Real-time simulation

This notebook introduces quantum simulation, and explores simulating the real-time dynamics of a spin-ring Ising system. We demonstrate classical analytic and numerical treatments, then study Trotterisation in the absence and presence of decoherence.

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```
Import["https://qtechtheory.org/questlink.m"];
CreateDownloadedQuESTEnv[];
```

Analytic

In quantum simulation, we are interested in studying the properties of a time-dependent state $|\psi(t)\rangle$ as it evolves according to the physics of some Hamiltonian \hat{H} . Consider this arbitrary 3-qubit Hamiltonian specified in the Pauli basis:

```
nQb = 3;
h = X<sub>0</sub> Y<sub>1</sub> + 2 Y<sub>2</sub> Z<sub>0</sub> - 3 Z<sub>0</sub> Z<sub>1</sub> Z<sub>2</sub>;
hMatr = CalcPauliExpressionMatrix[h]
SparseArray
Specified elements: 24
Dimensions: {8, 8}
```

We'll study the evolution of $|\psi(t)\rangle$ from initial state $|\psi(0)\rangle = |0\rangle$ initial state.

```
\psi 0 = \text{UnitVector}[2^{\text{nQb}}, 1]
{1, 0, 0, 0, 0, 0, 0, 0}
```

One way to obtain the future states $\mid \psi(t)
angle$ is to numerically solve the Schrödinger equation:

$$\bar{i} \frac{d}{dt} \left| \psi(t) \right\rangle = \hat{H} \left| \psi(0) \right\rangle$$

NDSolve[{
$$i \psi$$
'[t] == hMatr. ψ [t], ψ [0] == ψ 0}, ψ , {t, 0, 4}]; ψ = %[1, 1, 2]

InterpolatingFunction Domain: {{0., 4.}}
Output dimensions: {8}

 $\psi[0]$ // Chop

 $\{1., 0, 0, 0, 0, 0, 0, 0, 0\}$

 ψ [.3] // Chop

 $\{0.444122 + 0.700796 i, 0, 0, 0.170249 + 0.216967 i, 0.483035, 0, 0, 0. - 0.0475127 i\}$

We could instead obtain an analytic expression for $|\psi(t)\rangle = \hat{U}(t) |\psi(0)\rangle$ by symbolically constructing the unitary time evolution operator $\hat{U}(t) = e^{-it\hat{H}}$

u[t_] = MatrixExp[-itCalcPauliExpressionMatrix[h]];

MatrixForm@u[t]

We can then obtain analytic expressions for the Z-basis amplitudes of $|\psi(t)\rangle$ as functions of t

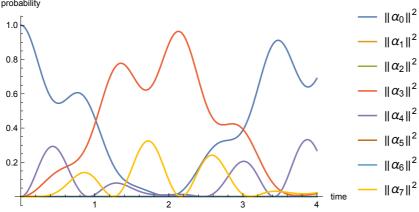
Clear[#]

$$\psi[t] = u[t] \cdot \psi0$$
 // Simplify

$$\begin{split} &\left\{\frac{1}{20} \, \left(10 \, \mathsf{Cos} \big[2 \, \sqrt{2} \, \, \mathsf{t} \big] + 10 \, \mathsf{Cos} \big[2 \, \sqrt{5} \, \, \mathsf{t} \big] + 5 \, \mathrm{i} \, \sqrt{2} \, \mathsf{Sin} \big[2 \, \sqrt{2} \, \, \mathsf{t} \big] + 4 \, \mathrm{i} \, \sqrt{5} \, \mathsf{Sin} \big[2 \, \sqrt{5} \, \, \mathsf{t} \big] \right), \, 0 \, , \, 0 \, , \\ &\frac{1}{20} \, \left(10 \, \mathrm{i} \, \mathsf{Cos} \big[2 \, \sqrt{2} \, \, \mathsf{t} \big] - 10 \, \mathrm{i} \, \mathsf{Cos} \big[2 \, \sqrt{5} \, \, \mathsf{t} \big] - 5 \, \sqrt{2} \, \mathsf{Sin} \big[2 \, \sqrt{2} \, \, \mathsf{t} \big] + 4 \, \sqrt{5} \, \mathsf{Sin} \big[2 \, \sqrt{5} \, \, \mathsf{t} \big] \right), \\ &\frac{1}{20} \, \left(5 \, \sqrt{2} \, \mathsf{Sin} \big[2 \, \sqrt{2} \, \, \mathsf{t} \big] + 2 \, \sqrt{5} \, \mathsf{Sin} \big[2 \, \sqrt{5} \, \, \mathsf{t} \big] \right), \, 0 \, , \\ &0 \, , \, -\frac{1}{20} \, \, \mathrm{i} \, \left(5 \, \sqrt{2} \, \mathsf{Sin} \big[2 \, \sqrt{2} \, \, \mathsf{t} \big] - 2 \, \sqrt{5} \, \mathsf{Sin} \big[2 \, \sqrt{5} \, \, \mathsf{t} \big] \right) \right\} \end{split}$$

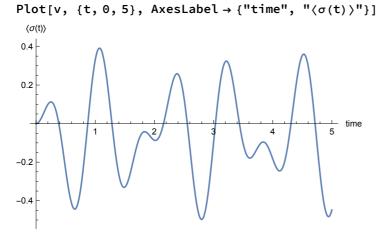
Here's how the probability of the basis states, with amplitudes α_i , evolve from $\delta_{i,0}$

