Hamiltonian Simulation H=Z

§4.7 Simulation of quantum systems, Nielsen & Chuang

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Introduction

Quantum circuit for simulating the Hamiltonian H=$\underline{\otimes}$Z for time Δt.
Get the Quantum Mathematica package at https://homepage.cem.itesm.mx/lgomez/

- Structure of H=$\underline{\otimes}$Z for time Δt, operator and matrix form
- Equivalence between circuits with CNOT connected directly to the last/ancilla qubit or with intermediate connections (both forms are used in the literature)

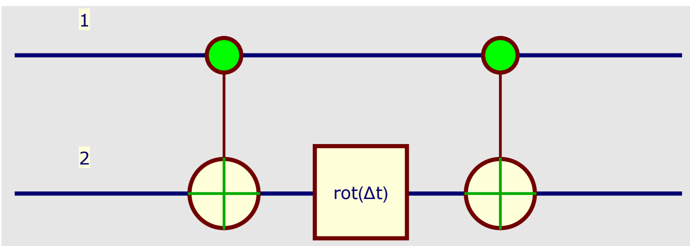
In[5]:=
```
(* import package *)
Needs["Quantum`Computing`"];
```

SetQuantumGate: Symbol SetQuantumGate appears in multiple contexts {Quantum`Computing`, Global`}; definitions in context Quantum`Computing` may shadow or be shadowed by other definitions.

n=1

In[∘]:=
```
Clear[Δt, I2, Z, RZ, U1, U2, rot, psi]
I2 = PauliMatrix[0];
Z = PauliMatrix[3];

(* direct method *)
U1 = MatrixExp[-I KroneckerProduct[Z, I2] Δt];

(* define Rz rotation *)
SetQuantumGate[rot, 1,
  Function[{q1},
   Function[{Δt},
    ⅇ^(-ⅈ Δt) |0_q̂1⟩ · ⟨0_q̂1| + ⅇ^(+ⅈ Δt) |1_q̂1⟩ · ⟨1_q̂1| ]]];
QuantumTableForm[rot_1̂[Δt]];
QuantumMatrixForm[rot_1̂[Δt]];
QuantumMatrixForm[C^{3̂}[NOT_4̂]];

(* build circuit *)
circ = C^{1̂}[NOT_2̂] · rot_2̂[Δt] · C^{1̂}[NOT_2̂];
(* plot *)
QuantumPlot[circ]
U2 = QuantumMatrix[circ];
(* compare unitaries *)
Print["U1=", U1]
Print["U2=", U2]
(* define test ket. We are only interested on the effect of the operators
 on an arbitrary ket (where the ancilla is supposed to start as 0) *)
psi = ArrayFlatten[KroneckerProduct[{a[0], a[1]}, {1, 0}], 1];
Print["ψ=", psi]
(* the non-zero entries of this ket
  will select the relevant entries of the operators *)
(* because of zero entries in U1,U2,
we need to add ϵ to the operators and then take the limit ϵ→0 *)
Limit[(U1.psi + ϵ) / (U2.psi + ϵ), ϵ → 0]
(* the resulting kets are the same *)
```

Out[∘]=



```
U1={{e^(-i Δt), 0, 0, 0}, {0, e^(-i Δt), 0, 0}, {0, 0, e^(i Δt), 0}, {0, 0, 0, e^(i Δt)}}
U2={{e^(-i Δt), 0, 0, 0}, {0, e^(i Δt), 0, 0}, {0, 0, e^(i Δt), 0}, {0, 0, 0, e^(-i Δt)}}
ψ={a[0], 0, a[1], 0}
```

