QM dynamics

Connectivity (hopping) matrix

```
H = {{0, 1, 0, 0, 0, 1}, {1, 0, 1, 0, 0, 0}, {0, 1, 0, 1, 0, 0},
   {0, 0, 1, 0, 1, 0}, {0, 0, 0, 1, 0, 1}, {1, 0, 0, 0, 1, 0}};
H2 = {{0, 0, 1, 0, 1, 0}, {0, 0, 0, 1, 0, 1}, {1, 0, 0, 0, 1, 0},
   {0, 1, 0, 0, 0, 1}, {1, 0, 1, 0, 0, 0}, {0, 1, 0, 1, 0, 0}};
MatrixForm[
 H]
```

$$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

Transfer matrix of Markov proces

```
T = (1 - 2 x^2) * IdentityMatrix[6] + x^2 * H;
MatrixForm[T]
```

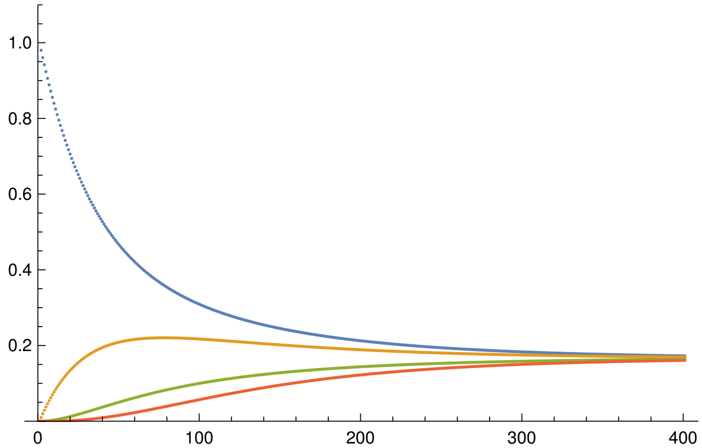
$$\begin{pmatrix} 1-2x^2 & x^2 & 0 & 0 & 0 & x^2 \\ x^2 & 1-2x^2 & x^2 & 0 & 0 & 0 \\ 0 & x^2 & 1-2x^2 & x^2 & 0 & 0 \\ 0 & 0 & x^2 & 1-2x^2 & x^2 & 0 \\ 0 & 0 & 0 & x^2 & 1-2x^2 & x^2 \\ x^2 & 0 & 0 & 0 & x^2 & 1-2x^2 \end{pmatrix}$$

Time step

```
x = 0.1;
```

Markov process starting with particle on site #1

```
Markov[n_, m_] := Module[{x = {1, 0, 0, 0, 0, 0}, u = {0}}, For[i = 0, i < n, i++, x = T.x;
    y = x[[m]];
    AppendTo[u, y]]; u];
ListPlot[{Markov[400, 1], Markov[400, 2], Markov[400, 3], Markov[400, 4]},
 PlotRange → {0, 1.1}]
```



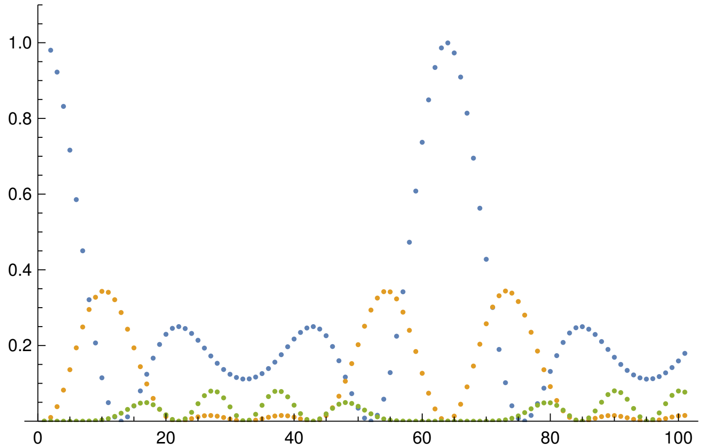
Unitary matrix of QM time evolution U=exp(itH) from particle localized on site #1

```
U = N[MatrixExp[i * x * H]];
MatrixForm[U]
```

