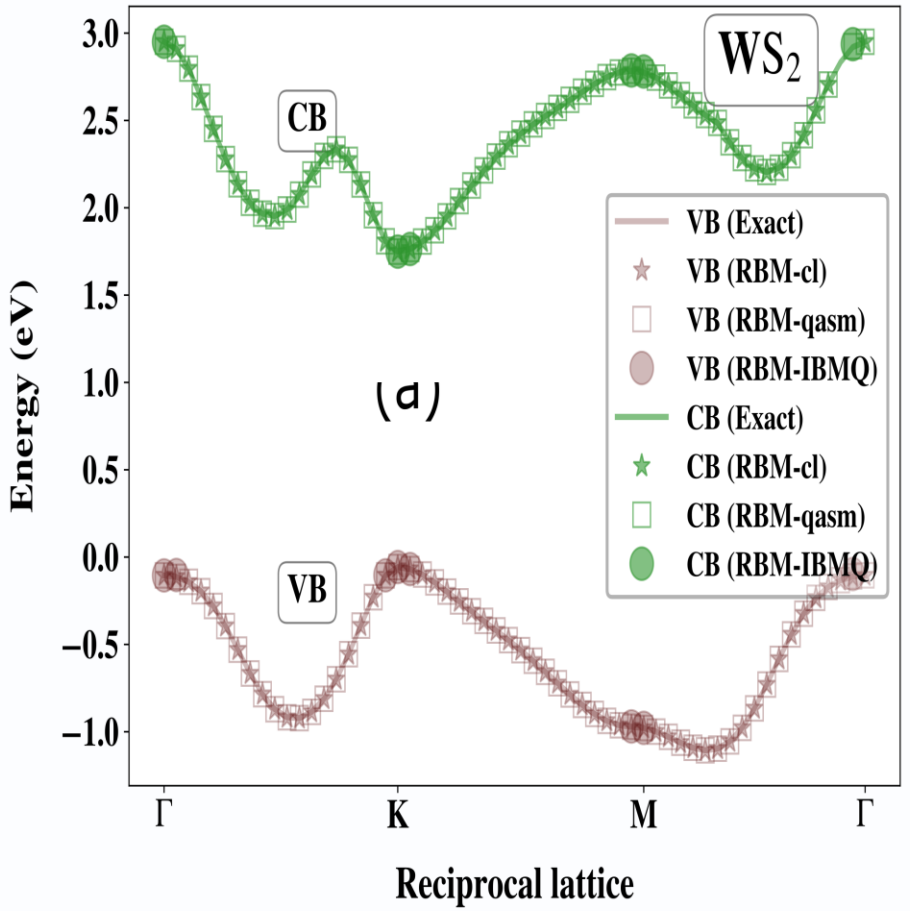
VALENCE AND CONDUCTION BAND - RESULTS FOR MoS_2

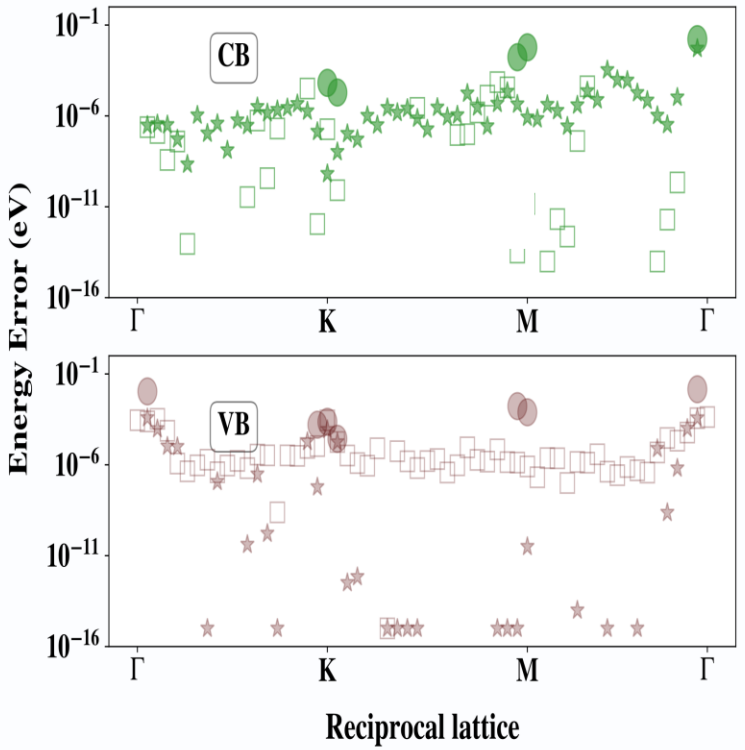


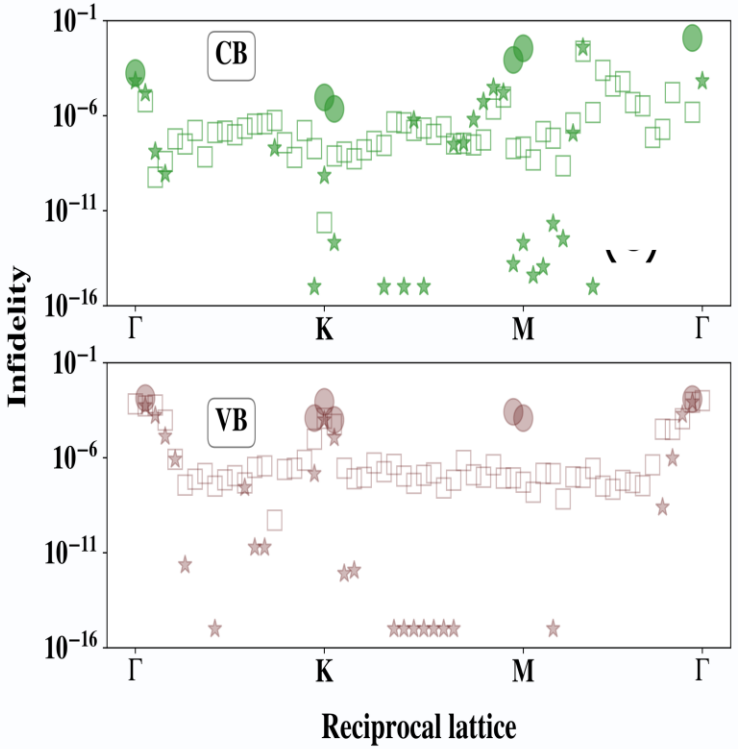




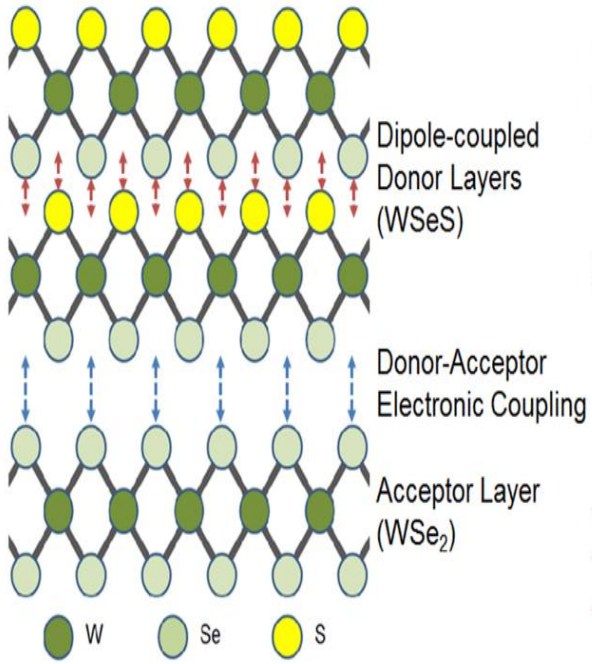
VALENCE AND CONDUCTION BAND- RESULTS FOR WS_2



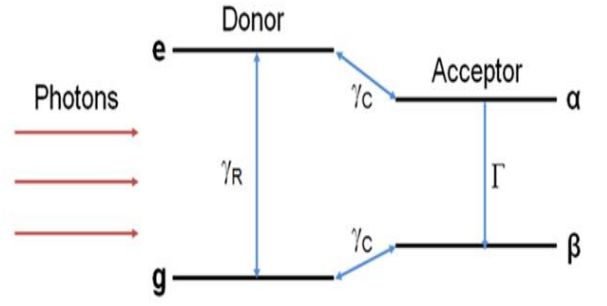




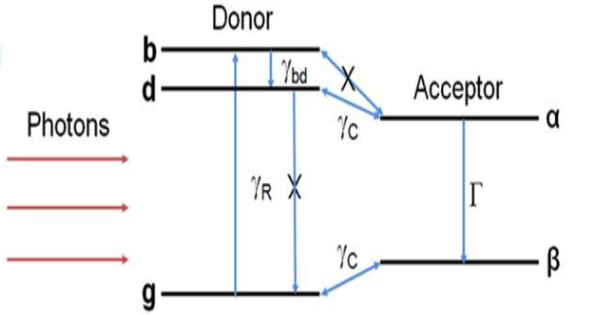
Enhancement of Photovoltaic Current through Dark States in Donor-Acceptor Pairs of Tungsten-Based Transition Metal Di-Chalcogenides



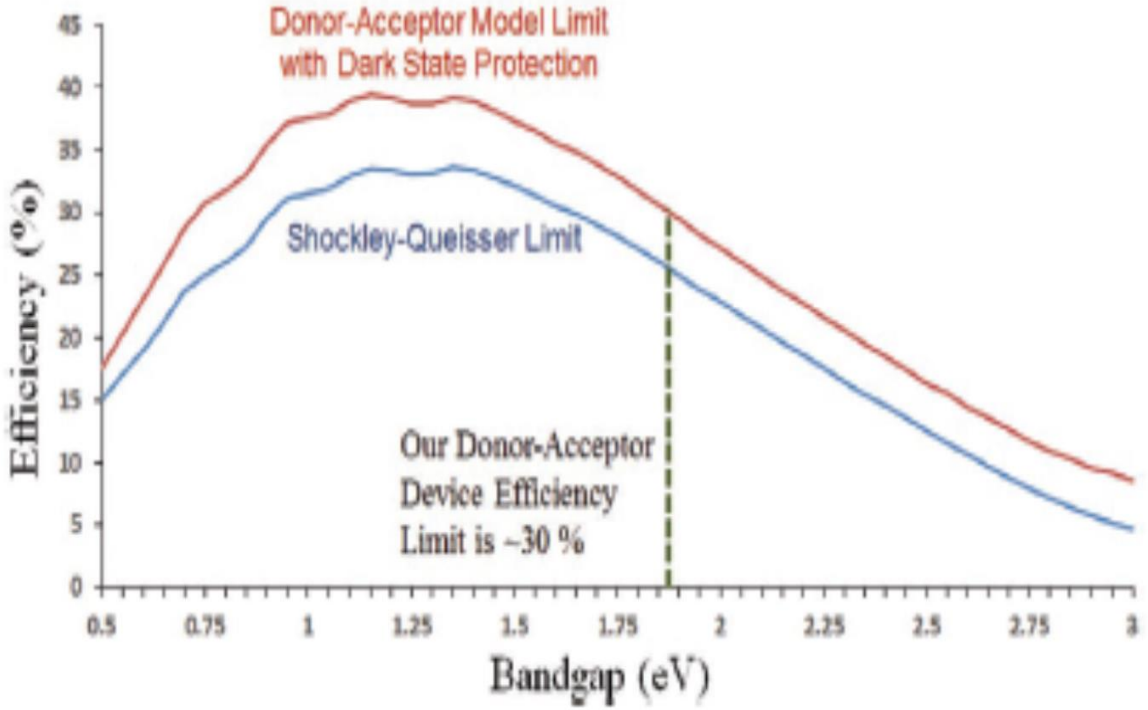
(A) Structure Model



(B) Standard photon-to-electron conversion with donor and acceptor



(C) New bright and dark states arise from strong excitonic coupling due to dipole interactions



