Qiskit Advocate Mentorship Program

#20

Implement new features and improve documentation in Operators



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Overloading `@` for Operator class



Motivation

To make easier to read the code, overloading `@` and make it work the same as *Operator.dot()*

If you want to get the right multiplied operator,

As is : a.dot(b)

To be : a @ b

Implement argsort and sort method to SparsePauliOp



[SparsePauliOp]

This is a sparse representation of an N-qubit matrix Operator in terms of N-qubit PauliList and complex coefficients.



[Motivation]

PauliList has argosort() method and sort() method .

We need these features in SparcePauliOp .

[Doing]

- 1. Understanding PauliList and SparcePauliOp
- 2. Implementing SparsePauliOp.argsort() and SparcePauliOp.sort()

【ToDo】

- 1. Sending a pull request.
- 2. Development of other issues.

Efficient Evaluation of Observable



Background

Evaluation of observable requires multiple measurement, where commutating observable can be evaluated simultaneously (grouping).

e.g. H = <I@Z> + <X@X> + <I@X> can be evaluated only by calculating <I@Z> and <X@X>





Existing Algorithm

qubit-wide commutation is inspected



Efficient Evaluation of Observable



New Algorithm

General commutating rule is employed

e.g. <X@X> and <Y@Y> are commutating but qubit-wise commutating rule cannot detect.

Impact

Grouping observable reduce the number of required measurement.

Its reduction contributes to **faster** VQE.

Pull Request

→ <u>https://github.com/Qiskit/qiskit-terra/pull/7874</u>

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Molecule	Transformation	Number of Groups		
		No-grouping	Qubit-wide Commutation	General Commutation
LiH	JW	631	136	35
	Parity		165	35
	ВК		211	35
BeH ₂	JW	1150	215	58
	Parity		323	58
	ВК		341	58
H ₂ O	JW	1858	380	84
	Parity		495	82
	ВК		515	82
NH_3	JW	4973	1052	117
	Parity		1091	115
	ВК		1086	115
HCl	JW	4427	906	110
	Parity		1098	112
	ВК		1434	112

*value referenced from Ikko Hamamura and Takashi Imamichi, npj Quant. Info. 6, 56 (2020)





- We are aiming to contribute Qiskit.quantum_info
 - Multiply operator method [a.dot(b) \rightarrow a @ b]
 - Sort Pauli operators
 - Grouping Pauli operator for simultaneous measurement

• Our contributions will appear on github pull-request soon!!



Thank you