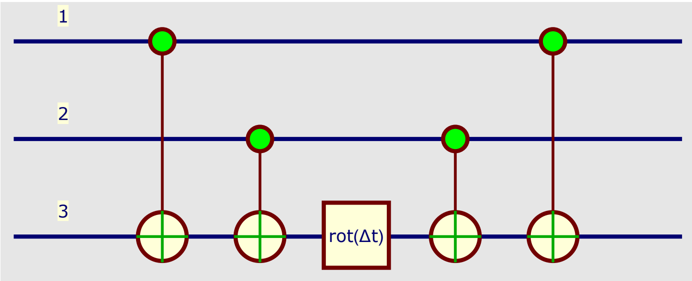
Out[•]= {1, 1, 1, 1}

n=2

In[•]:=

```
Clear[Δt, I2, Z, RZ, U1, U2, rot, psi]
I2 = PauliMatrix[0];
Z = PauliMatrix[3];

(* direct method *)
U1 = MatrixExp[-I KroneckerProduct[Z, Z, I2] Δt];

(* define Rz rotation *)
SetQuantumGate[rot, 1,
  Function[{q1},
   Function[{Δt},
    e^(-i Δt) |0_q1^⟩ · ⟨0_q1^| + e^(+i Δt) |1_q1^⟩ · ⟨1_q1^| ]]];
QuantumTableForm[rot_1^[Δt]];
QuantumMatrixForm[rot_1^[Δt]];
QuantumMatrixForm[C^{3^}[NOT_4^]];

(* build circuit *)
circ = C^{1^}[NOT_3^] · C^{2^}[NOT_3^] · rot_3^[Δt] · C^{2^}[NOT_3^] · C^{1^}[NOT_3^];
(* plot *)
QuantumPlot[circ]
U2 = QuantumMatrix[circ];
(* compare unitaries *)
psi = ArrayFlatten[KroneckerProduct[{a[0], a[1]}, {a[2], a[3]}, {1, 0}], 1];
Limit[(U1.psi + ϵ) / (U2.psi + ϵ), ϵ → 0]
```

Out[•]=

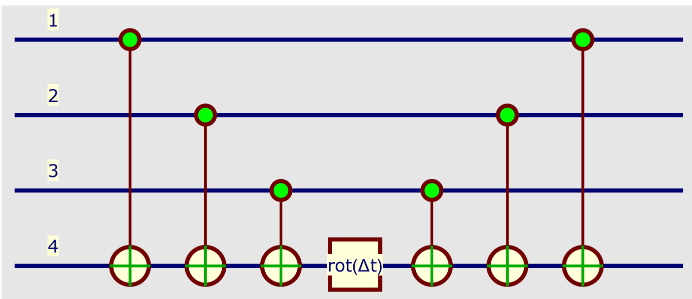


Out[•]= {1, 1, 1, 1, 1, 1, 1, 1}

n=3

In[∘]:=
```
Clear[Δt, I2, Z, RZ, U1, U2, psi]
I2 = PauliMatrix[0];
Z = PauliMatrix[3];

(* direct method *)
U1 = MatrixExp[-I KroneckerProduct[Z, Z, Z, I2] Δt];

(* define Rz rotation *)
SetQuantumGate[rot, 1,
  Function[{q1},
   Function[{Δt},
    e^(-ⅈ Δt) |0_q̂1⟩ · ⟨0_q̂1| + e^(+ⅈ Δt) |1_q̂1⟩ · ⟨1_q̂1| ]]];
QuantumTableForm[rot_1̂[Δt]];
QuantumMatrixForm[rot_1̂[Δt]];
QuantumMatrixForm[C^{3̂}[NOT_4̂]];

(* build circuit *)
circ =
  C^{1̂}[NOT_4̂] · C^{2̂}[NOT_4̂] · C^{3̂}[NOT_4̂] · rot_4̂[Δt] · C^{3̂}[NOT_4̂] · C^{2̂}[NOT_4̂] · C^{1̂}[NOT_4̂];

(* plot *)
QuantumPlot[circ]
U2 = QuantumMatrix[circ];
(* compare unitaries *)
psi = ArrayFlatten[
   KroneckerProduct[{a[0], a[1]}, {a[2], a[3]}, {a[4], a[5]}, {1, 0}], 1];
Limit[(U1.psi + ϵ) / (U2.psi + ϵ), ϵ → 0]
```

Out[∘]=



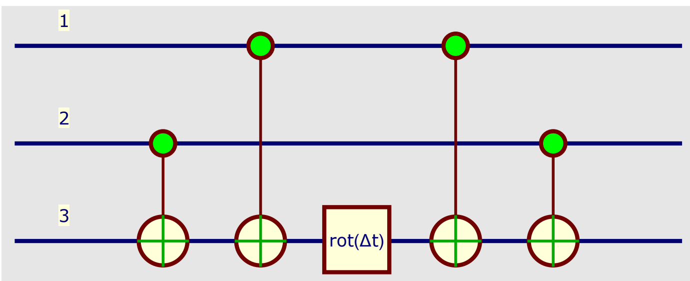
Out[∘]= {1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1}