Sayan Roy; Zixuan Hu; Sabre Kais; Peter Bermel (ECE-Purdue)

Advanced Functional Materials, 2100387, (2021)

Current / Future work using RBM

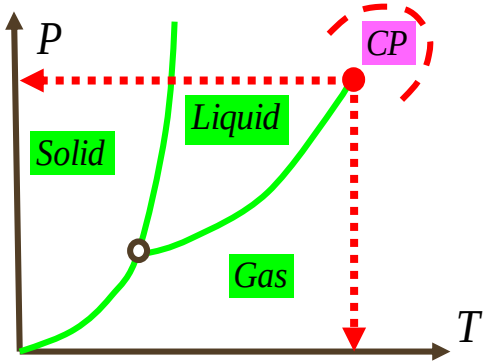
- Reduction of cost of the algorithm
- Band-gap engineering
- Studying energy-splitting like Spin-Orbit coupling
- Quantum phase-transitions using finite size scaling
- Quantum thermodynamics and renormalization group
- Quantum states classifications and tomography (Maximal Entropy Approach)
- Open quantum dynamics and RBM

Quantum Phase Transitions

- **Classical:** Classical phase transitions are driven by thermal energy fluctuations

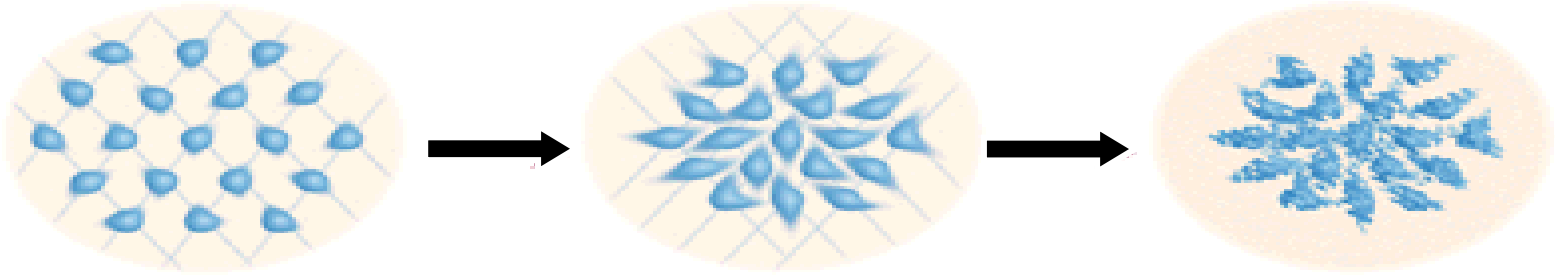
Like the melting of an ice cube:

$$\text{Solid} \rightarrow \text{Liquid} \rightarrow \text{Gas}$$



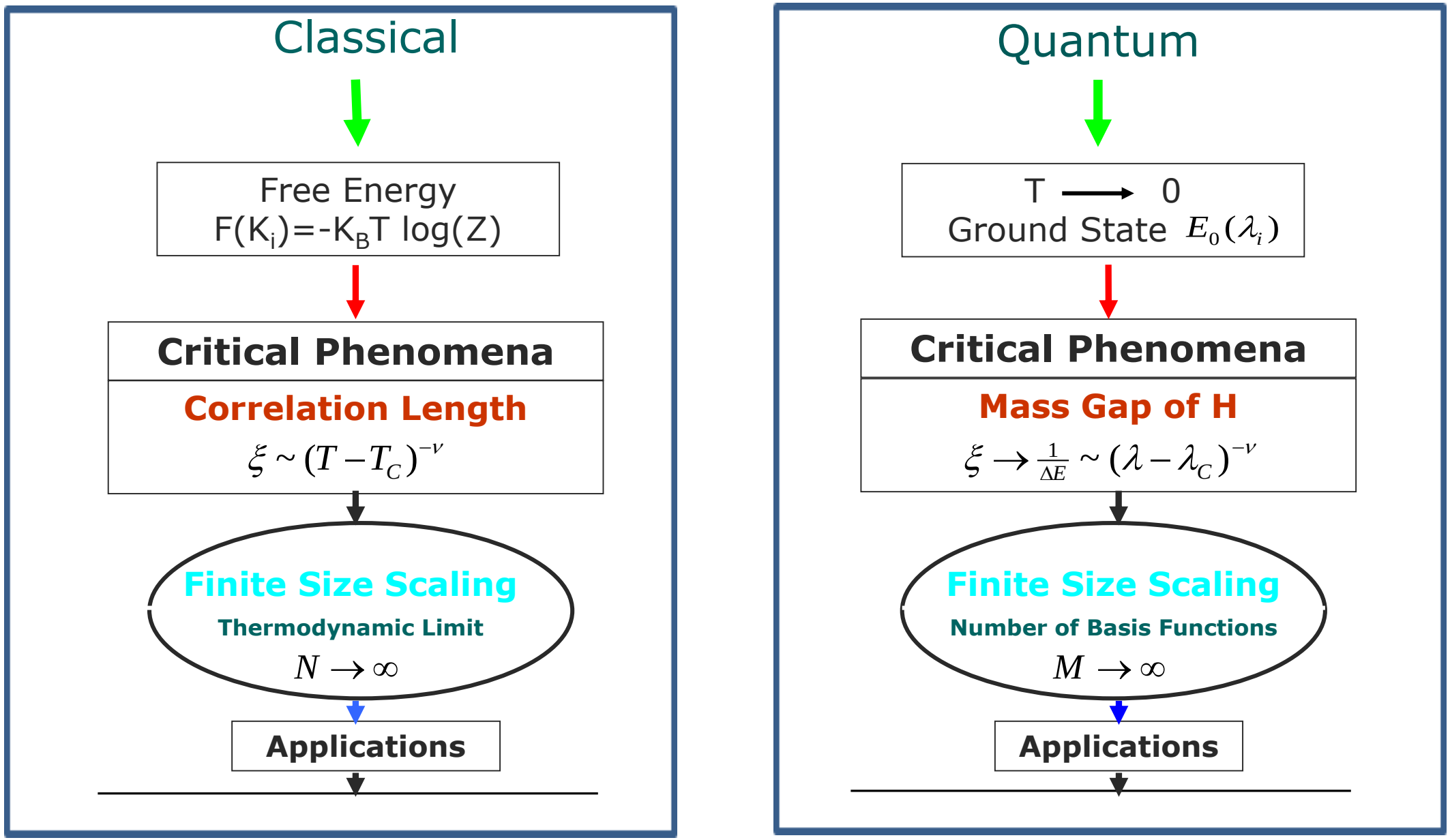
- **Quantum:** Quantum phase transitions, at T=0, are driven by the Heisenberg uncertainty principle

Like the melting of a Wigner crystal: Two dimensional electron layer trapped in a quantum well



$$E_0(\lambda)$$

Statistical Mechanics



In the present approach, the finite size corresponds not to the spatial dimension, as in statistics, but to the number of elements in a complete basis set used to expand the exact eigenfunction of a given Hamiltonian.

Quantum Mechanics

$$\psi = \sum_{n=0}^{\infty} a_n \phi_n \cong \sum_{n=0}^{M} a_n \phi_n$$

(Variational Calculations)

Classical $(N \to \infty)$ $\Leftrightarrow$ Quantum $(M \to \infty)$

Phys. Rev. Letters 79, 3142 (1997)

$$\psi_\lambda^{(N)} = \sum_{n}^{M(N)} a_n^{(N)}(\lambda)\phi_n$$

$$\langle O \rangle_\lambda^{(N)} = \sum_{n,m}^{N} a_n^{(N)}(\lambda)\, a_m^{(N)}(\lambda) O_{n,m}$$

The FSS ansatz

$$\langle O \rangle_\lambda^{(N)} \sim \langle O \rangle_\lambda F_O\left(N|\lambda - \lambda_C|^\nu\right)$$

$$\Delta_O(\lambda; N, N') = \frac{\ln\left(\langle O \rangle_\lambda^{(N)} / \langle O \rangle_\lambda^{(N')}\right)}{\ln(N'/N)}$$

$$\Delta_O(\lambda_C; N, N') = \Delta_O(\lambda_C; N'', N)$$

Finite Size Scaling and Quantum Phase Transitions

$$H(\lambda) = -\frac{1}{2}\nabla^2 - \lambda\frac{e^{-r}}{r}$$

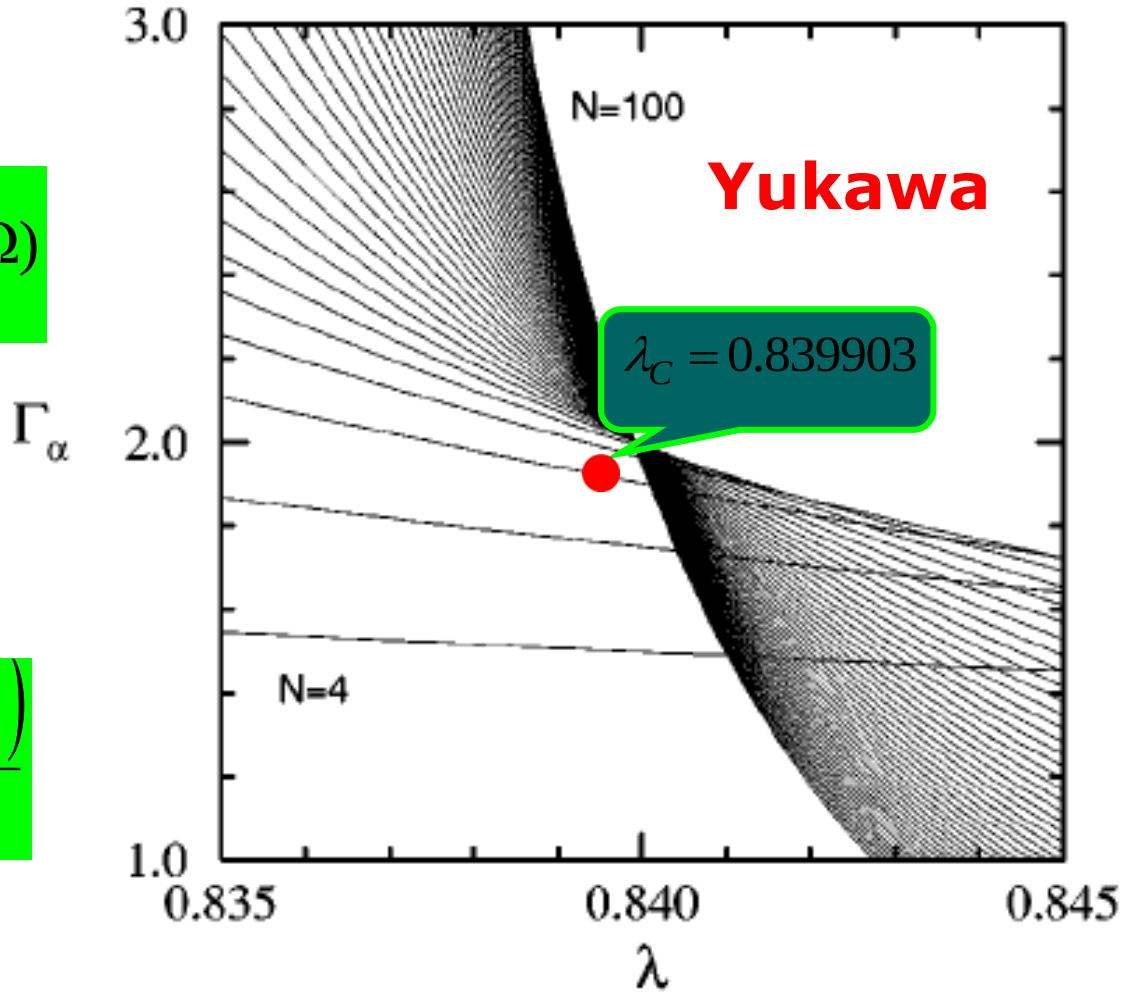
$$\phi_n(r,\Omega) = \frac{1}{\sqrt{(n-l+1)(n-l+2)}} e^{-r/2} L_{n-l}^{(2)}(r) Y_{l,m}(\Omega)$$

$$\Delta_O(\lambda; N, N') = \frac{\ln\left(\langle O\rangle_\lambda^{(N)} / \langle O\rangle_\lambda^{(N')}\right)}{\ln(N'/N)}$$

$$\Gamma_\alpha = \frac{\Delta_H}{\Delta_H - \Delta_{\frac{\partial V}{\partial \lambda}}}$$

$$\Delta_O(\lambda; N, N') = \frac{\ln\left(\langle O\rangle_\lambda^{(N)} / \langle O\rangle_\lambda^{(N')}\right)}{\ln(N'/N)}$$

$$\Delta_O(\lambda_C; N, N') = \Delta_O(\lambda_C; N'', N)$$



Finite Size Scaling for Atomic and Molecular Systems",
Sabre Kais and Pablo Serra
Advances in Chemical Physics, Volume 125, 1-100 (2003)