$$\begin{pmatrix} 0.990025 + 0.\, i & 0. + 0.0995009\, i & -0.0049792 + 0.\, i & 0. - 0.000332501\, i & -0.0049792 + 0. \\ 0. + 0.0995009\, i & 0.990025 + 0.\, i & 0. + 0.0995009\, i & -0.0049792 + 0.\, i & 0. - 0.000332501 \\ -0.0049792 + 0.\, i & 0. + 0.0995009\, i & 0.990025 + 0.\, i & 0. + 0.0995009\, i & -0.0049792 + 0. \\ 0. - 0.000332501\, i & -0.0049792 + 0.\, i & 0. + 0.0995009\, i & 0.990025 + 0.\, i & 0. + 0.0995009\, i \\ -0.0049792 + 0.\, i & 0. - 0.000332501\, i & -0.0049792 + 0.\, i & 0. + 0.0995009\, i & 0.990025 + 0.\, i \\ 0. + 0.0995009\, i & -0.0049792 + 0.\, i & 0. - 0.000332501\, i & -0.0049792 + 0.\, i & 0. + 0.0995009\, i \end{pmatrix}$$

QM time evolution + measurement x(n)=U^n x(0), y=|x_m(n)|^2

```
Quant[n_, m_] := Module[{x = {1, 0, 0, 0, 0, 0}, u = {0}}, For[i = 0, i < n, i++, x = U.x;
    y = Abs[x[[m]]]^2;
    AppendTo[u, y]]; u];
ListPlot[{Quant[100, 1], Quant[100, 2], Quant[100, 3] Quant[100, 4]},
 PlotRange → {0, 1.1}]
```



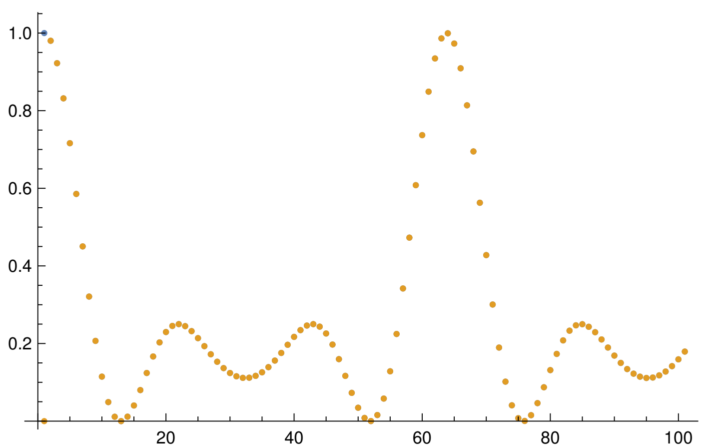
Eigenvalues and eigenvectors of the Hamiltonian H

```
eig = Eigensystem[N[H]];
ee = eig[[1]]
```

```
{2., -2., 1., 1., -1., -1.}
```

Time evolution as above obtained using eigenstates x_m(n)=sum_i <m|i><i|1>exp(itE_i)

```
evec = Module[{x = eig[[2]]}, For[i = 1, i < 7, i++, y = Sqrt[x[[i]].x[[i]]];
    x[[i]] = x[[i]] / y]; x];
Quant2[n_, m_] := Sum[evec[[i]][[1]] * evec[[i]][[m]] * Exp[ⅈ * n * x * ee[[i]]], {i, 1, 6}];
ListPlot[{Table[Abs[Quant2[n, 1]]^2, {n, 0, 100}], Quant[100, 1]}]
```