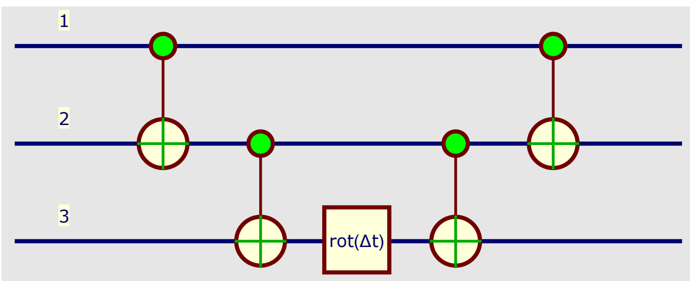
Equivalence between circuits with CNOT connected directly to the ancilla qubit or with

intermediate connections

n=2

In[•]:=
```
Clear[Δt, I2, Z, RZ, U1, U2, rot, psi, circ1, circ2]

I2 = PauliMatrix[0];
Z = PauliMatrix[3];
(* define Rz rotation *)
SetQuantumGate[rot, 1,
  Function[{q1},
   Function[{Δt},
    ⅇ^(-ⅈ Δt) |0_q̂1⟩ · ⟨0_q̂1| + ⅇ^(+ⅈ Δt) |1_q̂1⟩ · ⟨1_q̂1|]]];

(* build circuit *)
circ1 = C^{2̂}[NOT_3̂] · C^{1̂}[NOT_3̂] · rot_3̂[Δt] · C^{1̂}[NOT_3̂] · C^{2̂}[NOT_3̂];
circ2 = C^{1̂}[NOT_2̂] · C^{2̂}[NOT_3̂] · rot_3̂[Δt] · C^{2̂}[NOT_3̂] · C^{1̂}[NOT_2̂];

(* plot *)
QuantumPlot[circ1]
QuantumPlot[circ2]
U1 = QuantumMatrix[circ1];
U2 = QuantumMatrix[circ2];
(* compare unitaries *)
psi = ArrayFlatten[KroneckerProduct[{a[0], a[1]}, {a[2], a[3]}, {1, 0}], 1];
Limit[(U1.psi + ϵ) / (U2.psi + ϵ), ϵ → 0]
```