Juan Pablo Neirotti, Math, Aston University
Pablo Serra, Physics, U. Cordoba

Physical Review Letters, 79, 3142 (1997)

PRL 115, 180404 (2015) PHYSICAL REVIEW LETTERS week ending 30 OCTOBER 2015

Quantum Phase Transition and Universal Dynamics in the Rabi Model

Myung-Joong Hwang, Ricardo Puebla, and Martin B. Plenio
Institut für Theoretische Physik and IQST, Albert-Einstein-Allee 11, Universität Ulm, D-89069 Ulm, Germany
(Received 10 March 2015; revised manuscript received 29 September 2015; published 29 October 2015)

We consider the Rabi Hamiltonian, which exhibits a quantum phase transition (QPT) despite consisting only of a single-mode cavity field and a two-level atom. We prove QPT by deriving an exact solution in the limit where the atomic transition frequency in the unit of the cavity frequency tends to infinity. The effect of

ARTICLE

https://doi.org/10.1038/s41467-021-21425-8 OPEN

Check for updates

Observation of a quantum phase transition in the quantum Rabi model with a single trapped ion

M.-L. Cai[1,4], Z.-D. Liu[1,4], W.-D. Zhao[1,4], Y.-K. Wu[1], Q.-X. Mei[1], Y. Jiang[1], L. He[1], X. Zhang[1,2], Z.-C. Zhou[1,3] & L.-M. Duan[1✉]

Quantum phase transitions (QPTs) are usually associated with many-body systems in the thermodynamic limit when their ground states show abrupt changes at zero temperature with variation of a parameter in the Hamiltonian. Recently it has been realized that a QPT can also occur in a system composed of only a two-level atom and a single-mode bosonic field, described by the quantum Rabi model (QRM). Here we report an experimental demonstration of a QPT in the QRM using a $^{171}Yb^{+}$ ion in a Paul trap. We measure the spin-up state

nature COMMUNICATIONS

Quantum Rabi Model

Bilal Khalid

- Two-level system interacting with a bosonic mode:

$$H = \frac{\Delta}{2}\sigma_z + \omega_0 a^\dagger a - \lambda\sigma_x(a + a^\dagger)$$

- Second order quantum phase transition in the limit $\Delta/\omega_0 \to \infty$.
- For g defined as $g = 2\lambda/\sqrt{\omega_0\Delta}$, there is a phase transition around $g = 1$.
- For $g < 1$, the spin system is frozen in its ground state.
- For $g > 1$, the spin system points along the x-axis and the environment is in a super-radiant phase.

They report an experimental demonstration of a QPT in the QRM using a 171Yb+ ion in a Paul trap.

Quantum Rabi Model

$$H_{\text{Rabi}} = \omega_0 a^\dagger a + \frac{\Omega}{2}\sigma_z - \lambda(a + a^\dagger)\sigma_x$$

$g = \frac{2\lambda}{\sqrt{\omega_0 \Omega}} < 1$

$$H_{np} = \omega_0 a^\dagger a - \frac{\omega_0 g^2}{4}(a + a^\dagger)^2 - \frac{\Omega}{2}$$

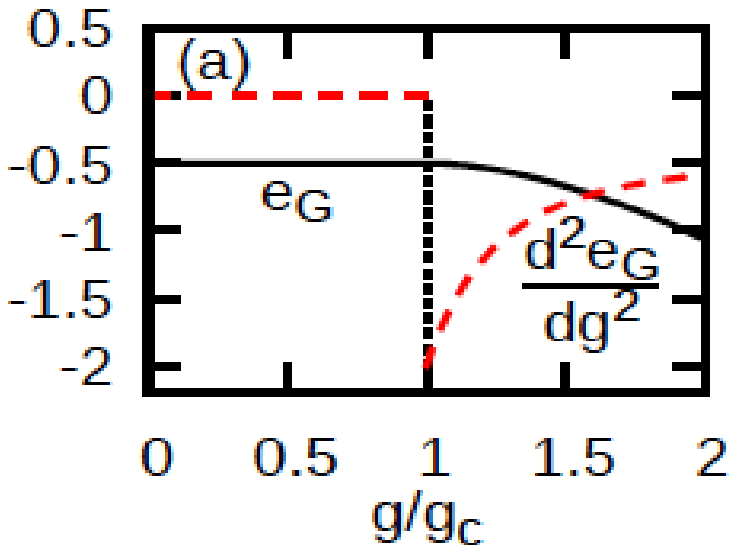
Normal Phase

- Scaled ground state energy:

$$e_G(g) = \frac{\omega_0}{\Omega} E_G(g) = -\frac{\omega_0}{2}$$

- Scaled photon number:

$$n_c = \frac{\omega_0}{\Omega}\langle a^\dagger a\rangle = 0$$



$g = \frac{2\lambda}{\sqrt{\omega_0 \Omega}} > 1$

$$H_{sp} = \omega_0 a^\dagger a - \frac{\omega_0}{4g^4}(a + a^\dagger)^2 - \frac{\Omega}{4}(g^2 + g^{-2})$$

Superradiant Phase

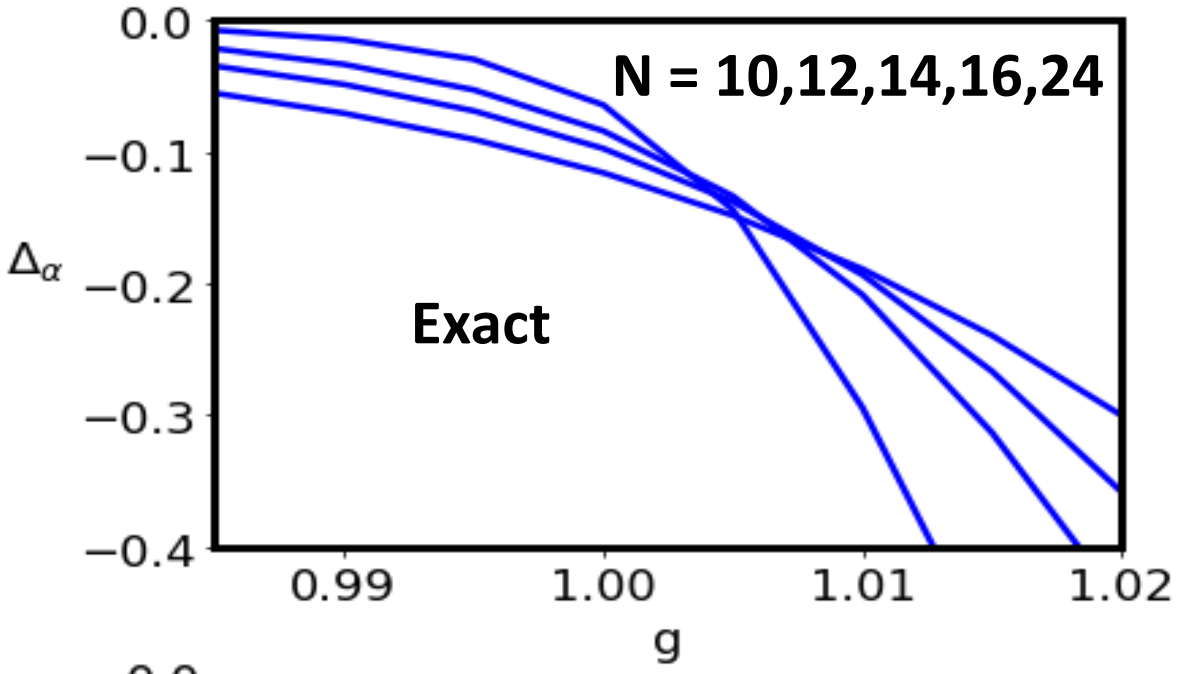
- Scaled ground state energy:

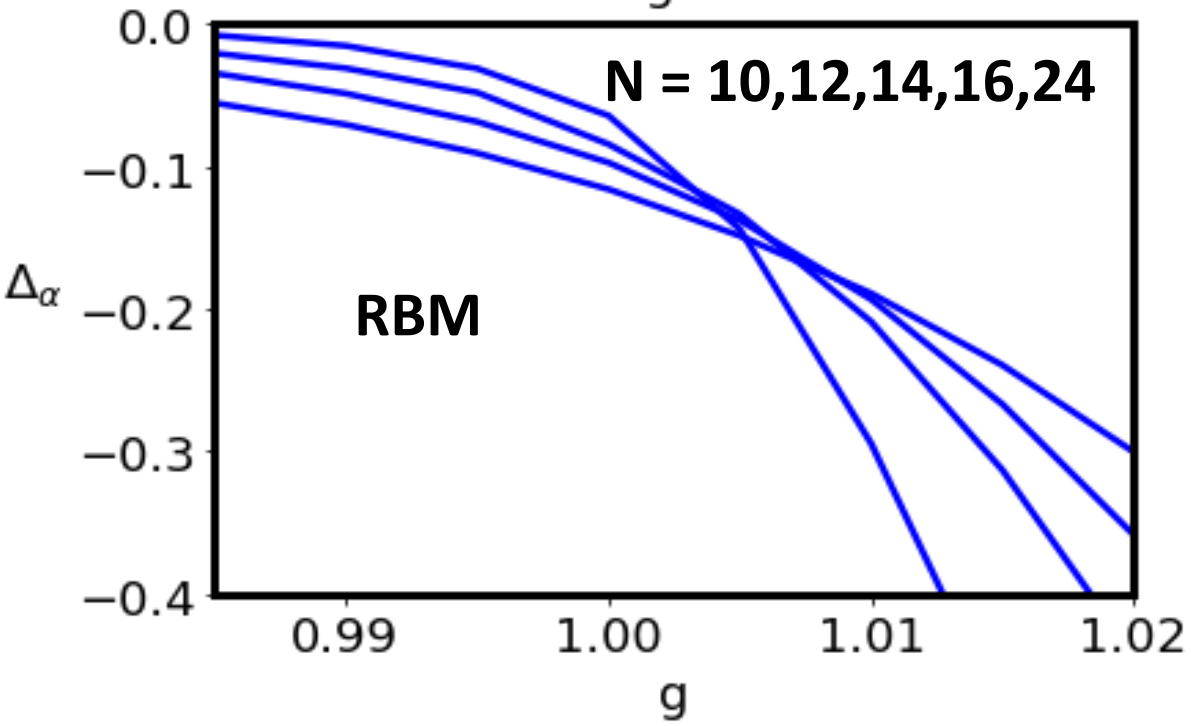
$$e_G(g) = \frac{\omega_0}{\Omega} E_G(g) = -\frac{\omega_0(g^4 + 1)}{4g^2}$$

- Scaled photon number:

$$n_c = \frac{\omega_0}{\Omega}\langle a^\dagger a\rangle = \frac{(g^4 - 1)}{4g^2}$$

Quantum Rabi Model





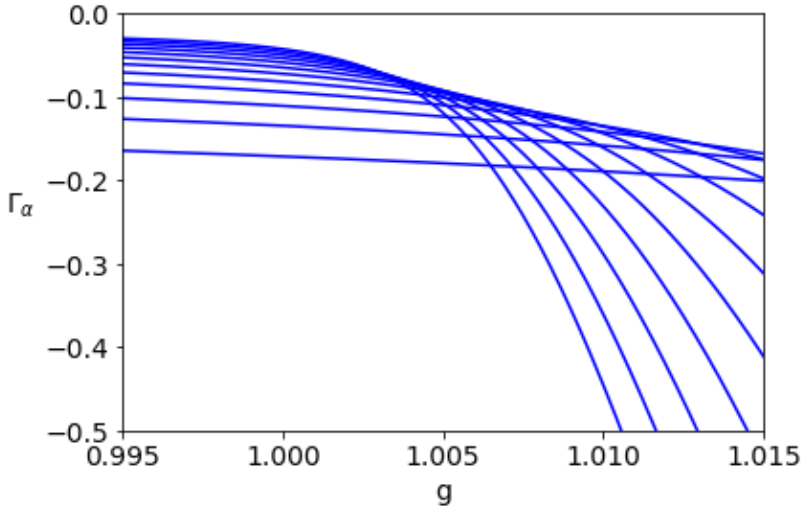
- **Number of qubits:**
  - 4 qubits for visible units (n)
  - 8 qubits for hidden units (m)
  - 12 ancillary qubits (n+m)
- **Number of gates:**
  - 12 single qubit rotations (n+m)
  - 32 Controlled-Controlled rotations (n×m)
  - 192 X (bit-flip) gates (6×n×m)
  - Total ~ 240
- **Number of iterations** = ~ 40,000 for each *g* value

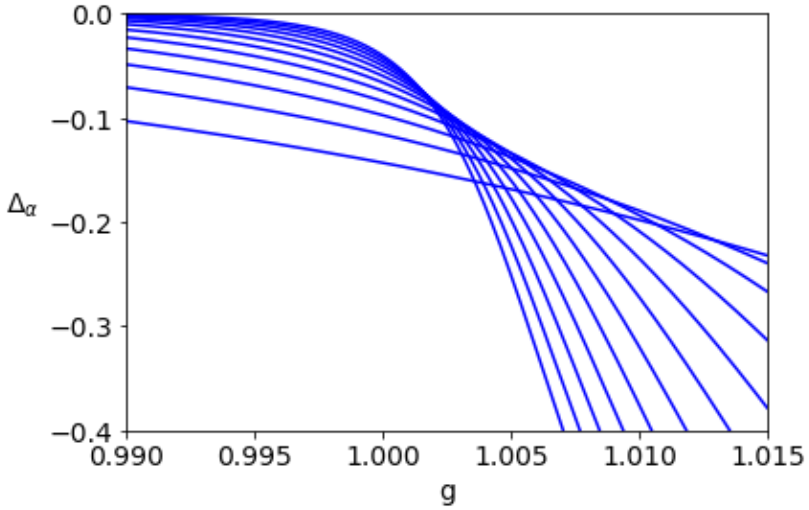
Shree Hari Sureshbabu

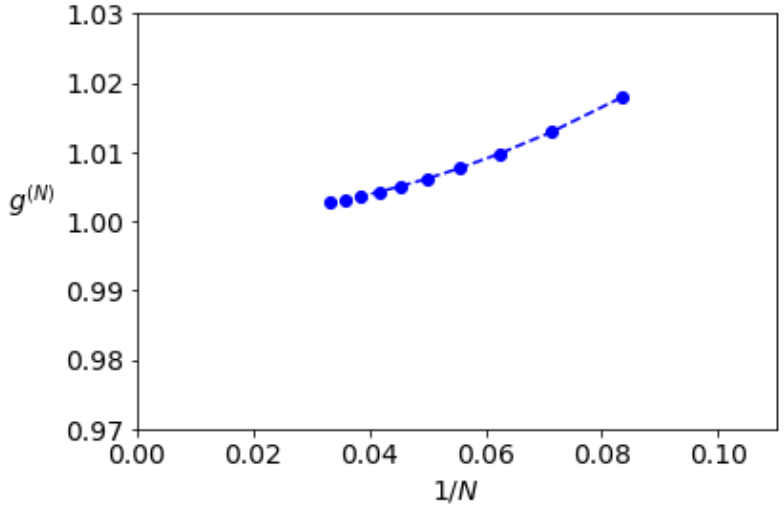
Finite-size scaling

Normal Phase

$$H_{np} = \omega_0 a^\dagger a - \frac{\omega_0 g^2}{4}(a + a^\dagger)^2 - \frac{\Omega}{2}$$