Gauge freedom - change the phase of each orbital arbitrarily

```
phase = {0.2, 5, 3.45, 1.2, 2, 0};
Regauge[H_, phase_] := Module[{New = H}, For[i = 1, i < 7, i++, For[j = 1, j < 7,
      j++, New[[i]][[j]] = H[[i]][[j]] * Exp[ⅈ * (phase[[j]] - phase[[i]])]]];
   New];
MatrixForm[Regauge[H, phase]]
Eigenvalues[Regauge[H, phase]]
```

$$\begin{pmatrix} 0.+0.\,i & 0.087499-0.996165\,i & 0.+0.\,i & 0.+0.\,i \\ 0.087499+0.996165\,i & 0 & 0.0207948-0.999784\,i & 0.+0.\,i \\ 0.+0.\,i & 0.0207948+0.999784\,i & 0.+0.\,i & -0.628174-0.778073\,i \\ 0.+0.\,i & 0.+0.\,i & -0.628174+0.778073\,i & 0.+0.\,i \\ 0.+0.\,i & 0 & 0.+0.\,i & 0.696707-0.717356\,i \\ 0.980067+0.198669\,i & 0 & 0.+0.\,i & 0.+0.\,i \end{pmatrix}$$

```
{2., -2., -1., 1., -1., 1.}
```

```
Htest = Regauge[H, {1, 2, 3, 4, 5, 6}];
MatrixForm[Htest]
Eigenvalues[Htest]
```

$$\begin{pmatrix} 0 & e^{i} & 0 & 0 & 0 & e^{5i} \\ e^{-i} & 0 & e^{i} & 0 & 0 & 0 \\ 0 & e^{-i} & 0 & e^{i} & 0 & 0 \\ 0 & 0 & e^{-i} & 0 & e^{i} & 0 \\ 0 & 0 & 0 & e^{-i} & 0 & e^{i} \\ e^{-5i} & 0 & 0 & 0 & e^{-i} & 0 \end{pmatrix}$$

```
{-2, 2, -1, -1, 1, 1}
```

This is not a gauge change (each hopping right adds a phase exp(i)). This corresponds to a system with magnetic flux through the ring.

```
Htest2 = {{0, E^I, 0, 0, 0, E^(- I)}, {E^-I, 0, E^I, 0, 0, 0}, {0, E^-I, 0, E^I, 0, 0},
    {0, 0, E^-I, 0, E^I, 0}, {0, 0, 0, E^-I, 0, E^I}, {E^(I), 0, 0, 0, E^-I, 0}};
MatrixForm[Htest2]
Eigenvalues[N[Htest2]]
```

$$\begin{pmatrix} 0 & e^{i} & 0 & 0 & 0 & e^{-i} \\ e^{-i} & 0 & e^{i} & 0 & 0 & 0 \\ 0 & e^{-i} & 0 & e^{i} & 0 & 0 \\ 0 & 0 & e^{-i} & 0 & e^{i} & 0 \\ 0 & 0 & 0 & e^{-i} & 0 & e^{i} \\ e^{i} & 0 & 0 & 0 & e^{-i} & 0 \end{pmatrix}$$

```
{1.99777, -1.99777, -1.0806, 1.0806, 0.917168, -0.917168}
```

Symmetry

Translation to the right

```
P = {{0, 1, 0, 0, 0, 0}, {0, 0, 1, 0, 0, 0}, {0, 0, 0, 1, 0, 0},
   {0, 0, 0, 0, 1, 0}, {0, 0, 0, 0, 0, 1}, {1, 0, 0, 0, 0, 0}};
MatrixForm[
 P]
```

$$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

Abelian group of translations {I,p,p^2,p^3,p^4,p^5}

```
{MatrixForm[P.P], MatrixForm[P.P.P], MatrixForm[P.P.P.P],
 MatrixForm[P.P.P.P.P], MatrixForm[P.P.P.P.P.P]}
```

$$\left\{\begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}\right\}$$

```
{MatrixForm[P.H - H.P], MatrixForm[P.Htest2 - Htest2.P]}
```

$$\left\{\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}\right\}$$

Reflection symmetry 1<->1, 2<->6, 3<->5, 4<->4

```
M = {{1, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 1}, {0, 0, 0, 0, 1, 0},
   {0, 0, 0, 1, 0, 0}, {0, 0, 1, 0, 0, 0}, {0, 1, 0, 0, 0, 0}};
MatrixForm[
 M]
```