```
probs = Abs[u[t] \cdot \psi 0]^2;
Plot[probs, {t, 0, 4},
       PlotRange → All,
       AxesLabel → {"time", "probability"},
       PlotLegends \rightarrow Table [Norm[\alpha_i]<sup>2</sup>, {i, 0, 2<sup>nQb</sup> - 1}]]
probability
```



In quantum simulation, we are more often interested in the time evolution of the expectation value of some observable $\langle \sigma(t) \rangle = \langle \psi(t) | \hat{\sigma} | \psi(t) \rangle$. Consider this arbitrary Pauli operator:

```
\sigma = X_0 X_1 X_2;
v = Simplify[
           Conjugate [\psi[t]]. CalcPauliExpressionMatrix [\sigma]. \psi[t],
           t ≥ 0]
\frac{1}{20} \left( -1 + 5 \cos \left[ 4 \sqrt{2} \ t \right] - 4 \cos \left[ 4 \sqrt{5} \ t \right] \right)
```



Numerical

Let's switch to numerical simulation and choose a more interesting, physically-meaningful problem. We will simulate an Ising spin-ring, nominated for its potential utility in demonstrating quantum advantage, with (periodic) Hamiltonian:

$$\hat{H} = \sum_{i=0}^{\mathsf{nQb-1}} \vec{\sigma}_i \cdot \vec{\sigma}_{i+1} + B\hat{Z}_i + d_i \hat{Z}_i$$

where B = 4 is the strength of a transverse magnetic field, and $d_i \in [-d, d]$

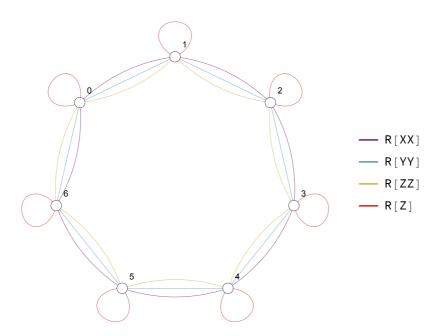
nQb = 7;Clear[h]

$$\begin{split} h[d_{-}] &= \text{Expand} \Big[\\ &\quad \text{Sum}[\, (4 + d \, \text{RandomReal}[\, \{-1,\, 1\}]) \, Z_i, \, \, \{i,\, 0,\, nQb - 1\}] \, + \\ &\quad \text{Sum} \Big[s_i \, s_{\text{Mod}[\, i+1,\, nQb]} \,, \, \, \{i,\, 0,\, nQb - 1\}, \, \, \{s,\, \{X,\, Y,\, Z\}\} \Big] \Big] \end{split}$$

$$\begin{array}{l} X_{0}\;X_{1}\;+\;X_{1}\;X_{2}\;+\;X_{2}\;X_{3}\;+\;X_{3}\;X_{4}\;+\;X_{4}\;X_{5}\;+\;X_{0}\;X_{6}\;+\;X_{5}\;X_{6}\;+\;Y_{0}\;Y_{1}\;+\;Y_{1}\;Y_{2}\;+\;Y_{2}\;Y_{3}\;+\;Y_{3}\;Y_{4}\;+\\ Y_{4}\;Y_{5}\;+\;Y_{0}\;Y_{6}\;+\;Y_{5}\;Y_{6}\;+\;4\;Z_{0}\;+\;0.889235\;d\;Z_{0}\;+\;4\;Z_{1}\;+\;0.115662\;d\;Z_{1}\;+\;Z_{0}\;Z_{1}\;+\;4\;Z_{2}\;+\\ 0.15242\;d\;Z_{2}\;+\;Z_{1}\;Z_{2}\;+\;4\;Z_{3}\;-\;0.917439\;d\;Z_{3}\;+\;Z_{2}\;Z_{3}\;+\;4\;Z_{4}\;-\;0.606932\;d\;Z_{4}\;+\\ Z_{3}\;Z_{4}\;+\;4\;Z_{5}\;+\;0.411064\;d\;Z_{5}\;+\;Z_{4}\;Z_{5}\;+\;4\;Z_{6}\;+\;0.0813288\;d\;Z_{6}\;+\;Z_{0}\;Z_{6}\;+\;Z_{5}\;Z_{6} \end{array}$$

A quick way to confirm the ring topology of this system is to plot the connectivity of its Trotter circuit.

DrawCircuitTopology @ GetKnownCircuit["Trotter", h[1], 1, 1, t]



The uniformly random real scalars $d_i \in [-d, d]$ in \hat{H} vary the effective magnetic field experienced by the spins. The scalar d > 0 is the strength of the disorder of the field.

CalcPauliStringMinEigVal@h[1]

-21.6352

CalcPauliStringMinEigVal@h[10]

-41.2231

This greatly affects the spectrum λ_i