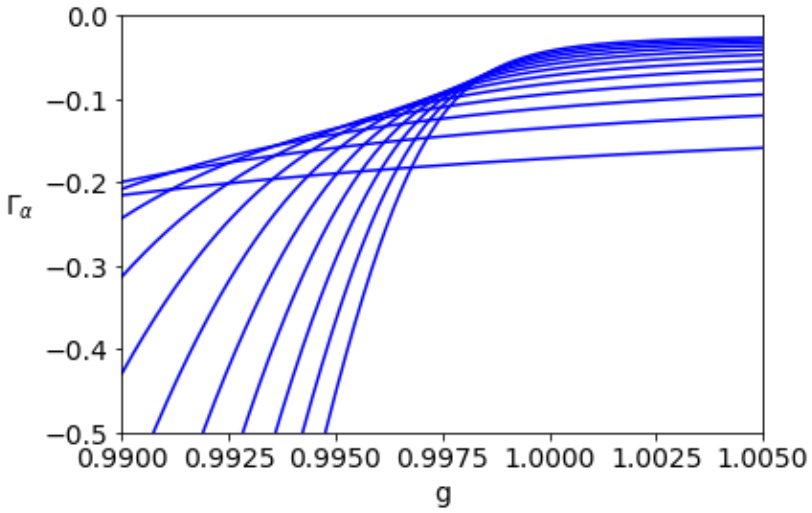


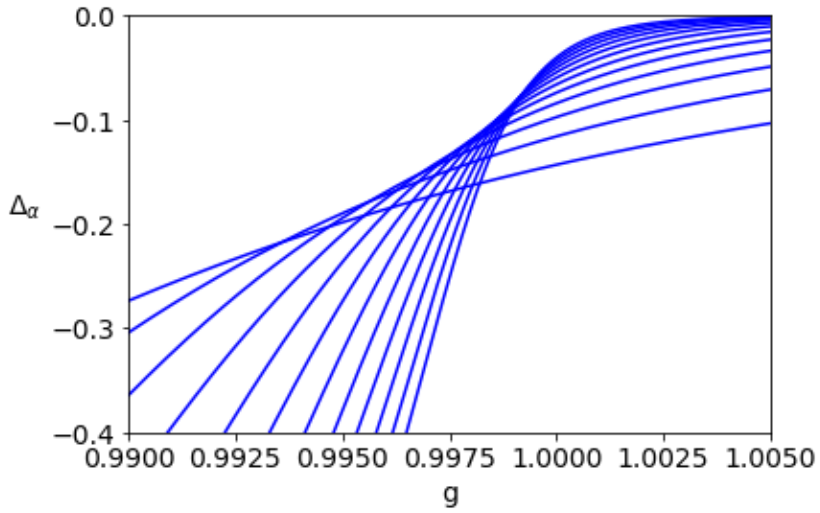
$$g_c = 1.00008$$

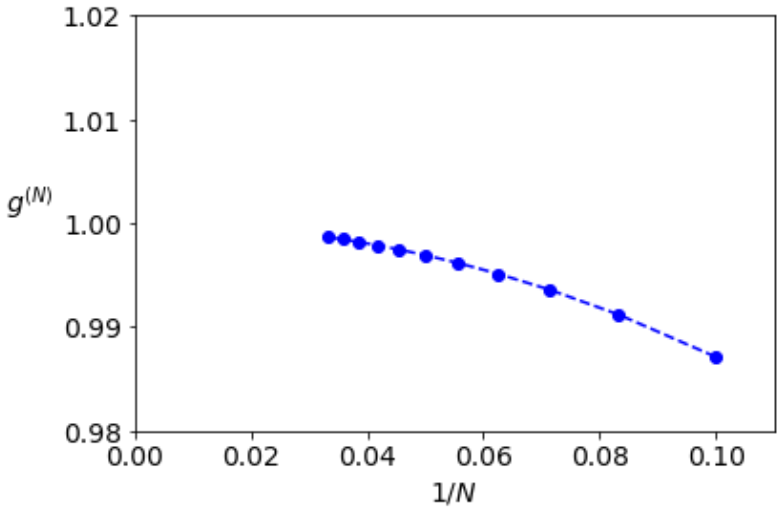
Finite-size scaling

Superrradiant Phase

$$H_{sp} = \omega_0 a^\dagger a - \frac{\omega_0}{4g^4}(a + a^\dagger)^2 - \frac{\Omega}{4}(g^2 + g^{-2}),$$







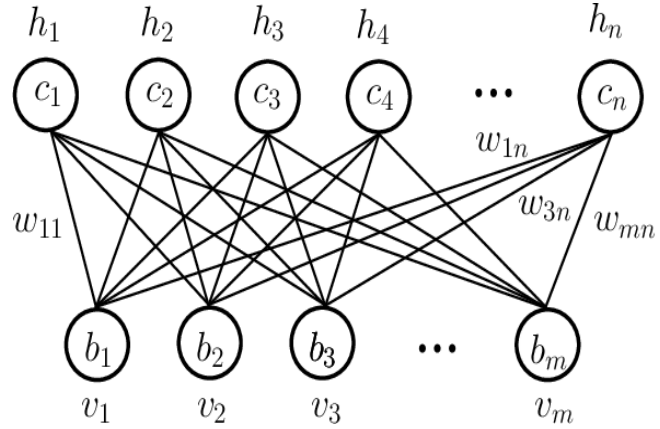
$$g_c = 0.99996$$

Renormalization Group (RG) and Machine Learning

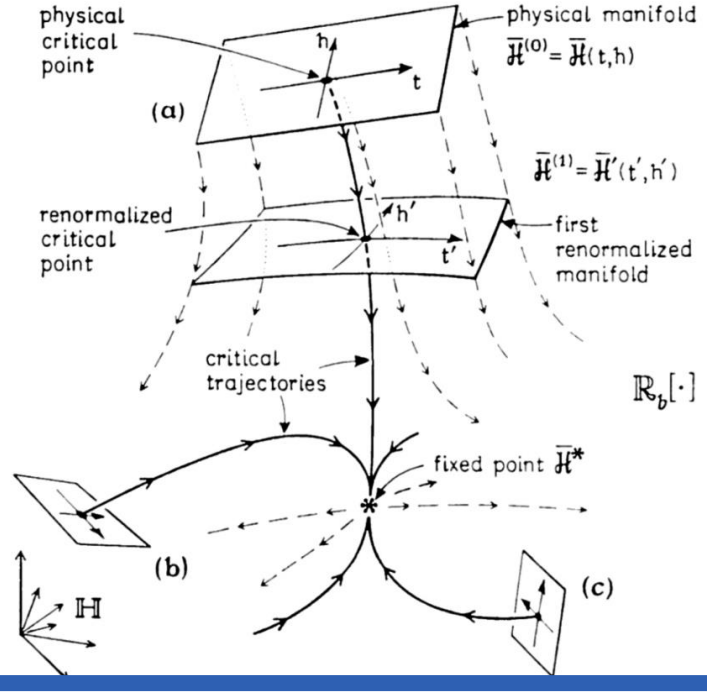
- A good understanding for the powerful representation and classification of neural networks is still missing!
- In physics, RG introduced by Wilson has provided for effective coarse grain descriptions of Hamiltonians
- Maps that retain partition functions are used in RG. Exact mapping to RBM hasn't been solved for beyond one-d Ising chains. The hidden layer in RBM samples coarse description of RG. Approximate solutions are likely to reveal interesting details about learning near critical points in general.
- Relative entropy over the layers of the neural network might provide for a better theoretical understanding about the strengths and limits of neural networks in terms of training time and achievable accuracy for unsupervised learning

