SimplifyPaulis

```
SetDirectory @ NotebookDirectory[];
Import["../Link/QuESTlink.m"];
```

QuESTlink: Bug alert! Prior to this version (v0.19), SimplifyPaulis[] contained a bug whereby multiplying X and Z operators (targeting the same qubit) produced a Y operator with an incorrect sign. This bug occurred only when multiplying Pauli strings together, and did not affect other algebraic forms (like summing or exponentiation), though did affect the downstream function CalcPauliExpressionMatrix[]. Please check any previous calculations which passed products of Pauli–strings to SimplifyPaulis[] and CalcPauliExpressionMatrix[]. We sincerely apologise for any arising issues! Silence this warning using Quiet[].

Doc

```
? SimplifyPaulis
```

Symbol

SimplifyPaulis[expr] freezes commutation and analytically simplifies the given expression of Pauli operators, and expands it in the Pauli basis. The input expression can include sums, products, non–commuting products, and powers (with nonzero integer exponents) of (subscripted) Id, X, Y and Z operators and other Mathematica symbols (including variables defined as Pauli expressions, and functions thereof).

Be careful of performing algebra with Pauli operators outside of SimplifyPaulis[], since Mathematica may erroneously automatically commute them.

Correctness

```
SetAttributes[evalExprAsMatrix, HoldAll]
SetAttributes[test, HoldAll]

pauliOpToMatrix[p_{q_},n_] := KroneckerProduct @@ ReplaceAll[
    {IdentityMatrix[2^{n-q-1}], PauliMatrix[p/.{Id→0,X→1,Y→2,Z→3}], IdentityMatrix[2^{q}]},
    {{1}} → Nothing] /. KroneckerProduct[m_] :→ m // Quiet

evalExprAsMatrix[expr_] := (With[
    {numQb = 1 + Max @ Cases[Unevaluated[expr], (Id|X|Y|Z)_{q_Integer}:→q, {0,Infinity}]},
    Hold[expr]
        (* replace auto-commuting Times with non-commuting matrix-multiply (Dot) *)
        /. Times → Dot
        (* replace element-wise powers with matrix exponentiation *)
        //. Power[b_, n_Integer?NonNegative] :→ MatrixPower[b,n]
        (* replace every Pauli operator with full-state matrix *)
        /. σ:(Id|X|Y|Z)_{_Integer} :→ pauliOpToMatrix[σ,numQb]
        (* remove scalars from Dots with (functions of) matrices; preserve matrix orde
        //. Dot[a___?(FreeQ[#,List]&), m__?(Not@FreeQ[#,List]&), b___?(FreeQ[#,List]&)
            /; (Length@{a,b}>0) :→ Times[a,b] Dot[m,r]
        (* perform evaluation of matrix multiplications *)
        // ReleaseHold]
        (* restore Times of any remaining scalars *)
        /. Dot → Times
        (* restore MatrixPower of scalars to scalar exponent *)
        /. MatrixPower[a_,b_] :→ a^b)

test[expr_] := Module[
    {out, matrOut, matrEval, error},
    out = SimplifyPaulis[expr];
    matrOut = CalcPauliExpressionMatrix[out];
    matrEval = evalExprAsMatrix[expr];
    error = matrOut - matrEval // Abs // Max // Simplify;
    Echo[out, "output: "];
    Echo[error, "error: "];
    If[error =!= 0, Style["ERRONEOUS SIMPLIFICATION!", Red]]
]
```

Stable expressions

```
test[X_{4}]
```

» output: X_4

» error: 0

test[a X_4 a]

» output: $a^2 X_4$

» error: 0

test[a X_0 b Y_1 + c]

» output: $c + a\, b\, X_0\, Y_1$

» error: 0

test[a X_0 Y_1 + b Z_0 Z_1 Z_2 – Id_2]

» output: $-Id_2 + a\, X_0\, Y_1 + b\, Z_0\, Z_1\, Z_2$

» error: 0

Products

test[X_0 Y_0]
test[Y_0 X_0]

» output: $i\, Z_0$

» error: 0

» output: $-i\, Z_0$

» error: 0

test[Z_2 X_2]
test[X_2 Z_2]

» output: $i\, Y_2$

» error: 0

» output: $-i\, Y_2$

» error: 0

test[Y_0 Z_0]
test[Z_0 Y_0]

» output: $i\, X_0$

» error: 0

» output: $-i\, X_0$

» error: 0

test[Id_0 X_0]

» output: X_0

» error: 0

test[Id_2 X_4]

» output: X_4

» error: 0

SimplifyPaulis[X_0 Id_{10}]

X_0

test[$X_0\ X_0$]

test[$Y_0\ Y_0$]

test[$Z_0\ Z_0$]

» output: Id_0

» error: 0

» output: Id_0

» error: 0

» output: Id_0

» error: 0

test[$a\ X_0\ b\ Y_0\ Z_0\ X_0\ c\ X_0\ X_0$]

» output: ⅈ $a\ b\ c\ X_0$

» error: 0

test[$X_0\ X_1\ Y_0\ Y_1$]