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}$$

```
{MatrixForm[M.H - H.M], MatrixForm[M.Htest2 - Htest2.M]}
```

$$\left\{\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -e^{-i}+e^{i} & 0 & 0 & 0 & e^{-i}-e^{i} \\ -e^{-i}+e^{i} & 0 & 0 & 0 & e^{-i}-e^{i} & 0 \\ 0 & 0 & 0 & e^{-i}-e^{i} & 0 & -e^{-i}+e^{i} \\ 0 & 0 & e^{-i}-e^{i} & 0 & -e^{-i}+e^{i} & 0 \\ 0 & e^{-i}-e^{i} & 0 & -e^{-i}+e^{i} & 0 & 0 \\ e^{-i}-e^{i} & 0 & -e^{-i}+e^{i} & 0 & 0 & 0 \end{pmatrix}\right\}$$

For Htest2 clockwise and anti-clockwise hopping is not equivalent (particle picks a phase), therefore Htest2 does not commute with M

```
{MatrixForm[M.Htest2.Inverse[M]], MatrixForm[Htest2]}
```

$$\left\{\begin{pmatrix} 0 & e^{-i} & 0 & 0 & 0 & e^{i} \\ e^{i} & 0 & e^{-i} & 0 & 0 & 0 \\ 0 & e^{i} & 0 & e^{-i} & 0 & 0 \\ 0 & 0 & e^{i} & 0 & e^{-i} & 0 \\ 0 & 0 & 0 & e^{i} & 0 & e^{-i} \\ e^{-i} & 0 & 0 & 0 & e^{i} & 0 \end{pmatrix}, \begin{pmatrix} 0 & e^{i} & 0 & 0 & 0 & e^{-i} \\ e^{-i} & 0 & e^{i} & 0 & 0 & 0 \\ 0 & e^{-i} & 0 & e^{i} & 0 & 0 \\ 0 & 0 & e^{-i} & 0 & e^{i} & 0 \\ 0 & 0 & 0 & e^{-i} & 0 & e^{i} \\ e^{i} & 0 & 0 & 0 & e^{-i} & 0 \end{pmatrix}\right\}$$

Translation and Reflection do not commute

```
MatrixForm[M.P - P.M]
```

$$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 \\ 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}$$

Eigenvalues of P are non-degenerate

```
Eigenvalues[N[P]]
```

$\{-0.5 + 0.866025\, i,\ -0.5 - 0.866025\, i,\ 1. + 0.\, i,\ -1. + 0.\, i,\ 0.5 + 0.866025\, i,\ 0.5 - 0.866025\, i\}$

```
pvec = Transpose[Eigenvectors[N[P]]];
MatrixForm[pvec]
```

$$\begin{pmatrix} -0.204124 - 0.353553\, i & -0.204124 + 0.353553\, i & -0.408248 + 0.\, i & 0.408248 + 0.\, i & \\ 0.408248 + 0.\, i & 0.408248 + 0.\, i & -0.408248 + 0.\, i & -0.408248 + 0.\, i & - \\ -0.204124 + 0.353553\, i & -0.204124 - 0.353553\, i & -0.408248 + 0.\, i & 0.408248 + 0.\, i & 0 \\ -0.204124 - 0.353553\, i & -0.204124 + 0.353553\, i & -0.408248 + 0.\, i & -0.408248 + 0.\, i & 0.4 \\ 0.408248 + 1.11022 \times 10^{-16}\, i & 0.408248 - 1.11022 \times 10^{-16}\, i & -0.408248 + 0.\, i & 0.408248 + 0.\, i & 0 \\ -0.204124 + 0.353553\, i & -0.204124 - 0.353553\, i & -0.408248 + 0.\, i & -0.408248 + 0.\, i & - \end{pmatrix}$$

```
MatrixForm[Round[ConjugateTranspose[pvec].H.pvec, 0.01]]
```