Out[•]=


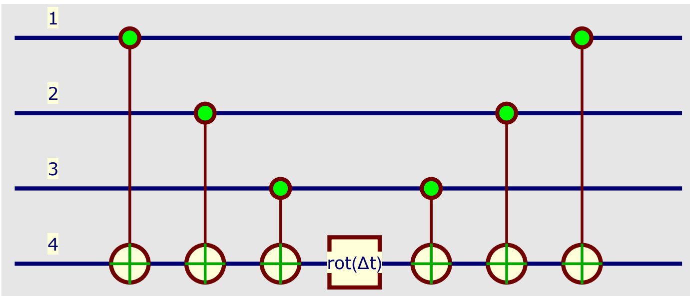
Out[•]=


Out[•]= {1, 1, 1, 1, 1, 1, 1, 1}

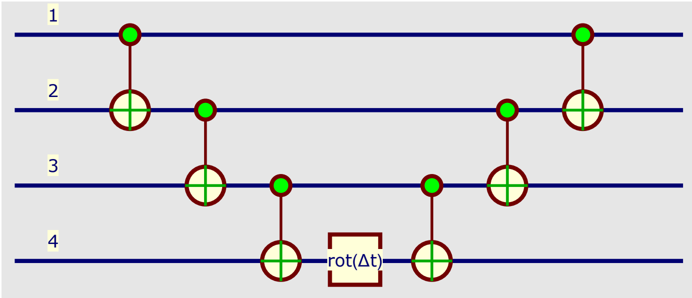
n=3

In[∘]:=
```
Clear[Δt, I2, Z, RZ, U1, U2, rot, psi, circ1, circ2]

I2 = PauliMatrix[0];
Z = PauliMatrix[3];
(* define Rz rotation *)
SetQuantumGate[rot, 1,
  Function[{q1},
   Function[{Δt},
    ⅇ^(-ⅈ Δt) |0_q̂1⟩·⟨0_q̂1| + ⅇ^(+ⅈ Δt) |1_q̂1⟩·⟨1_q̂1|]]];

(* build circuit *)
circ1 =
  C^{1̂}[NOT_4̂] · C^{2̂}[NOT_4̂] · C^{3̂}[NOT_4̂] · rot_4̂[Δt] · C^{3̂}[NOT_4̂] · C^{2̂}[NOT_4̂] · C^{1̂}[NOT_4̂];
circ2 = C^{1̂}[NOT_2̂] · C^{2̂}[NOT_3̂] · C^{3̂}[NOT_4̂] · rot_4̂[Δt] ·
   C^{3̂}[NOT_4̂] · C^{2̂}[NOT_3̂] · C^{1̂}[NOT_2̂];

(* plot *)
QuantumPlot[circ1]
QuantumPlot[circ2]
U1 = QuantumMatrix[circ1];
U2 = QuantumMatrix[circ2];
(* compare unitaries *)
psi = ArrayFlatten[
   KroneckerProduct[{a[0], a[1]}, {a[2], a[3]}, {a[4], a[5]}, {1, 0}], 1];
Limit[(U1.psi + ϵ) / (U2.psi + ϵ), ϵ → 0]
```

Out[∘]=



Out[∘]=

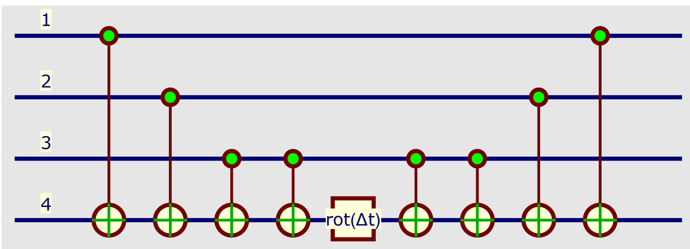


Out[∘]= {1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1}

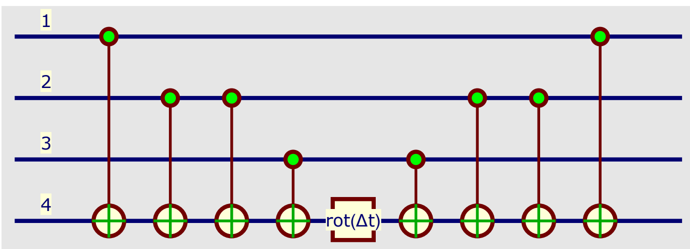
ZZ operations in different pairs of qubits commute -> there is no specific order for the ZZ operations

```
Clear[Δt, I2, Z, RZ, U1, U2, psi]
(* define Rz rotation *)
SetQuantumGate[rot, 1,
  Function[{q1},
   Function[{Δt},
    ⅇ^(-ⅈ Δt) |0_q1̂⟩ · ⟨0_q1̂| + ⅇ^(+ⅈ Δt) |1_q1̂⟩ · ⟨1_q1̂|]]];

(* build circuit *)
circ12 = C^{1̂}[NOT_4̂] · C^{2̂}[NOT_4̂] · C^{3̂}[NOT_4̂] · C^{3̂}[NOT_4̂] ·
   rot_4̂[Δt] · C^{3̂}[NOT_4̂] · C^{3̂}[NOT_4̂] · C^{2̂}[NOT_4̂] · C^{1̂}[NOT_4̂];
circ13 = C^{1̂}[NOT_4̂] · C^{2̂}[NOT_4̂] · C^{2̂}[NOT_4̂] · C^{3̂}[NOT_4̂] ·
   rot_4̂[Δt] · C^{3̂}[NOT_4̂] · C^{2̂}[NOT_4̂] · C^{2̂}[NOT_4̂] · C^{1̂}[NOT_4̂];

(* plot *)
QuantumPlot[circ12]
U12 = QuantumMatrix[circ12];
QuantumPlot[circ13]
U13 = QuantumMatrix[circ13];

(* commutator is zero *)
Abs[U12.U13 - U13.U12] // Total // Total
```