» output: $-Z_0\ Z_1$

» error: 0

Sums

test[$a\ X_0 + Y_0 + Z_0 + b\ X_0$]

» output: $(a+b)\ X_0 + Y_0 + Z_0$

» error: 0

test[$a\ (X_0 + Y_0) - b\ (X_0 + Z_0) + c\ (Y_0 + Z_0)$]

» output: $(a-b)\ X_0 + (a+c)\ Y_0 + (-b+c)\ Z_0$

» error: 0

test[$X_0\ Y_1 + Y_1\ X_0$]

» output: $2\ X_0\ Y_1$

» error: 0

Powers

SimplifyPaulis[$(X_0\ Y_0\ Z_0)^0$]

1

test[$\text{Id}_0{}^3$]

» output: Id_0

» error: 0

test[$X_0{}^2$]

test[$Y_0{}^2$]

test[$Z_0{}^2$]

» output: Id_0

» error: 0

» output: Id_0

» error: 0

» output: Id_0

» error: 0

$\mathrm{test}[X_0{}^5]$
$\mathrm{test}[Y_0{}^5]$
$\mathrm{test}[Z_0{}^5]$

» output: X_0

» error: 0

» output: Y_0

» error: 0

» output: Z_0

» error: 0

$\mathrm{test}[(a\,X_0\,)^3]$

» output: $a^3\,X_0$

» error: 0

$\mathrm{test}\left[\left(a\,X_0\,Y_0{}^2\right)^3\right]$

» output: $a^3\,X_0$

» error: 0

$\mathrm{test}\left[\left(a\,X_2\,Y_1{}^2\right)^3\right]$

» output: $a^3\,X_2$

» error: 0

$\mathrm{test}[(a\,X_0\,b\,Y_0\,c\,Z_0\,Z_1\,Z_2)^3]$

» output: $-i\,a^3\,b^3\,c^3\,Z_1\,Z_2$

» error: 0

Expressions

$\mathrm{test}[(a\,X_0\;+\;b\,X_0\,c\,Y_1\,d\,Z_2)^3\;(f\,X_0+e\,Y_0)]$

» output: $a\left(a^2+3\,b^2\,c^2\,d^2\right)\,f\,\mathrm{Id}_0+i\,a\left(a^2+3\,b^2\,c^2\,d^2\right)\,e\,Z_0+$
$b\,c\,d\left(3\,a^2+b^2\,c^2\,d^2\right)\,f\,Y_1\,Z_2+i\,b\,c\,d\left(3\,a^2+b^2\,c^2\,d^2\right)\,e\,Y_1\,Z_0\,Z_2$

» error: 0

$\mathrm{test}\left[\left((Y_0+c\,Y_1)^3\;(X_0+X_1)\right)^2\right]$

» output: 0

» error: 0

$$\texttt{test}\left[\left((a\,X_0\ +\ b\,X_0\,c\,Y_1\,d\,Z_2)^3\,h^3\ (f\,X_0+e\,Y_0)\right)^3\right]$$

» output: $a\left(a^2+3\,b^2\,c^2\,d^2\right)\,f$
$\left(-3\,b^6\,c^6\,d^6\,e^2+9\,a^2\,b^4\,c^4\,d^4\left(-5\,e^2+f^2\right)+a^6\left(-3\,e^2+f^2\right)+3\,a^4\,b^2\,c^2\,d^2\left(-15\,e^2+2\,f^2\right)\right)\,h^9\,\text{Id}_0+$
$3\,a\left(a^2+3\,b^2\,c^2\,d^2\right)\left(3\,a^2\,b\,c\,d+b^3\,c^3\,d^3\right)^2\,f\left(-2\,e^2+f^2\right)\,h^9\,\text{Id}_2-$
$\mathbb{i}\,a\left(a^2+3\,b^2\,c^2\,d^2\right)\left(a^6+33\,a^4\,b^2\,c^2\,d^2+27\,a^2\,b^4\,c^4\,d^4+3\,b^6\,c^6\,d^6\right)\,e\left(e^2-3\,f^2\right)\,h^9\,Z_0+$
$b\,c\,d\left(3\,a^2+b^2\,c^2\,d^2\right)\left(3\,a^6+27\,a^4\,b^2\,c^2\,d^2+33\,a^2\,b^4\,c^4\,d^4+b^6\,c^6\,d^6\right)\,f\left(-3\,e^2+f^2\right)\,h^9\,Y_1\,Z_2-$
$\mathbb{i}\,b\,c\,d\left(3\,a^2+b^2\,c^2\,d^2\right)\left(3\,a^6+27\,a^4\,b^2\,c^2\,d^2+33\,a^2\,b^4\,c^4\,d^4+b^6\,c^6\,d^6\right)\,e\left(e^2-3\,f^2\right)\,h^9\,Y_1\,Z_0\,Z_2$