$$\begin{pmatrix} -1. & 0. & 0. & 0. & 0. & 0. \\ 0. & -1. & 0. & 0. & 0. & 0. \\ 0. & 0. & 2. & 0. & 0. & 0. \\ 0. & 0. & 0. & -2. & 0. & 0. \\ 0. & 0. & 0. & 0. & 1. & 0. \\ 0. & 0. & 0. & 0. & 0. & 1. \end{pmatrix}$$

```
H3 = 0.25 H - 0.32 H2;
MatrixForm[H3]
MatrixForm[Round[ConjugateTranspose[pvec].H3.pvec, 0.0001]]
```

$$\begin{pmatrix} 0. & 0.25 & -0.32 & 0. & -0.32 & 0.25 \\ 0.25 & 0. & 0.25 & -0.32 & 0. & -0.32 \\ -0.32 & 0.25 & 0. & 0.25 & -0.32 & 0. \\ 0. & -0.32 & 0.25 & 0. & 0.25 & -0.32 \\ -0.32 & 0. & -0.32 & 0.25 & 0. & 0.25 \\ 0.25 & -0.32 & 0. & -0.32 & 0.25 & 0. \end{pmatrix}$$

$$\begin{pmatrix} 0.07 & 0. & 0. & 0. & 0. & 0. \\ 0. & 0.07 & 0. & 0. & 0. & 0. \\ 0. & 0. & -0.14 & 0. & 0. & 0. \\ 0. & 0. & 0. & -1.14 & 0. & 0. \\ 0. & 0. & 0. & 0. & 0.57 & 0. \\ 0. & 0. & 0. & 0. & 0. & 0.57 \end{pmatrix}$$

```
Eigenvalues[N[M]]
mvec = Transpose[Eigenvectors[N[M]]];
MatrixForm[mvec]
```

{-1., -1., 1., 1., 1., 1.}

$$\begin{pmatrix} 0. & 0. & 1. & 0. & 0. & 0. \\ 0. & 0. & 0. & 0.707107 & 0. & -0.707107 \\ 0.707107 & 0. & 0. & 0. & 0.707107 & 0. \\ 0. & 1. & 0. & 0. & 0. & 0. \\ 0.707107 & 0. & 0. & 0. & -0.707107 & 0. \\ 0. & 0. & 0. & 0.707107 & 0. & 0.707107 \end{pmatrix}$$

```
MatrixForm[Round[ConjugateTranspose[mvec].H3.mvec, 0.0001]]
```

$$\begin{pmatrix} -0.32 & 0.3536 & -0.4525 & 0.25 & 0. & 0. \\ 0.3536 & 0. & 0. & -0.4525 & 0. & 0. \\ -0.4525 & 0. & 0. & 0.3536 & 0. & 0. \\ 0.25 & -0.4525 & 0.3536 & -0.32 & 0. & 0. \\ 0. & 0. & 0. & 0. & 0.32 & -0.25 \\ 0. & 0. & 0. & 0. & -0.25 & 0.32 \end{pmatrix}$$

```
MatrixForm[Round[ConjugateTranspose[pvec].M.pvec, 0.0001]]
```

$$\begin{pmatrix} 0. & -0.5-0.866\,i & 0. & 0. & 0. & 0. \\ -0.5+0.866\,i & 0. & 0. & 0. & 0. & 0. \\ 0. & 0. & 1. & 0. & 0. & 0. \\ 0. & 0. & 0. & 1. & 0. & 0. \\ 0. & 0. & 0. & 0. & 0. & 1. \\ 0. & 0. & 0. & 0. & 1. & 0. \end{pmatrix}$$

```
{MatrixForm[Round[Conjugate[evec].H.Transpose[evec], 0.0001]],
 MatrixForm[Round[Conjugate[evec].P.Transpose[evec], 0.0001]]}
```