```
vals = Transpose @ Table[
           - Eigenvalues[
                   - CalcPauliExpressionMatrix @ h[d], 5,
                   Method → {"Arnoldi", "Criteria" → "RealPart"}],
           {d, .1, 5, .1}];
ListLinePlot[
      vals,
      AxesLabel → {"disorder (10 d)", "energy"},
      PlotLegends \rightarrow Table[\lambda_i, {i, 5}]]
energy
                                                disorder (10 d)
                    20
-20
                                                                  -\lambda_2
-22

    λ<sub>3</sub>

-24
                                                                 -\lambda_4
                                                                -\lambda_5
-26
-28
```

To simulate time evolution under \hat{H} , we will make use of its Z-basis matrix representation. Here we use a Mathematica trick to save the matrix being computed for a given value of d so that repeated calls to hMatr[d] below don't repeat the computation.

```
Clear[hMatr]
hMatr[d_] := hMatr[d] = CalcPauliExpressionMatrix @ h[d]
First @ Timing @ hMatr[.1]
0.03099
First @ Timing @ hMatr[.1]
First @ Timing @ hMatr[.1]
First @ Timing @ hMatr[.1]
8. \times 10^{-6}
6.\times10^{-6}
5. \times 10^{-6}
```

Let's consider an initial state whereby half of the spins are excited against the external field; this is the "Néel ordered state".

```
in\psi = CreateQureg[nQb];
ApplyCircuit[in\psi, Table[X_q, {q, 0, nQb - 1, 2}]];
GetQuregState[inψ, "ZBasisKets"]
1010101
```

We now *numerically* construct the time evolution operator in order to obtain future states.

```
true\psi = CreateQureg[nQb];
setTrueState[true\(\psi_\), in\(\psi_\), hMatr_, t_] :=
     SetQuregMatrix[trueψ, MatrixExp[-ithMatr].GetQuregState[inψ]]
```

Time evolution under this Hamiltonian quickly excites the other spins:

```
setTrueState[trueψ, inψ, hMatr[.1], 0];
GetQuregState[trueψ, "ZBasisKets"]
1010101
setTrueState[true\psi, in\psi, hMatr[.1], 10<sup>-6</sup>];
GetQuregState[trueψ, "ZBasisKets"] // Chop
 (0.-2.\times10^{-6}~\text{i})~|0110101\rangle-(0.+2.\times10^{-6}~\text{i})~|1001101\rangle-
     (0. + 2. \times 10^{-6} i) | 1010011 \rangle + (1. + 9.09068 \times 10^{-6} i) | 1010101 \rangle -
      \begin{array}{c|c} (\textbf{0.} + \textbf{2.} \times \textbf{10}^{-6} \ \text{i}) & | \ \textbf{1010110} \ \rangle - (\textbf{0.} + \textbf{2.} \times \textbf{10}^{-6} \ \text{i}) & | \ \textbf{1011001} \ \rangle - (\textbf{0.} + \textbf{2.} \times \textbf{10}^{-6} \ \text{i}) & | \ \textbf{1100101} \ \rangle \end{array} 
setTrueState[trueψ, inψ, hMatr[.1], 1];
GetQuregState[trueψ, "ZBasisKets"][;; 10]
(-0.0233376 + 0.0143622 i) | 0001111 \rangle - (0.0870519 + 0.171909 i) | 0010111 \rangle +
     (0.0767504 - 0.0120878 \pm) \mid 0011011 \rangle - (0.0531524 + 0.103575 \pm) \mid 0011101 \rangle - (0.0767504 - 0.0120878 \pm) \mid 0011101 \rangle - (0.0767504 - 0.012088 \pm) \mid 0011101 \rangle - (0.0767504 - 0.012088 \pm) \mid 0011101 \rangle - (0.0767504 - 0.012088 \pm) \mid 0011101 \rangle - (0.0767504 - 0.01208 \pm) \mid 0011101 - 0.01208 \pm
     (0.103286 - 0.0211168 i) |0011110\rangle - (0.120611 - 0.0299637 i) |0100111\rangle -
      (\textbf{0.0736363} - \textbf{0.129366}\,\,\dot{\textbf{1}}) \,\,\, \big|\, \textbf{0101011} \,\big\rangle \,-\, (\textbf{0.197389} - \textbf{0.338313}\,\,\dot{\textbf{1}}) \,\,\, \big|\, \textbf{0101101} \,\big\rangle \,\,+\, 
     (0.167059 - 0.0165693 i) | 0101110 \rangle + (0.0198486 - 0.0990428 i) | 0110011 \rangle
```

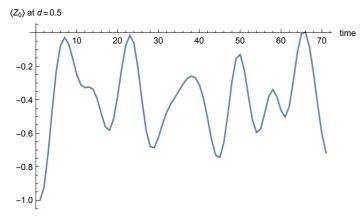
In this system, we are interested in the single-site magnetisation of the spins, $\langle Z_i \rangle$.

