Quantum simulation of the single-particle Schrödinger equation

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Introduction

In this notebook we simulate 1D linear Schrödinger equation with different external potentials.

Fig. 3. a) Linear potential

In[1]:=
```
(* clear variables *)
Clear[psi0, n, Nv, psi, x, x0, FN, expK, expV, U, FNinv, p]

(* normalization *)
ℏ = m = 1;
(* parameters *)
n = 7; x0 = -2.5; p0 = 0; σ = 0.5;

(* coordinate domain *)
Nv = 2^n;
x = Table[x, {x, -5, 5, 10 / (Nv - 1)}] // N;
p = 2 π RotateLeft[x, Nv / 2];

(* initial wavefunction *)
psi0 = 1/(Sqrt[Sqrt[π] σ]) Exp[-((x - x0)^2)/(2 σ^2) + I/ℏ (p0 (x - x0))];(**)
(* normalization will depend on resolution n *)
η = (psi0 // Conjugate).psi0;
psi0 = 1 / Sqrt[η] psi0;

(* time evolve *)
tdim = 50;
ϵ = π / 100;
tmax = tdim ϵ;
```

```
dt = tmax / tdim // N;

(* partial operators *)
expK = MatrixExp[-I DiagonalMatrix[ p^2 / (2 m)  ] 1 / ℏ ϵ];
expV = MatrixExp[-I DiagonalMatrix[ -4.8 x  ] 1 / ℏ ϵ];

(*Fourier matrix*)
FN = FourierMatrix[Nv, FourierParameters → {0, -1}];
FNinv  = ConjugateTranspose[FN];
(* one time-step evolution *)
U = FNinv.expK.FN.expV;

(* lists *)
psilst = {};
normlst = {};

(* time evolve *)
psi  = psi0;
For[t = 0, t < tdim, t++,
 AppendTo[psilst, Abs[psi] ^ 2];
 AppendTo[normlst, (psi // Conjugate).psi];
 psi = U.psi;
]

(* plot *)
MatrixPlot[psilst // Transpose, AspectRatio → 1,
 ColorFunction → "SunsetColors", PlotLegends → Automatic]
```