$$\left\{\begin{pmatrix} 2. & 0. & 0. & 0. & 0. & 0. \\ 0. & -2. & 0. & 0. & 0. & 0. \\ 0. & 0. & 1. & 0. & 0. & 0. \\ 0. & 0. & 0. & 1. & 0. & 0. \\ 0. & 0. & 0. & 0. & -1. & 0. \\ 0. & 0. & 0. & 0. & 0. & -1. \end{pmatrix}, \begin{pmatrix} 1. & 0. & 0. & 0. & 0. & 0. \\ 0. & -1. & 0. & 0. & 0. & 0. \\ 0. & 0. & 0.5 & 0.866 & 0. & 0. \\ 0. & 0. & -0.866 & 0.5 & 0. & 0. \\ 0. & 0. & 0. & 0. & -0.5 & 0.866 \\ 0. & 0. & 0. & 0. & -0.866 & -0.5 \end{pmatrix}\right\}$$

Translational symmetry

```
klist = Table[Exp[ⅈ * 2 π / 6 * n], {n, 0, 5}]
```

$\left\{1,\ e^{\frac{i\pi}{3}},\ e^{\frac{2i\pi}{3}},\ -1,\ e^{-\frac{2i\pi}{3}},\ e^{-\frac{i\pi}{3}}\right\}$

```
init = {1, 4, ⅈ + 2, 2 - ⅈ * 0.3, 2, 0};
norm = Abs[Conjugate[init].init];
init = init / norm;
init
```

```
{0.0332336, 0.132935, 0.0664673 + 0.0332336 ⅈ, 0.0664673 - 0.00997009 ⅈ, 0.0664673, 0.}
```

```
{0.03323363243602526`, 0.13293452974410103`,
 0.06646726487205051` + 0.03323363243602526` ⅈ,
 0.06646726487205051` - 0.009970089730807577` ⅈ, 0.06646726487205051`, 0.`}
```

```
{0.0332336, 0.132935, 0.0664673 + 0.0332336 ⅈ, 0.0664673 - 0.00997009 ⅈ, 0.0664673, 0.}
```

```
Plist = {IdentityMatrix[6], P, P.P, P.P.P, P.P.P.P, P.P.P.P.P};
```

```
Bloch[n_] := Module[{x = {0, 0, 0, 0, 0, 0}, y = klist[[n + 1]]},
   For[i = 0, i < 6, i++, x = x + y^i * Plist[[i + 1]].init];
   norm = Abs[Conjugate[x].x];
   If[norm > 0.0001, x = x / Sqrt[norm]];
   Round[x, 0.00000001]];
```

```
Conjugate[Bloch[2]].Bloch[2]
```

```
1. + 0. ⅈ
```

```
U = Transpose[{Bloch[0], Bloch[1], Bloch[2], Bloch[3], Bloch[4], Bloch[5]}];
MatrixForm[Round[ConjugateTranspose[U].H3.U, 0.01]]
```

$$\begin{pmatrix} -0.14 & 0. & 0. & 0. & 0. & 0. \\ 0. & 0.57 & 0. & 0. & 0. & 0. \\ 0. & 0. & 0.07 & 0. & 0. & 0. \\ 0. & 0. & 0. & -1.14 & 0. & 0. \\ 0. & 0. & 0. & 0. & 0.07 & 0. \\ 0. & 0. & 0. & 0. & 0. & 0.57 \end{pmatrix}$$

Double chain - the size of the Hilbert space doubles, we can construct the matrices by using tensor products of the 6-site chain and 2-site local problem (You can think about this structure, but there is nothing fundamental in it. It is a trick to generate this particular 12x12 matrices with little effort).

```
hop = {{1, 0.1}, {0.1, 1.5}};
MatrixForm[TensorProduct[H3, hop]]
H3double = ArrayFlatten[TensorProduct[H3, hop], 2];
Hrag = 0.2 * ArrayFlatten[TensorProduct[IdentityMatrix[6], {{0, 1}, {1, 0}}], 2];
Udouble = ArrayFlatten[TensorProduct[U, IdentityMatrix[2]], 2];
MatrixForm[H3double + Hrag]
MatrixForm[Udouble]
```