```
\phi = CreateQureg[nQb];
CalcExpecPauliString[true\psi, Z<sub>0</sub>, \phi]
-0.163828
```

Let's check how the magnetisation of the first qubit (which started anti-aligned with the transverse magnetic field) evolves in time, for a specific choice of disorder d.

```
pureData = Table[
        setTrueState[trueψ, inψ, hMatr[.5], t];
        CalcExpecPauliString[true\psi, Z<sub>0</sub>, \phi],
        {t, 0, nQb, .1}];
```

ListLinePlot[pureData, AxesLabel \rightarrow {"time", " $\langle Z_0 \rangle$ at d = 0.5"}]



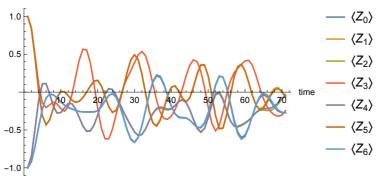
Here's how the magnetisation of *all* spins evolve in time, when the field has small disorder.

```
data = Transpose@ Table[
         setTrueState[trueψ, inψ, hMatr[.01], t];
        CalcExpecPauliString[true\psi, Z_q, \phi],
         {t, 0, nQb, .1},
         {q, 0, nQb-1}];
```

ListLinePlot[data,

```
AxesLabel → {"time", "magnetisation (when d = .05)"},
PlotLegends \rightarrow Table[Row@{"\langle ", Z_i, "\rangle "}, \ \{i, \ 0, \ nQb-1\}]]
```

magnetisation (when d = .05)



We see that the strong ±1 magnetisation of our initial state is quickly thermalized, and averages around zero. As reported here, the reason that this system is interesting is because as the disorder d of the transverse magnetic field is increased, the spins take significantly longer to thermalize. A strongly disordered external field sees the spins remain localized, retaining information about their original magnetisation. Here's the magnetisation in-time when the disorder is d = 3...

-0.5

```
data = Transpose@ Table[
             setTrueState[trueψ, inψ, hMatr[5], t];
            CalcExpecPauliString[true\psi, Z_q, \phi],
             {t, 0, nQb, .1},
             {q, 0, nQb-1}];
ListLinePlot[data,
       AxesLabel \rightarrow {"time", "magnetisation (when d = 3)"},
        PlotLegends \rightarrow Table[Row@{"\langle", Z<sub>i</sub>, "\rangle"}, {i, 0, nQb - 1}]]
magnetisation (when d=3)
       1.0
                                                                        ---\langle Z_0\rangle
                                                                        --\langle Z_1\rangle
       0.5
                                                                        --\langle Z_2\rangle
                                                                         --\langle Z_3\rangle
                                                                         --\langle Z_4\rangle
                                                                        --\langle Z_5\rangle
      -0.5
                                                                         --\langle Z_6\rangle
 and when d = 10...
data = Transpose@ Table[
             setTrueState[trueψ, inψ, hMatr[10], t];
            CalcExpecPauliString[true\psi, Z_q, \phi],
             {t, 0, nQb, .1},
             {q, 0, nQb-1}];
ListLinePlot[data,
       AxesLabel → {"time", "magnetisation (when d = 10)"},
       PlotLegends \rightarrow Table[Row@{"\langle", Z<sub>i</sub>, "\rangle"}, {i, 0, nQb - 1}]]
magnetisation (when d = 10)
        1.0
                                                                        ---\langle Z_0\rangle
                                                                          -\langle Z_1\rangle
       0.5
                                                                        --\langle Z_2\rangle
                                                                          — ⟨Z<sub>3</sub>⟩
                                                              70
                                30
                                               50
                                                                         --\langle Z_4\rangle
```

There is in fact a *phase transition* in the magnetisation occurring over *d*.

 $-\langle Z_5\rangle$

 $-\langle Z_6 \rangle$