Raja Selvarajan

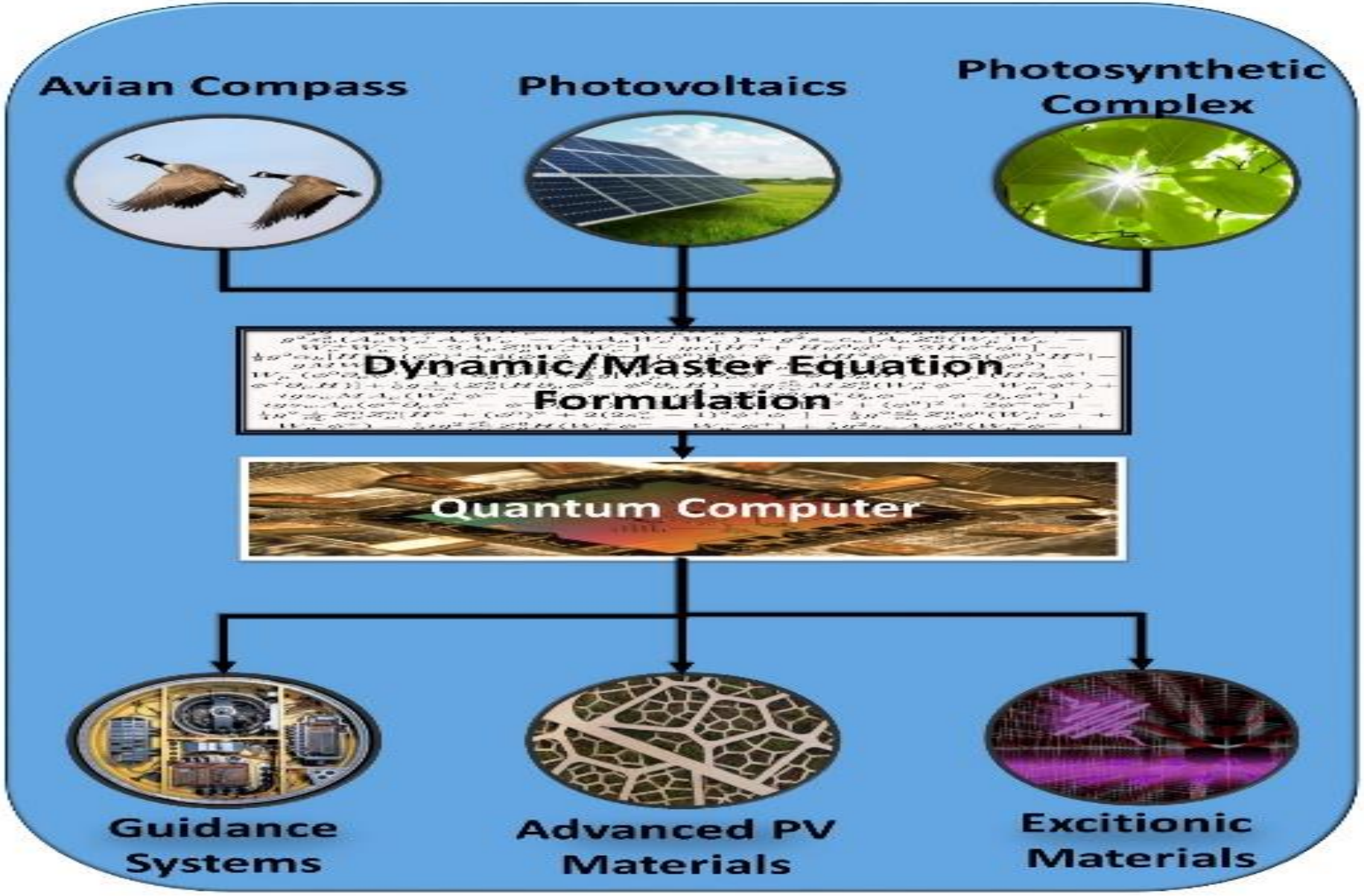
Sangchul Oh

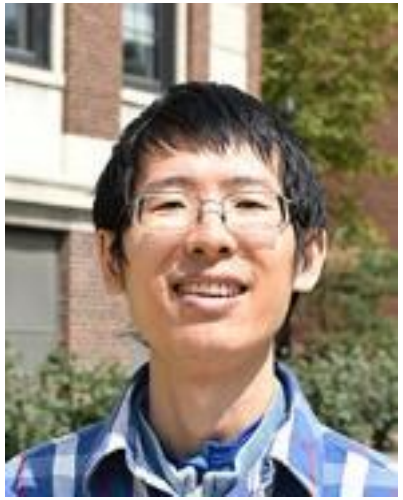


Deep Learning and Renormalization Group Flow



Quantum Computing for Open Quantum Systems





Andrew Hu

A=System of interest B= Bath, Environment,

$$H_{AB} = H_0 + V_{AB}, \qquad \text{where} \qquad H_0 = H_A \otimes 1_B + 1_A \otimes H_B,$$

V_{AB} is the hamiltonian describing the interaction between two parts

Von Neumann Equation

$$i\hbar \frac{d}{dt} \rho_{AB}(t) = [\, H_{AB},\, \rho_{AB}(t)\,],$$

Focusing on the system A

$$\rho_A(t) = \mathrm{Tr}_B\{\rho_{AB}(t)\}.$$

Quantum Master Equation

Unitary Hamiltonian Evolution **Dissipator**

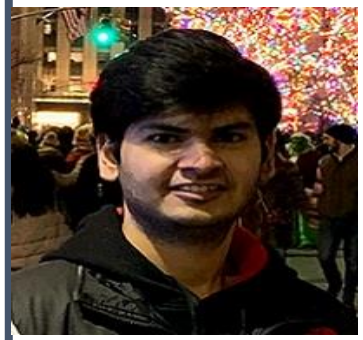
$$\frac{d}{dt}\rho_A(t) = \frac{1}{i\hbar}[H,\, \rho_A(t)] + \sum_{ij} a_{ij}\left(F_i\, \rho_A(t)\, F_j^\dagger - \tfrac{1}{2}[F_j^\dagger F_i,\, \rho_A(t)]_+ \right).$$

$$\dot{\rho}(t) = \mathcal{L}\rho(t) \longrightarrow \rho(t) = \sum_k \rho_k(t) = \sum_k \mathbf{M}_k \rho \mathbf{M}_k^\dagger$$