$$\begin{pmatrix}
\begin{pmatrix} 0. & 0. \\ 0. & 0. \end{pmatrix} & \begin{pmatrix} 0.25 & 0.025 \\ 0.025 & 0.375 \end{pmatrix} & \begin{pmatrix} -0.32 & -0.032 \\ -0.032 & -0.48 \end{pmatrix} & \begin{pmatrix} 0. & 0. \\ 0. & 0. \end{pmatrix} & \begin{pmatrix} -0.32 & -0.03 \\ -0.032 & -0.4 \end{pmatrix} \\
\begin{pmatrix} 0.25 & 0.025 \\ 0.025 & 0.375 \end{pmatrix} & \begin{pmatrix} 0. & 0. \\ 0. & 0. \end{pmatrix} & \begin{pmatrix} 0.25 & 0.025 \\ 0.025 & 0.375 \end{pmatrix} & \begin{pmatrix} -0.32 & -0.032 \\ -0.032 & -0.48 \end{pmatrix} & \begin{pmatrix} 0. & 0. \\ 0. & 0. \end{pmatrix} \\
\begin{pmatrix} -0.32 & -0.032 \\ -0.032 & -0.48 \end{pmatrix} & \begin{pmatrix} 0.25 & 0.025 \\ 0.025 & 0.375 \end{pmatrix} & \begin{pmatrix} 0. & 0. \\ 0. & 0. \end{pmatrix} & \begin{pmatrix} 0.25 & 0.025 \\ 0.025 & 0.375 \end{pmatrix} & \begin{pmatrix} -0.32 & -0.03 \\ -0.032 & -0.4 \end{pmatrix} \\
\begin{pmatrix} 0. & 0. \\ 0. & 0. \end{pmatrix} & \begin{pmatrix} -0.32 & -0.032 \\ -0.032 & -0.48 \end{pmatrix} & \begin{pmatrix} 0.25 & 0.025 \\ 0.025 & 0.375 \end{pmatrix} & \begin{pmatrix} 0. & 0. \\ 0. & 0. \end{pmatrix} & \begin{pmatrix} 0.25 & 0.02 \\ 0.025 & 0.37 \end{pmatrix} \\
\begin{pmatrix} -0.32 & -0.032 \\ -0.032 & -0.48 \end{pmatrix} & \begin{pmatrix} 0. & 0. \\ 0. & 0. \end{pmatrix} & \begin{pmatrix} -0.32 & -0.032 \\ -0.032 & -0.48 \end{pmatrix} & \begin{pmatrix} 0.25 & 0.025 \\ 0.025 & 0.375 \end{pmatrix} & \begin{pmatrix} 0. & 0. \\ 0. & 0. \end{pmatrix} \\
\begin{pmatrix} 0.25 & 0.025 \\ 0.025 & 0.375 \end{pmatrix} & \begin{pmatrix} -0.32 & -0.032 \\ -0.032 & -0.48 \end{pmatrix} & \begin{pmatrix} 0. & 0. \\ 0. & 0. \end{pmatrix} & \begin{pmatrix} -0.32 & -0.032 \\ -0.032 & -0.48 \end{pmatrix} & \begin{pmatrix} 0.25 & 0.02 \\ 0.025 & 0.37 \end{pmatrix}
\end{pmatrix}$$