```
data = Transpose @ Table[
           Abs /@ Mean /@ Transpose @ Table[
                 setTrueState[true\(\psi\), in\(\psi\), hMatr[d], t];
                 CalcExpecPauliString[true\psi, Z_q, \phi],
                 \{t, 0, nQb/2, .1\},\
                 \{q, 0, nQb-1\},
           {d, .01, 30, 1}];
ListLinePlot[data,
      AxesLabel → {"disorder (d)", "average magnetisation strength"},
      PlotMarkers → Automatic
1
average magnetisation strength
                                                               - \mathbb{E}_t |\langle Z_0(t) \rangle|
        1.0
                                                               - \mathbb{E}_t |\langle Z_1(t) \rangle|
        0.8
                                                               -\!\!\!\!-\!\!\!\!\!- \mathbb{E}_t |\langle Z_2(t) \rangle|
        0.6
                                                               - \mathbb{E}_t |\langle Z_4(t) \rangle|
                                                               - \mathbb{E}_t |\langle Z_5(t) \rangle|
        0.2
                                                               \blacksquare \mathbb{E}_t |\langle Z_6(t) \rangle|
                                                     disorder (d)
ListLogLinearPlot[
      Mean @ data,
      AxesLabel → {"disorder (d)", "average magnetisation strength"},
      Joined → True, PlotMarkers → Automatic,
      PlotStyle → Directive[Black, Dashed]
]
average magnetisation strength
        8.0
        0.6
                                                    disorder (d)
```

Trotterisation

Pure

Let's pretend the previous section's spin-ring Hamiltonian was sadly too big to process by the classical numerics above, though it remains tractable to describe as a Pauli string:

h1 = h[1]

$$\begin{array}{l} X_0 \ X_1 + X_1 \ X_2 + X_2 \ X_3 + X_3 \ X_4 + X_4 \ X_5 + X_0 \ X_6 + X_5 \ X_6 + Y_0 \ Y_1 + Y_1 \ Y_2 + Y_2 \ Y_3 + Y_3 \ Y_4 + Y_4 \ Y_5 + Y_6 \ Y_6 + Y_5 \ Y_6 + 4.88923 \ Z_0 + 4.11566 \ Z_1 + Z_0 \ Z_1 + 4.15242 \ Z_2 + Z_1 \ Z_2 + 3.08256 \ Z_3 + Z_2 \ Z_3 + 3.39307 \ Z_4 + Z_3 \ Z_4 + 4.41106 \ Z_5 + Z_4 \ Z_5 + 4.08133 \ Z_6 + Z_0 \ Z_6 + Z_5 \ Z_6 \end{array}$$

Suppose the Z-basis representation of \hat{H} is classically computationally intractable, so we could not evaluate this:

h1Matr = CalcPauliExpressionMatrix[h1]



Imagine that we fortunately we have a quantum computer at our disposal, with which to perform quantum simulation! The canonical method of quantumly simulating the real-time unitary dynamics of a system is to evaluate the circuit produced by *Trotterising* its unitary time evolution operator:

$$e^{-it\hat{H}} \approx \prod_{i} \hat{U}_{i}[t]$$

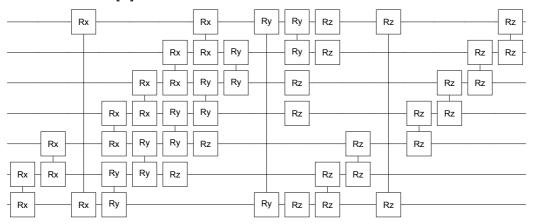
Clear[u]

```
u[t_] = GetKnownCircuit["Trotter", h1, 1, 1, t]
```

```
\{R[2t, X_0 X_1], R[2t, X_1 X_2], R[2t, X_2 X_3], R[2t, X_3 X_4], R[2t, X_4 X_5],
R[2t, X_0 X_6], R[2t, X_5 X_6], R[2t, Y_0 Y_1], R[2t, Y_1 Y_2], R[2t, Y_2 Y_3],
R[2t, Y_3 Y_4], R[2t, Y_4 Y_5], R[2t, Y_0 Y_6], R[2t, Y_5 Y_6], R[9.77847t, Z_0],
R[8.23132t, Z_1], R[2t, Z_0Z_1], R[8.30484t, Z_2], R[2t, Z_1Z_2],
 R[6.16512t, Z_3], R[2t, Z_2Z_3], R[6.78614t, Z_4], R[2t, Z_3Z_4],
 R[8.82213t, Z_5], R[2t, Z_4Z_5], R[8.16266t, Z_6], R[2t, Z_0Z_6], R[2t, Z_5Z_6]
```

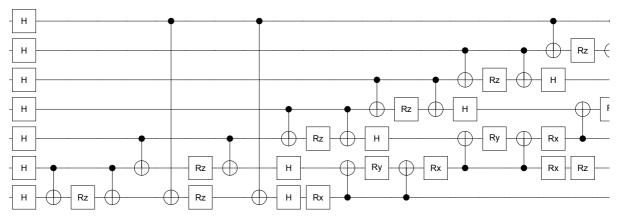
This is a circuit with gate parameters dependent upon the coefficients of our Hamiltonian, and the target simulation time t.

DrawCircuit@u[t]

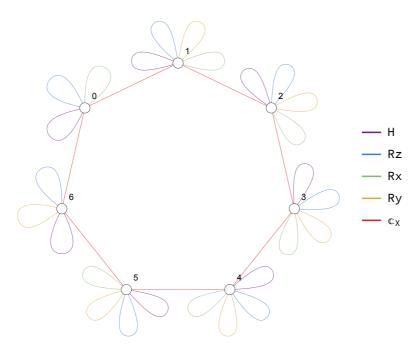


If necessary, we could recompile this circuit into the native operations of our hardware...

v = SimplifyCircuit@RecompileCircuit[u[t], "SingleQubitAndCNOT"]; DrawCircuit[v]



DrawCircuitTopology@v



but for convenience, let's assume our hardware can perform the original two-qubit Pauli gadgets. The Trotter circuit \hat{U} , applied to the initial state $|\psi(0)\rangle$, produces a direct approximation to the state $|\psi(t)\rangle = e^{-it\hat{H}} |\psi(0)\rangle$

```
\psi = CreateQureg[nQb];
CloneQureg[\psi, in\psi];
{\tt GetQuregState[}\psi, \ "{\tt ZBasisKets"}]
1010101
```

```
\tau = 0.1;
ApplyCircuit[\psi, u[\tau]];
setTrueState[true\psi, in\psi, h1Matr, \tau];
CalcFidelity[\psi, true\psi]
0.992173
```

An experimentalist can ergo apply circuit $\hat{U}(t)$, with rotations informed by the desired simulation time t, and thereafter measure their observable of interest, like the spin-ring magnetisation.