Out[∘]=



Out[∘]=



Out[∘]= 0

Procedurally building a circuit implementing the k^2 operator

In[173]:=
```
(* agrees with Figure 4.3 of Eltohfa
 "Quantum Simulation of Schrödinger's Equation" *)
Clear[Δt, I2, Z, RZ, U1, U2, psi, n, circ]

n = 4;
Δt = π;

(* define Rz rotation *)
SetQuantumGate[rot, 1,
  Function[{q1},
   Function[{Δt},
    e^(-i Δt) |0_q̂1⟩·⟨0_q̂1| + e^(+i Δt) |1_q̂1⟩·⟨1_q̂1|]]];

cnot[i_, j_] := Module[{},
  Return[
   C^{î}[NOT_(n+1)^] · C^{ĵ}[NOT_(n+1)^] · rot_(n+1)^[2^(4 - i - j) Δt] · C^{ĵ}[NOT_(n+1)^] · C^{î}[NOT_(n+1)^]]
 ]

circ = ⊗_{j=1}^{n} rot_ĵ[2^(-n + 4 - j) Δt] · ⊗_{j=1}^{n} ⊗_{m=j+1}^{n} cnot[j, m]

QuantumPlot[circ]
```

Out[178]=

$$\text{rot}_{\hat{1}}\left[\frac{\pi}{2}\right] \cdot \text{rot}_{\hat{2}}\left[\frac{\pi}{4}\right] \cdot \text{rot}_{\hat{3}}\left[\frac{\pi}{8}\right] \cdot \text{rot}_{\hat{4}}\left[\frac{\pi}{16}\right] \cdot C^{\{\hat{1}\}}\left[NOT_{\hat{5}}\right] \cdot C^{\{\hat{2}\}}\left[NOT_{\hat{5}}\right] \cdot \text{rot}_{\hat{5}}[2\,\pi] \cdot$$
$$C^{\{\hat{2}\}}\left[NOT_{\hat{5}}\right] \cdot C^{\{\hat{1}\}}\left[NOT^{2}_{\hat{5}}\right] \cdot C^{\{\hat{3}\}}\left[NOT_{\hat{5}}\right] \cdot \text{rot}_{\hat{5}}[\pi] \cdot C^{\{\hat{3}\}}\left[NOT_{\hat{5}}\right] \cdot C^{\{\hat{1}\}}\left[NOT^{2}_{\hat{5}}\right] \cdot$$
$$C^{\{\hat{4}\}}\left[NOT_{\hat{5}}\right] \cdot \text{rot}_{\hat{5}}\left[\frac{\pi}{2}\right] \cdot C^{\{\hat{4}\}}\left[NOT_{\hat{5}}\right] \cdot C^{\{\hat{1}\}}\left[NOT_{\hat{5}}\right] \cdot C^{\{\hat{2}\}}\left[NOT_{\hat{5}}\right] \cdot C^{\{\hat{3}\}}\left[NOT_{\hat{5}}\right] \cdot$$
$$\text{rot}_{\hat{5}}\left[\frac{\pi}{2}\right] \cdot C^{\{\hat{3}\}}\left[NOT_{\hat{5}}\right] \cdot C^{\{\hat{2}\}}\left[NOT^{2}_{\hat{5}}\right] \cdot C^{\{\hat{4}\}}\left[NOT_{\hat{5}}\right] \cdot \text{rot}_{\hat{5}}\left[\frac{\pi}{4}\right] \cdot C^{\{\hat{4}\}}\left[NOT_{\hat{5}}\right] \cdot$$
$$C^{\{\hat{2}\}}\left[NOT_{\hat{5}}\right] \cdot C^{\{\hat{3}\}}\left[NOT_{\hat{5}}\right] \cdot C^{\{\hat{4}\}}\left[NOT_{\hat{5}}\right] \cdot \text{rot}_{\hat{5}}\left[\frac{\pi}{8}\right] \cdot C^{\{\hat{4}\}}\left[NOT_{\hat{5}}\right] \cdot C^{\{\hat{3}\}}\left[NOT_{\hat{5}}\right]$$

Out[179]=