Out[23]=

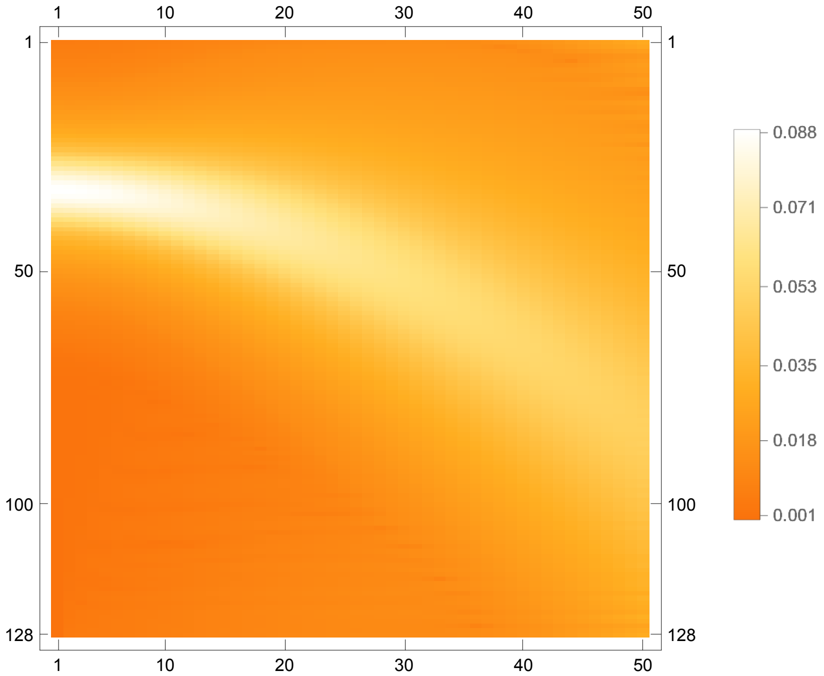

Fig. 3. b) Square barrier potential

```
In[24]:= (* clear variables *)
Clear[psi0, n, Nv, psi, x, x0, FN, expK, expV, U, FNinv, p]

(* normalization *)
ℏ = m = 1;
(* parameters *)
n = 7; x0 = 3; p0 = -10; σ = 0.5;

(* coordinate domain *)
Nv = 2^n;
x = Table[x, {x, -5, 5, 10 / (Nv - 1)}] // N;
p = 2 π RotateLeft[x, Nv / 2];

(* initial wavefunction *)
psi0 = 1/(Sqrt[Sqrt[π] σ]) Exp[-(x - x0)^2/(2 σ^2) + I/ℏ (p0 (x - x0))]; (**)
(* normalization will depend on resolution n *)
η = (psi0 // Conjugate).psi0;
psi0 = 1 / Sqrt[η] psi0;

(* time evolve *)
tdim = 100;
ϵ = π / 200;
tmax = tdim ϵ;
dt = tmax / tdim // N;

(* partial operators *)
expK = MatrixExp[-I DiagonalMatrix[ p^2 / (2 m) ] 1 / ℏ ϵ];
expV = MatrixExp[-I DiagonalMatrix[
      Table[If[-2.66 < x[[i]] < -1.875, 43.9, 0], {i, 1, Nv}] ] 1 / ℏ ϵ];

(*Fourier matrix*)
FN = FourierMatrix[Nv, FourierParameters → {0, -1}];
FNinv = ConjugateTranspose[FN];
(* one time-step evolution *)
U = FNinv.expK.FN.expV;

(* lists *)
psilst = {};
normlst = {};

(* time evolve *)
psi = psi0;
For[t = 0, t < tdim, t++,
```

```
 AppendTo[psilst, Abs[psi]^2];
 AppendTo[normlst, (psi // Conjugate).psi];
 psi = U.psi;
]

(* plot *)
MatrixPlot[psilst // Transpose, AspectRatio → 1,
 ColorFunction → "SunsetColors", PlotLegends → Automatic]
```

Out[46]=

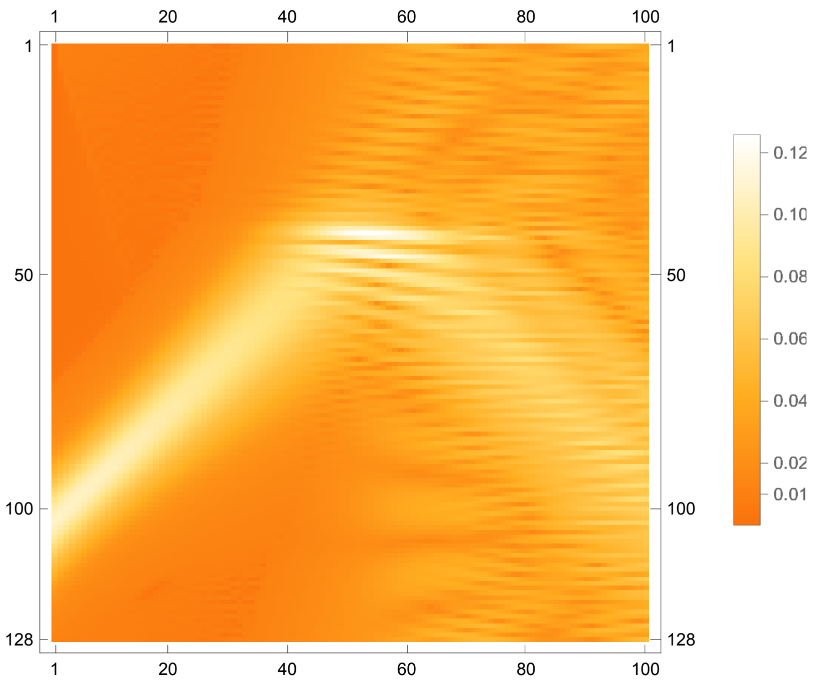

Fig. 3. c) Quadratic potential

In[47]:=

```
(* clear variables *)
Clear[psi0, n, Nv, psi, x, x0, FN, expK, expV, U, FNinv, p]

(* normalization *)
ℏ = m = 1;
(* parameters *)
n = 7; x0 = -2.5; p0 = 0; σ = 2;

(* coordinate domain *)
Nv = 2^n;
x = Table[x, {x, -5, 5, 10 / (Nv - 1)}] // N;
p = 2 π RotateLeft[x, Nv / 2];

(* initial wavefunction *)
psi0 = 1/Sqrt[Sqrt[π] σ] Exp[-(x - x0)^2/(2 σ^2) + I/ℏ (p0 (x - x0))]; (**)
(* normalization will depend on resolution n *)
η = (psi0 // Conjugate).psi0;
```

```
psi0 = 1 / Sqrt[η] psi0;

(* time evolve *)
tdim = 50;
ϵ = π / 10;
tmax = tdim ϵ;
dt = tmax / tdim // N;

(* partial operators *)
expK = MatrixExp[-I DiagonalMatrix[ p^2 / (2 m)  ] 1 / ℏ ϵ];
expV = MatrixExp[-I DiagonalMatrix[ x^2 / 2  ] 1 / ℏ ϵ];

(*Fourier matrix*)
FN = FourierMatrix[Nv, FourierParameters → {0, -1}];
FNinv = ConjugateTranspose[FN];
(* one time-step evolution *)
U = FNinv.expK.FN.expV;

(* lists *)
psilst = {};
normlst = {};

(* time evolve *)
psi = psi0;
For[t = 0, t < tdim, t++,
 AppendTo[psilst, Abs[psi] ^ 2];
 AppendTo[normlst, (psi // Conjugate).psi];
 psi = U.psi;
]

(* plot *)
MatrixPlot[psilst // Transpose, AspectRatio → 1,
 ColorFunction → "SunsetColors", PlotLegends → Automatic]
```