```
data = Table[
           CloneQureg[\psi, in\psi];
           ApplyCircuit[\psi, u[t]];
           CalcExpecPauliString[\psi, Z<sub>0</sub>, \phi],
           {t, 0, nQb, .01}];
ListLinePlot[data, AxesLabel \rightarrow {"Trotter time", "\langle Z_{\theta} \rangle at d = 1"}]
\langle Z_0 \rangle at d=1
                                                             Trotter time
                                                 600
                          300
                                          500
                  200
-0.2
-0.4
-0.6
-0.8
-1.0
```

This doesn't look how we expected - it is suspiciously periodic (as the Trotter circuit is as a function of t), whereas we earlier witnessed thermalisation. Indeed the fidelity is imperfect -Trotterisation can only approximate the evolution when the Hamiltonian contains non-commuting terms.

```
\tau = 0.3;
ApplyCircuit[CloneQureg[\psi, in\psi], u[\tau]];
setTrueState[true\psi, in\psi, h1Matr, \tau];
CalcFidelity[\psi, true\psi]
0.812077
```

```
The fidelity \left| \left\langle \psi(0) \right| e^{it\hat{H}} \hat{U}(t) \left| \psi(0) \right\rangle \right|^2 drops quickly with increasing t.
```

```
Bra[\psi]
```

⟨32|

```
fid = Table[
        ApplyCircuit[CloneQureg[\psi, in\psi], u[t]];
        setTrueState[trueψ, inψ, h1Matr, t];
        CalcFidelity[\psi, true\psi],
        {t, 0, 1, .05}];
ListLinePlot[fid,
     AxesLabel → {"time (x20)", "fidelity"},
     PlotMarkers → Automatic
]
fidelity
1.0
8.0
0.6
0.2
```

We can improve the fidelity by using more Trotter *repetitions*, or using a *higher order* method.

```
order = 4;
reps = 3;
u[t_] = GetKnownCircuit["Trotter", h1, order, reps, t]
```

$$\left\{ \mathsf{R} \left[\frac{\mathsf{t}}{3 \, \left(4 - 2^{2/3} \right)} \,,\, \mathsf{X}_0 \, \mathsf{X}_1 \right] \,,\, \mathsf{R} \left[\frac{\mathsf{t}}{3 \, \left(4 - 2^{2/3} \right)} \,,\, \mathsf{X}_1 \, \mathsf{X}_2 \right] \,,\, \mathsf{R} \left[\frac{\mathsf{t}}{3 \, \left(4 - 2^{2/3} \right)} \,,\, \mathsf{X}_2 \, \mathsf{X}_3 \right] \,,\, \mathsf{R} \left[\frac{\mathsf{t}}{3 \, \left(4 - 2^{2/3} \right)} \,,\, \mathsf{X}_3 \, \mathsf{X}_4 \right] \,,\, \ldots \,,\, \mathsf{R} \left[\frac{\mathsf{t}}{3 \, \left(4 - 2^{2/3} \right)} \,,\, \mathsf{X}_2 \, \mathsf{X}_3 \right] \,,\, \mathsf{R} \left[\frac{\mathsf{t}}{3 \, \left(4 - 2^{2/3} \right)} \,,\, \mathsf{X}_1 \, \mathsf{X}_2 \right] \,,\, \mathsf{R} \left[\frac{\mathsf{t}}{3 \, \left(4 - 2^{2/3} \right)} \,,\, \mathsf{X}_0 \, \mathsf{X}_1 \right] \right\}$$
 large output show less show more show all set size limit...

```
fid = Table[
        ApplyCircuit[CloneQureg[\psi, in\psi], u[t]];
        setTrueState[trueψ, inψ, h1Matr, t];
        CalcFidelity[\psi, true\psi],
         {t, 0, 1, .05}];
ListLinePlot[fid,
      AxesLabel → {"time (x20)", "fidelity"},
      PlotMarkers → Automatic
]
  fidelity
1.000
0.999
0.998
0.997
0.996
0.995
                                                 time (×20)
                       10
                                  15
```

Of course, this means increasing the number of gates in the circuit.

```
Length @ GetKnownCircuit["Trotter", h1, 4, 1, t]
275
cost = Table[
        Length @ GetKnownCircuit["Trotter", h1, order, 1, t] / nQb,
        {order, {1, 2, 4, 6, 8, 10, 12}}];
ListLogPlot[cost,
     AxesLabel → {"Trotter order", "circuit depth"},
     Joined → True, PlotMarkers → Automatic,
     PlotStyle → Directive[Dashed]
]
circuit depth
10<sup>4</sup>
1000
100
 10
```

Let's simulate to fixed time t = nQb/2, and record the costs and performance of using Trotter

circuits of different order and repetitions.