$$\begin{pmatrix}
0. & 0.2 & 0.25 & 0.025 & -0.32 & -0.032 & 0. & 0. & -0.32 & -0.032 & 0.25 & 0. \\
0.2 & 0. & 0.025 & 0.375 & -0.032 & -0.48 & 0. & 0. & -0.032 & -0.48 & 0.025 & 0. \\
0.25 & 0.025 & 0. & 0.2 & 0.25 & 0.025 & -0.32 & -0.032 & 0. & 0. & -0.32 & -0 \\
0.025 & 0.375 & 0.2 & 0. & 0.025 & 0.375 & -0.032 & -0.48 & 0. & 0. & -0.032 & -0 \\
-0.32 & -0.032 & 0.25 & 0.025 & 0. & 0.2 & 0.25 & 0.025 & -0.32 & -0.032 & 0. & (\\
-0.032 & -0.48 & 0.025 & 0.375 & 0.2 & 0. & 0.025 & 0.375 & -0.032 & -0.48 & 0. & (\\
0. & 0. & -0.32 & -0.032 & 0.25 & 0.025 & 0. & 0.2 & 0.25 & 0.025 & -0.32 & -0 \\
0. & 0. & -0.032 & -0.48 & 0.025 & 0.375 & 0.2 & 0. & 0.025 & 0.375 & -0.032 & -0 \\
-0.32 & -0.032 & 0. & 0. & -0.32 & -0.032 & 0.25 & 0.025 & 0. & 0.2 & 0.25 & 0. \\
-0.032 & -0.48 & 0. & 0. & -0.032 & -0.48 & 0.025 & 0.375 & 0.2 & 0. & 0.025 & 0. \\
0.25 & 0.025 & -0.32 & -0.032 & 0. & 0. & -0.32 & -0.032 & 0.25 & 0.025 & 0. & 0 \\
0.025 & 0.375 & -0.032 & -0.48 & 0. & 0. & -0.032 & -0.48 & 0.025 & 0.375 & 0.2 & (
\end{pmatrix}$$

$$\begin{pmatrix}
0.407424 + 0.025927\,i & 0. + 0.\,i & -0.202615 + 0.35442\,i & 0. + 0.\,i \\
0. + 0.\,i & 0.407424 + 0.025927\,i & 0. + 0.\,i & -0.202615 + 0.35442 \\
0.407424 + 0.025927\,i & 0. + 0.\,i & 0.205629 + 0.35268\,i & 0. + 0.\,i \\
0. + 0.\,i & 0.407424 + 0.025927\,i & 0. + 0.\,i & 0.205629 + 0.35268\,i \\
0.407424 + 0.025927\,i & 0. + 0.\,i & 0.408245 - 0.00174006\,i & 0. + 0.\,i \\
0. + 0.\,i & 0.407424 + 0.025927\,i & 0. + 0.\,i & 0.408245 - 0.0017400 \\
0.407424 + 0.025927\,i & 0. + 0.\,i & 0.202615 - 0.35442\,i & 0. + 0.\,i \\
0. + 0.\,i & 0.407424 + 0.025927\,i & 0. + 0.\,i & 0.202615 - 0.35442\,i \\
0.407424 + 0.025927\,i & 0. + 0.\,i & -0.205629 - 0.35268\,i & 0. + 0.\,i \\
0. + 0.\,i & 0.407424 + 0.025927\,i & 0. + 0.\,i & -0.205629 - 0.35268 \\
0.407424 + 0.025927\,i & 0. + 0.\,i & -0.408245 + 0.00174006\,i & 0. + 0.\,i \\
0. + 0.\,i & 0.407424 + 0.025927\,i & 0. + 0.\,i & -0.408245 + 0.0017400
\end{pmatrix}$$

```
MatrixForm[Round[ConjugateTranspose[Udouble].(H3double + Hrag).Udouble, 0.00001]]
```

$$
\begin{pmatrix}
-0.14 & 0.186 & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. \\
0.186 & -0.21 & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. \\
0. & 0. & 0.57 & 0.257 & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. \\
0. & 0. & 0.257 & 0.855 & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. \\
0. & 0. & 0. & 0. & 0.07 & 0.207 & 0. & 0. & 0. & 0. & 0. & 0. \\
0. & 0. & 0. & 0. & 0.207 & 0.105 & 0. & 0. & 0. & 0. & 0. & 0. \\
0. & 0. & 0. & 0. & 0. & 0. & -1.14 & 0.086 & 0. & 0. & 0. & 0. \\
0. & 0. & 0. & 0. & 0. & 0. & 0.086 & -1.71 & 0. & 0. & 0. & 0. \\
0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0.07 & 0.207 & 0. & 0. \\
0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0.207 & 0.105 & 0. & 0. \\
0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0.57 & 0.257 \\
0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0.257 & 0.855
\end{pmatrix}
$$