Out[69]=

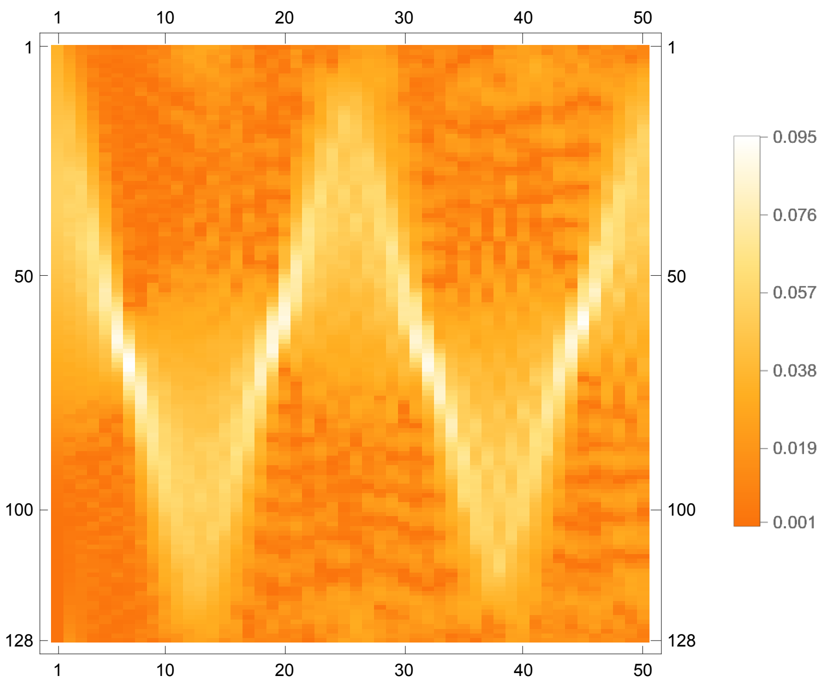

Fig. 3. d) Cubic potential

In[70]:=
```
(* clear variables *)
Clear[psi0, n, Nv, psi, x, x0, FN, expK, expV, U, FNinv, p]

(* normalization *)
ħ = m = 1;
(* parameters *)
n = 7; x0 = -2.5; p0 = 0; σ = 1;

(* coordinate domain *)
Nv = 2^n;
x = Table[x, {x, -5, 5, 10 / (Nv - 1)}] // N;
p = 2 π RotateLeft[x, Nv / 2];

(* initial wavefunction *)
psi0 = 1/(Sqrt[Sqrt[π] σ]) Exp[-((x - x0)^2)/(2 σ^2) + I/ħ (p0 (x - x0))]; (**)
(* normalization will depend on resolution n *)
η = (psi0 // Conjugate).psi0;
psi0 = 1 / Sqrt[η] psi0;

(* time evolve *)
tdim = 50;
ϵ = π / 10;
tmax = tdim ϵ;
dt  = tmax / tdim // N;
```

```
(* partial operators *)
expK = MatrixExp[-I DiagonalMatrix[ p^2 / (2 m) ] 1 / ℏ ϵ];
expV = MatrixExp[-I DiagonalMatrix[
      Table[If[x⟦i⟧ > 0, x⟦i⟧^2 / 2, -0.4 x⟦i⟧^3], {i, 1, Nv}] ] 1 / ℏ ϵ];

(*Fourier matrix*)
FN = FourierMatrix[Nv, FourierParameters → {0, -1}];
FNinv = ConjugateTranspose[FN];
(* one time-step evolution *)
U = FNinv.expK.FN.expV;

(* lists *)
psilst = {};
normlst = {};

(* time evolve *)
psi = psi0;
For[t = 0, t < tdim, t++,
 AppendTo[psilst, Abs[psi]^2];
 AppendTo[normlst, (psi // Conjugate).psi];
 psi = U.psi;
]

(* plot *)
MatrixPlot[psilst // Transpose, AspectRatio → 1,
 ColorFunction → "SunsetColors", PlotLegends → Automatic]
```

Out[92]=