```
\tau = nQb / 2;
setTrueState[trueψ, inψ, h1Matr, τ];
data = Table[
       u = GetKnownCircuit["Trotter", h1, order, reps, N@τ];
        ApplyCircuit[CloneQureg[\psi, in\psi], u];
        {Length[u], CalcFidelity[\psi, true\psi]},
        {order, {1, 2, 4, 6, 8}},
        {reps, 1, Floor[100/order]}];
```

We can see that higher-order Trotter quickly becomes expensive:

```
ListLogLinearPlot data,
       AxesLabel \rightarrow {"number of gates", "fidelity at t=nQb/2"},
       Joined → True, PlotRange → \{\{.5 \times 10^2, 10^5\}, All\},
      PlotStyle \rightarrow Dashed, PlotMarkers \rightarrow {"\bullet", 7},
      Ticks \rightarrow {Table[{10<sup>i</sup>, "10"<sup>i</sup>}, {i, 1, 5}], Automatic},
       PlotLegends → Table["order " <> ToString[i], {i, {1, 2, 4, 6, 8}}]
fidelity at t=nQb/2
   1.0
                                                                --•-- order 1
   0.8
                                                                   •-- order 2
   0.6
                                                                    -- order 4
                                                                   •-- order 6
                                                                ---- order 8
   0.2
                                                  number of gates
```

yet it is our only hope if we wish to simulate far into the future!

```
\tau = 4 \text{ nQb};
setTrueState[true\psi, in\psi, h1Matr, \tau];
data = Table[
         u = GetKnownCircuit["Trotter", h1, order, reps, N@τ];
         ApplyCircuit[CloneQureg[\psi, in\psi], u];
          {Length[u], CalcFidelity[\psi, true\psi]},
          {order, {1, 2, 4, 6, 8}},
         {reps, 1, Floor[100/order]}];
ListLogLinearPlot[data,
      AxesLabel \rightarrow {"number of gates", "fidelity at t=4nQb"},
      Joined \rightarrow True, PlotRange \rightarrow \{\{.5 \times 10^2, 10^5\}, \{0, 1\}\},
      PlotStyle \rightarrow Dashed, PlotMarkers \rightarrow {"\bullet", 7},
      Ticks \rightarrow {Table[\{10^i, "10^{"i}\}, \{i, 1, 5\}], Automatic},
      PlotLegends → Table["order " <> ToString[i], {i, {1, 2, 4, 6, 8}}]
1
fidelity at t=4 nQb
   1.0

    - order 1

   0.8
                                                                    - order 2
   0.6
                                                                    - order 4
   0.4

    - order 6

                                                                   -- order 8
   0.2
                                  104
```

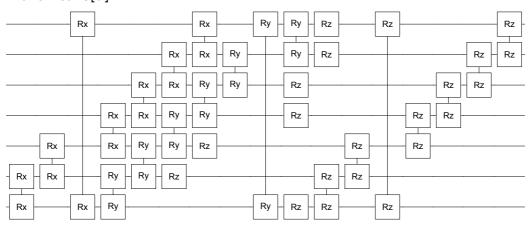
Noisy

There is yet another problem - what happens if our quantum hardware is imperfect and susceptible to decoherence? Let's now assume that parameter-dependent dephasing noise of probability $\xi \mid \theta \mid$ follows every Rz[θ] gate, and fixed two-qubit depolarising noise of strength ξ follows every two-qubit Pauli gadget.

```
noisify[u_, \xi_] := u /. {
           g: R[\theta_{-}, Z_{t_{-}}] \Rightarrow Sequence[g, Deph_{t}[Abs[\theta] \xi]],
           g: R[\theta_-, Verbatim[Times][_{t1\_}, _{t2\_}]] \Rightarrow Sequence[g, Depol_{t1,t2}[\xi]]
```

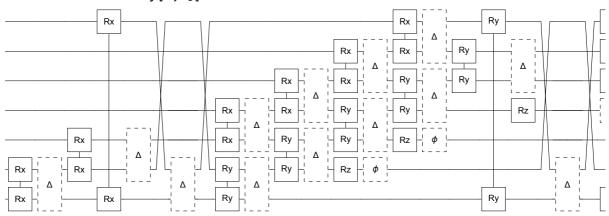
Attempting to perform the first-order single-repetition unitary Trotter circuit...

$\tau = 0.1;$ u = GetKnownCircuit["Trotter", h1, 1, 1, τ]; DrawCircuit[u]



would instead invoke the channel:

DrawCircuit @ noisify[u, ξ]



Simulating this channel will require we switch our quantum registers to be *density matrices*.

```
ρ = CreateDensityQureg[nQb];
InitPureState[\rho, in\psi];
ApplyCircuit[\rho, noisify[u, 10<sup>-3</sup>]];
CalcPurity[ρ]
0.953016
```

The decoherence (physical error) worsens our fidelity, compounding the existing inaccuracy of our Trotter truncation (algorithmic error)

```
setTrueState[trueψ, inψ, h1Matr, τ];
InitPureState[\rho, in\psi];
ApplyCircuit[\rho, noisify[u, 10^{-2}]];
CalcFidelity[\rho, true\psi]
0.824697
```

Here's first-order single-repetition Trotter simulation succumbing to increasing decoherence.