» error: 0

Variables and functions

$$\texttt{myPauli}\ =\ X_0\,Y_1\,Z_2\ +\ a\,X_0\,Z_1;$$
$$\texttt{myFunc[x\_]}\ :=\ b\,x^2+X_0$$
$$\texttt{out1}\ =\ \texttt{SimplifyPaulis}\left[X_0\ \texttt{myFunc}[\texttt{myPauli}]\ Y_0\ +\ a\left(Y_0-\texttt{myFunc}\left[\texttt{myPauli}^2\right]^2\right)^3\right]$$

$$a\left(-4-17\left(1+a^2\right)^4 b^2-13\left(1+a^2\right)^8 b^4\right)\text{Id}_0+a^3\left(-2-a^2\right)\left(1+a^2\right)^2 b^2\left(1+\left(1+a^2\right)^4 b^2\right)^2\text{Id}_1-$$
$$a\left(1+a^2\right)^2 b^2\left(1+\left(1+a^2\right)^4 b^2\right)^2\text{Id}_2+2\,a\left(1+a^2\right)^2 b\left(-4-10\left(1+a^2\right)^4 b^2-3\left(1+a^2\right)^8 b^4\right)X_0+$$
$$\left(1+a\left(4+10\left(1+a^2\right)^4 b^2+3\left(1+a^2\right)^8 b^4\right)\right)Y_0+\mathbb{i}\left(1+a^2\right)b\,Z_0$$

$$\texttt{out2}\ =\ \texttt{SimplifyPaulis}\Big[$$
$$X_0\ \left(b\ (X_0\,Y_1\,Z_2\ +\ a\,X_0\,Z_1)^2\ +\ X_0\right)\,Y_0\ +\ a\left(Y_0-\left(b\ (X_0\,Y_1\,Z_2\ +\ a\,X_0\,Z_1)^4+X_0\right)^2\right)^3\Big]$$

$$a\left(-4-17\left(1+a^2\right)^4 b^2-13\left(1+a^2\right)^8 b^4\right)\text{Id}_0+a^3\left(-2-a^2\right)\left(1+a^2\right)^2 b^2\left(1+\left(1+a^2\right)^4 b^2\right)^2\text{Id}_1-$$
$$a\left(1+a^2\right)^2 b^2\left(1+\left(1+a^2\right)^4 b^2\right)^2\text{Id}_2+2\,a\left(1+a^2\right)^2 b\left(-4-10\left(1+a^2\right)^4 b^2-3\left(1+a^2\right)^8 b^4\right)X_0+$$
$$\left(1+a\left(4+10\left(1+a^2\right)^4 b^2+3\left(1+a^2\right)^8 b^4\right)\right)Y_0+\mathbb{i}\left(1+a^2\right)b\,Z_0$$

$$\texttt{out1}-\texttt{out2}$$

0

Scalars

$$\texttt{SimplifyPaulis}[a\,X_0+a]$$
$$\texttt{SimplifyPaulis}[a\,X_0\,X_0\ +\ a]$$

$a+a\,X_0$

$a+a\,\text{Id}_0$

Errors

$\texttt{SimplifyPaulis}\left[(X_2 + Y_1\, Y_0)^{2.1}\, X_0 - 2\, X_0\right]$

SimplifyPaulis: Input contained the following sub–expression of Pauli operators which could not be simplified: $(X_2 + Y_0\, Y_1)^{2.1}$

$\texttt{SimplifyPaulis}[1 / X_0]$

SimplifyPaulis: Input contained the following sub–expression of Pauli operators which could not be simplified: $\frac{1}{X_0}$

$\texttt{SimplifyPaulis}\left[\mathrm{Id}_0^{3.5}\right]$

SimplifyPaulis: Input contained the following sub–expression of Pauli operators which could not be simplified: $\mathrm{Id}_0^{3.5}$

$\texttt{SimplifyPaulis}\left[\texttt{f@}\ \sqrt{X_0 - Y_2}\right]$

SimplifyPaulis: Input contained the following sub–expression of Pauli operators which could not be simplified: $f\left[\sqrt{X_0 - Y_2}\right]$

$\texttt{myvar = } X_0\texttt{;}$
$\texttt{SimplifyPaulis[f[myvar] + 2]}$

SimplifyPaulis: Input contained the following sub–expression of Pauli operators which could not be simplified: $f[X_0]$

```
SimplifyPaulis[a, b]
```

SimplifyPaulis: Invalid arguments. See ?SimplifyPaulis

```
$Failed
```

Downstream

$\texttt{CalcPauliExpressionMatrix}\left[\,(X_0 + Y_0)^{-1.4}\right]$

SimplifyPaulis: Input contained the following sub–expression of Pauli operators which could not be simplified:

$$\frac{1}{(X_0 + Y_0)^{1.4}}$$

$\texttt{CalcPauliExpressionMatrix[}\ X_0 + \texttt{Sqrt[}X_0 + Y_0\texttt{]}\texttt{, 10]}$

SimplifyPaulis: Input contained the following sub–expression of Pauli operators which could not be simplified: $\sqrt{X_0 + Y_0}$