Kraus Sum Operators

Quantum State Classifications and Tomography

Junxi Li



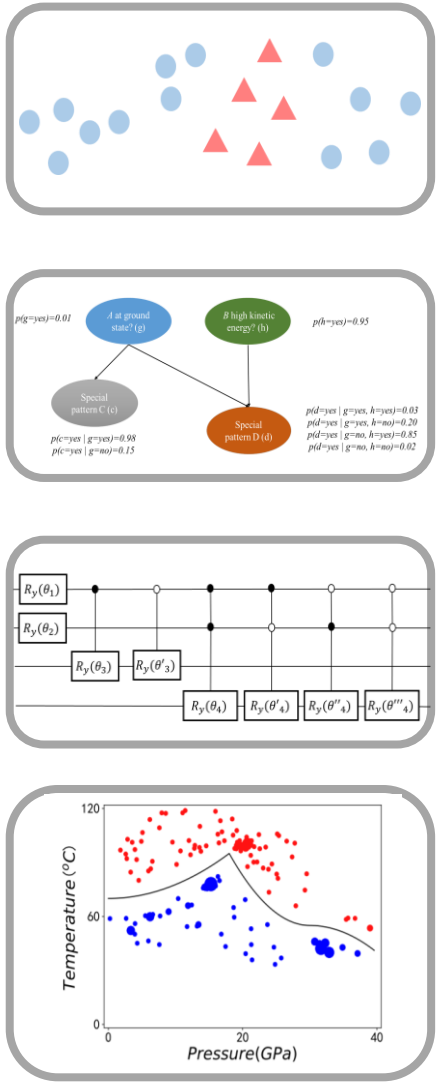
Rishabh Gupta

Sumit Suresh Kale

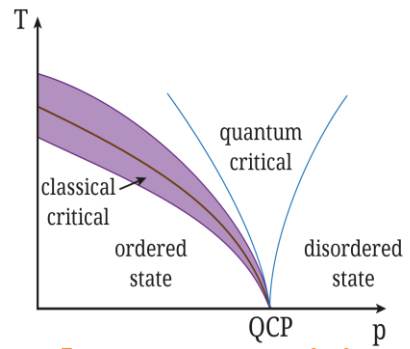
Data Driven

- Quantum Bayesian Network
- Quantum SVM
- Quantum kNN
- ••• •••
- Quantum RBM

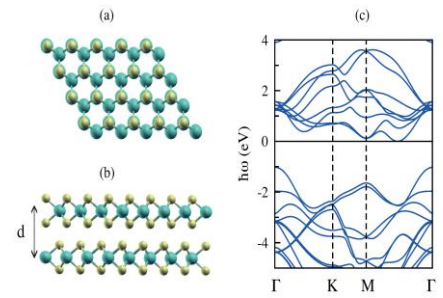
Collect Raw Data → Build Appropriate Model → Implement Quantum Circuit → Reveal Physics



Quantum Simulation → Comparing with Experiment → Predicting Signature → Implement Quantum Circuit → Physics Model



Phase Transition
Classical critical & Quantum critical



Energy Structure

Machine Learning Framework for Quantum Sampling of Highly-Constrained, Continuous Optimization Problems

Blake A. Wilson[1,3,*], Zhaxylyk A. Kudyshev[1,3,*], Alexander V. Kildishev[1], Sabre Kais[2,3], Vladimir M. Shalaev[1,3], and Alexandra Boltasseva[1,3]

[1]School of Electrical and Computer Engineering, Birck Nanotechnology Center and Purdue Quantum Science and Engineering Institute, Purdue University, West Lafayette, IN, USA

[2]School of Chemistry, Purdue University, West Lafayette, IN 47907, USA

[3]The Quantum Science Center (QSC), a National Quantum Information Science Research Center of the U.S. Department of Energy (DOE), Oak Ridge, TN 37931

[*]authors with equal contribution

arXiv:2105.02396, (2021)

Abstract

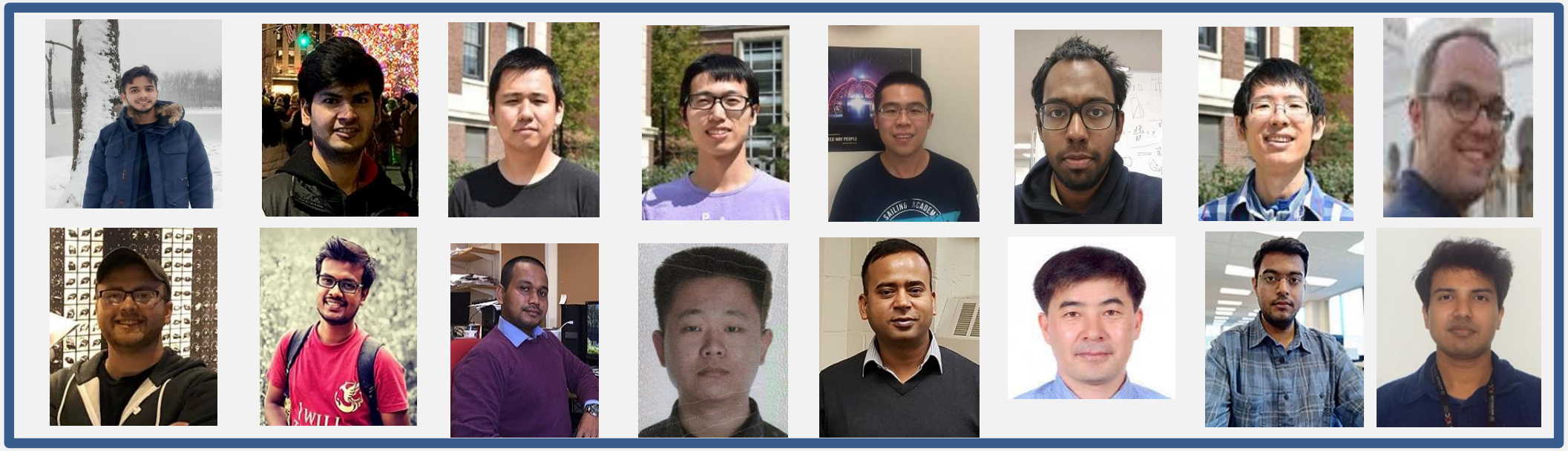
In the recent years, there is a growing interest in using quantum computers for solving combinatorial optimization problems. In this work, we developed a generic, machine learning-based framework for mapping continuous-space inverse design problems into surrogate quadratic unconstrained binary optimization (QUBO) problems by employing a binary variational autoencoder and a factorization machine. The factorization machine is trained as a low-dimensional, binary surrogate model for the continuous design space and sampled using various QUBO samplers. Using the D-Wave Advantage hybrid sampler and simulated annealing, we demonstrate that by repeated resampling and retraining of the factorization machine, our framework finds designs that exhibit figures of merit exceeding those of its training set. We showcase the framework's performance on two inverse design problems by optimizing (i) thermal emitter topologies for thermophotovoltaic applications and (ii) diffractive meta-gratings for highly efficient beam steering. This technique can be further scaled to leverage future developments in quantum optimization to solve advanced inverse design problems for science and engineering applications.

Blake Wilson
ECE-Purdue

Conclusion

- Restricted Boltzmann Machine (RBM) can be used to perform electronic structure calculations (ground and excited States) with chemical accuracy for molecules and materials: **H_2, H_2O, LiH, h-BN, graphene, Molybdenum disulfide(MoS2) and Tungsten disulfide (WS2)**
- The number of qubits required scales as *O(visible=m hidden=n),* the complexity of the gates turns out to be *O(mn)* for one sampling. So, we **have quadratic resource requirements** (circuit width, circuit depth, parameter count). We have a lower bound on the number successful sampling.
- FSS combined with RBM can be used to calculated **quantum critical parameters** and quantum phase transitions.
- We trained the network on various flavors of computation using not only a classical computer, **Qasm** backend quantum simulator in **Qiskit** but also a real **IBMQ machine** (IBM Sydney and IBM Toronto) with the objective to see the performance of the algorithm on actual NISQ devices.
- In all flavors of computation our algorithm demonstrated very high accuracy when compared to the exact values obtained from direct diagonalization.

Quantum Information and Quantum Computating for Complex Chemical Systems



Active Collaborations: Dudley Herschbach and Prineha Narang (Harvard); Raphy Levine (UCLA+FH-Jerusalem); David Mazziotti (U. Chicago); Yong Chen (Purdue); Bretislav Friedrich (FH-Berlin), Ruth Pachter (Air Force), Travis Humble (ORNL), …

https://www.chem.purdue.edu/kais/

Quantum Information and Quantum Computing for Complex Chemical Systems

Funding

Center for Quantum Technologies (CQT) - Purdue University

National Science Foundation-backed Center for Quantum Technologies (CQT) to develop novel quantum technologies to address significant industry challenges.
Purdue (Kais, Director) , IU, IUPUI and ND **https://www.purdue.edu/cqt/**

Phase I: NSF Center for Quantum Dynamics on Modular Quantum Devices (CQD-MQD)
Victor Batista, Michel Devoret (Yale) ; Sabre Kais (Purdue), Eitan Geva (U. Michigan) ; Lea Santos (Yeshiva)

Thank you

kais@purdue.edu