```
noise = Range[0, 10^{-2}, 10^{-3}];
data = Transpose @ Table[
          InitPureState[\rho, in\psi];
          ApplyCircuit[ρ, noisify[u, ξ]];
          {CalcFidelity[\rho, true\psi], CalcPurity[\rho]},
          \{\xi, \text{ noise}\}\];
ListLinePlot[
      Transpose[{noise, #}] & /@ data,
      AxesLabel → {"noise strength", "1st order Trotter"},
      PlotLegends → {"purity", "fidelity"},
      PlotMarkers → Automatic
]
1st order Trotter
  1.00
  0.95
  0.90
                                                            purity
  0.85
                                                              fidelity
  0.80
  0.75
  0.70
                                                noise strength
           0.002
                   0.004
                            0.006
                                    0.008
                                            0.010
```

While the algorithmic Trotter error worsens for increasing t, the physical error of decoherence worsens the fidelity at *all times*. Even a measly *t*=1 simulation is quickly ruined!

```
Clear[u];
u[t_] = GetKnownCircuit["Trotter", h1, 4, 1, t];
ch[t_{,\xi_{]}} = noisify[u[t], \xi];
time = Range[0, 1, 0.05];
noise = \{0, 10^{-4}, 10^{-3}, 2 \times 10^{-3}, 5 \times 10^{-3}, 10^{-2}\};
fid = Transpose @ Table[
          setTrueState[trueψ, inψ, h1Matr, t];
          ApplyCircuit[InitPureState[\rho, in\psi], ch[t, \xi]];
          CalcFidelity[\rho, true\psi],
          {t, time},
          \{\xi, \text{noise}\}\];
```

```
ListLinePlot[
      Transpose[{time, #}] & /@ fid,
      AxesLabel → {"time", "fidelity"},
      PlotLegends \rightarrow Table["\xi=" \leftrightarrow ToString[N@\xi], {\xi, noise}],
      PlotMarkers → Automatic
]
fidelity
                                                               --- \xi=0.
                                                               \xi = 0.0001
                                                               \leftarrow \xi=0.001
                                                               = \xi = 0.002
                                                               \xi=0.005
                                                               - \xi=0.01
```

Let's repeat our earlier resource-aware simulations of time t = nQb/2 using increasing Trotter orders and repetitions, but this time incorporating a modest physical error rate of $\xi = 10^{-4}$.

```
\tau = nQb / 2;
\xi = 10^{-4};
setTrueState[true\psi, in\psi, h1Matr, \tau];
data = Table[
        u = GetKnownCircuit["Trotter", h1, order, reps, N@τ];
        ApplyCircuit[InitPureState[\rho, in\psi], noisify[u, \xi]];
        {Length[u], CalcFidelity[\rho, true\psi]},
        {order, {1, 2, 4, 6, 8}},
        {reps, 1, Floor[100/order]}];
```

This reveals increasing the Trotter repetitions and order can actually worsen performance, because the additional gates introduce more opportunities for physical error:

```
ListLogLinearPlot[data,
      AxesLabel → {"number of gates", "fidelity at t=nQb/2"},
      Joined → True, PlotRange → \{\{.5 \times 10^2, 10^5\}, All\},
      PlotStyle → Dashed, PlotMarkers → {"•", 7},
      Ticks \rightarrow {Table[\{10^i, "10^{"i}\}, \{i, 1, 5\}], Automatic},
      PlotLegends → Table["order " <> ToString[i], {i, {1, 2, 4, 6, 8}}]
]
fidelity at t=nQb/2
   0.8
                                                                  -- order 1

    order 2

   0.6
                                                                  -- order 4
   0.4

    order 6

                                                                  -- order 8
   0.2
                     10<sup>3</sup>
                                  10<sup>4</sup>
```

This is why Trotterisation is believed to be incompatible with near-future noisy quantum hardware. It prescribes deep circuits leveraging precise interference effects, which are easily damaged by noise and the imperfections of near-future quantum computers.

How would the experimentalist fair attempting to use this hardware to study the dynamics of magnetisation in our spin-ring system?

```
\mu = CreateDensityQureg[nQb];
data = Table[
        u = GetKnownCircuit["Trotter", h1, 4, 1, t];
        ApplyCircuit[InitPureState[\rho, in\psi], noisify[u, 10<sup>-4</sup>]];
        CalcExpecPauliString[\rho, Z_0, \mu],
        {t, 0, nQb, .1}];
```

Well at least it more closely resembles thermalization! $^-\ (^\vee)_-/^-$

```
ListLinePlot[
        {data, pureData},
        AxesLabel \rightarrow {"time (×10)", "\langle Z_0 \rangle at d = 1"},
        PlotMarkers → Automatic,
        PlotLegends \rightarrow {"\xi=10<sup>-4</sup>", "\xi=0"}]
\langle Z_0 \rangle at d=1
 0.2
-0.2
-0.4
-0.6
-0.8
```