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Towards Optimal Quantum Simulations

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Quantum Simulations



If you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it does not look so easy.

---Richard Feynman, 1982

-conceptual perspectives

- Novel order and phenomena
- Unconventional couplings
- > Unprecedented functionality

-computational perspectives

- > **Precise** phase diagram computation
- Solving difficult problems
- Assisting material/drug design

Optimal Quantum Simulations

- Minimizing simulation time
- Precise calibration of the platform
- Improving the robustness against noise

Using quantum simulations for computational purposes Fundamentally related to computational complexity To make best use of quantum "advantage" or "supremacy"

Towards Universal Quantum Simulations



Universal Quantum Simulator

New physics beyond!!

Quantum Adiabatic Doping

Reference: Jian Lin, Jue Nan, Yuchen Luo, Xiaopeng Li, PRL XXX, XXXX (2019)

Status of OLE



Numerical Challenge:

- Exponential Hilbert space and sign problem; Quantum Monte Carlo simulations fail
- Gapless excitations; Tensor network methods not efficient

Atomic Simulations:

 Cooling, Heating problem, finite lifetime, calibration error, non-universal Rabl, Daley, Cirac, Zoller, Phys. Rev. Lett (2003) Greif, Esslinger et al., Science 340, 1307 (2013) Hart, Hulet et al., Nature 519, 211 (2015) Mazurenko, Greiner et al., Nature 545, 462 (2017)

Adiabatic doping with incommensurate optical lattices

[Jian Lin, Jue Nan, Xingcan Yao, Xiaopeng Li, PRL XXX, XXXX (2019)]

Band insulator with large gap



Potential: $V(x) = V_1 \cos\left(\frac{2\pi}{\lambda}x\right)$ **Filling: two particle per site**

Intermediate incommensurate lattice



$$V(x,t) = \left(1 - \frac{t}{T}\right) V_1 \cos\left(\frac{2\pi}{\lambda}x\right) + \left(\frac{t}{T}\right) V_2 \cos\left(\frac{2\pi}{\lambda v}x\right)$$

Doped lattice



Potential: $V(x) = V_2 \cos\left(\frac{2\pi}{\lambda v}x\right)$ **Filling:** (2 ν) **particle per site**

Half-filling/commensurate case: Trebst, Schollwock, Troyer, Zoller, PRL 96, 250402

Reaching adiabaticity in 1d

[Jian Lin, Jue Nan, Xingcan Yao, Xiaopeng Li, PRL XXX, XXXX (2019)]



Reaching adiabaticity in 1d

[Jian Lin, Jue Nan, Xingcan Yao, Xiaopeng Li, PRL XXX, XXXX (2019)]



Reaching adiabaticity in 2d

[Jian Lin, Jue Nan, Xingcan Yao, Xiaopeng Li, PRL XXX, XXXX (2019)]



Interaction comes to rescue

[Jian Lin, Jue Nan, Xingcan Yao, Xiaopeng Li, PRL XXX, XXXX (2019)]



Interactions make the adiabatic evolution much more efficient

Killing localization leads to an exponential speed up in the quantum simulation

Machine Learning Quantum Algorithms

Reference: Jian Lin, Zhong Yuan Lai, Xiaopeng Li, arXiv 1812.10797 (2018)

Recent advances in deep learning

Image/Speech Recognition

Language Translation

Game/Strategy making



2012 -Beat All Other Image Classification Methods

2014 -Human-level Image Classification

2016 -Human-level Translator on Isolated Sentences

2016 -Superhuman in Go

2019 -Human-level in Strategy Game

Motivation: automated algorithm design

* Algorithm configuration

- **SATEinstein** (Portfolio-based algorithm configuration for SAT) [A.R. Khudabukhsch et al., In Proc. IJCAI, 517-524 (2009)]
- Hydra (Automatically configuring algorithms for portfolio-based selection)
 [L. Xu et al., AAAI conference on artificial intelligence (2010)]
 - **ISAC** (Instance specific algorithm configuration) [S. Kadioglu et al., ECAI 751-756 (2010)]

Super Human intelligence algorithm design?

- Algorithm selection
 - SATzilla (Portfolio-based algorithm selection for SAT) [Lin Xu, F. Hutter, H.H. Hoos, K. Leyton-Brown, J. Artificial Intelligence (2007)]
 - Claspfolio (Portolio-based answer-set programming solver) [H. Hoos, M. Lindauer, T. Schaub, arXiv: 1405.1520 (2014)]

Our goal

AutoQA for development of quantum application design with less expert knowledge

Quantum Adiabatic Algorithm

In adiabatic quantum computing, the Hamiltonian can be written as a time-dependent combination of initial and final Hamiltonians,

$H = s(t/T)H_p + (1 - s(t/T))H_b$

Different choices for the path could lead to algorithms having dramatically **different performance** and even in the complexity scaling.

path
$$s(t/T)$$

Under this framework, the quantum algorithm design corresponds to the optimization of the Hamiltonian path (auto algorithm configuration)

References: Farhi, E. et al. Science 292, 472–475 (2001); Roland, J. et al., Phys. Rev. A 65, 042308 (2002)

Example: Grover Search

Problem: search x which satisfies a certain criterion, say f(x) = 1



Oracle: $U_{\omega}|x\rangle|y\rangle = |x\rangle|y\oplus f(x)\rangle$

But a linear quantum adiabatic algorithm has O(N) complexity

Reinforcement-learning adiabatic algorithm

[Jian Lin, Zhong Yuan Lai, Xiaopeng Li, arXiv 1812.10797 (2018)]

The form of the path :

$$s\left(\frac{t}{T}\right) = \frac{t}{T} + \sum_{m=1}^{C} b^{(m)} \sin(\frac{m\pi t}{T})$$

• Al agent exploration:

Take actions to path state

 $a^{(0)}(\mathbf{b}) = \mathbf{b}$ $[a^{(2m-1)}(\mathbf{b})]_n = b_n - \Delta \delta_{mn}, \ m \ge 1$ $[a^{(2m)}(\mathbf{b})]_n = b_n + \Delta \delta_{mn}$

Sample problem instances and average over certain number of instances

0

Reward:

problem solved

problem unsolved

Problems of our interest: hard to solve, but easy to check, e.g., Grover search, 3-SAT

Modified reinforcement learning

[Jian Lin, Zhong Yuan Lai, Xiaopeng Li, arXiv 1812.10797 (2018)] Action choose processing

 ϵ -greedy strategy

 $1-\epsilon$ choose action randomly

Agent with probability

 ϵ choose corresponding action with max Q

Modified simulation annealing

Acceptance probability function:

$$P(e,T) = \exp(\frac{e}{T})$$

$$e = \frac{Q(\mathbf{b}'|a', b_j + \Delta_0) - Q(\mathbf{b}|a)}{\Delta_0} * \Delta, \Delta \in [0, 0.01]$$

Performance on Grover search



Results for Grover search



Performance on Hard Grover search

[Jian Lin, Zhong Yuan Lai, Xiaopeng Li, arXiv: 1812.10797 (2018)]

Hard Grover Search



t

Scalability

[Jian Lin, Zhong Yuan Lai, Xiaopeng Li, arXiv: 1812.10797 (2018)]



3-SAT problem

Question:

Can you color the teddy bears such that every alien is holding at least one blue hand?

[*from https://math.stackexchange.com]

Formal definition:

A sequence to satisfy $C_1 \wedge C_2 \wedge C_3 \wedge C_4 \wedge C_5 \dots$

$$C = (x_1 \lor x_2 \lor x_3), (\neg x_1 \lor x_2 \lor x_3), \text{ or } ...$$

Hamiltonian encoding:

$$H_P^{\text{SAT}} = -\sum_{i=1}^{N_C} \sum_{\alpha} |\mathbf{q}_i; \mathbf{z}_{i\alpha}\rangle \langle \mathbf{q}_i; \mathbf{z}_{i\alpha}|$$



- All SAT problems
- Max-Cut problem
- Travel salesman problem

▶ ...

To demonstrate near-term quantum supremacy?

Performance on 3-SAT

[Jian Lin, Zhong Yuan Lai, Xiaopeng Li, arXiv: 1812.10797 (2018)]

3-SAT Problem 4 clauses 5 clauses Distribution 6 clauses 0.5 Success Probability **RL-design** 0 0.98 **RL** Algorithm 0 2 **Rescaled Infidelity** Linear Algorithm 0.96 1 **S** 0.5 4 clauses 5 clauses Distribution 0 6 clauses 0.5 t/T0.94 0.5 Linear 2 4 6 **Clause Number** 0 2 0 **Rescaled Infidelity**

Summary & Outlook

- Quantum adiabatic doping with incommensurate optical lattices
- Machine learning enabled automated quantum algorithm design (many open questions)
- > Application of algorithm design to quantum simulations

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Jian Lin, Jue Nan et al., PRL XXX, XXXX (2019)



Jian Lin, Zhong-Yuan Lai et al., arXiv: 1812.10797 (2019)