Quantum Computation and Visualization of Hamiltonians Using Discrete Quantum Mechanics and IBM QISKit

Raffaele Miceli and Michael McGuigan, arXiv:1812.01044v1 [quant-ph] (2018)
Notebook: Óscar Amaro, December 2022 @ GoLP-EPP

Introduction

In this notebook we reproduce some results from the paper.

Main takeaway:
- analytical equalities may be exact in theory, but in matrix form may lead to inconsistencies that then reflect on different eigenspectra.

Figure 1

In[160]:=
```
(* n=5 can be very slow on some computers *)
Clear[n, A, Adg, Id, Idtil, HhoEnergy,
 HhoPos, HhoEnergyE, X, P, Xpos, Ppos, F, Fdg]

(* number of qubits*)
n = 5;

Id = ParallelTable[δ_{i-j} , {i, 1, 2^n, 1}, {j, 1, 2^n, 1}];

(* equation 5: define A *)
A = ParallelTable[Sqrt[j] δ_{i-1-j} , {i, 1, 2^n, 1}, {j, 1, 2^n, 1}];

(* define A dagger *)
Adg = ConjugateTranspose[A];

(* equation 17 *)
Adg.A - A.Adg;

(* using this form would give the exact result for the eigenenergies*)
```

```
A.Adg + Id / 2 ;

(* equation 14: we use this instead  *)
HhoEnergy = 0.5 (A.Adg + Adg.A);
(* eigenvalues will appear in reverse order*)
HhoEnergyE = Eigenvalues[HhoEnergy];

ordE = Ordering[HhoEnergyE];
HhoEnergyE = HhoEnergyE[[ordE]];

(* equation 6: position momentum operators  *)
(*X=1/√2 (Adg+A);P=I/√2 (Adg-A);*)
```

$$\text{Xpos} = \text{Sqrt}\left[\frac{2\,\pi}{2\,\hat{}\,n}\right]\ \text{Table}\left[\frac{2\,j-1-2\,\hat{}\,n}{2}\ \delta_{i-j}\ ,\ \{i,\ 1,\ 2\,\hat{}\,n,\ 1\},\ \{j,\ 1,\ 2\,\hat{}\,n,\ 1\}\right];$$

$$\text{F} = \frac{1}{\text{Sqrt}[2\,\hat{}\,n]}\ \text{Table}\left[\text{Exp}\left[\frac{2\,\pi\,\text{I}}{2\,\hat{}\,n}\ \left(\frac{2\,i-1-2\,\hat{}\,n}{2}\right)\ \left(\frac{2\,j-1-2\,\hat{}\,n}{2}\right)\right]\ ,\ \{i,\ 1,\ 2\,\hat{}\,n,\ 1\},\ \{j,\ 1,\ 2\,\hat{}\,n,\ 1\}\right];$$

```
Fdg = ConjugateTranspose[F] // N;
Ppos = F.Xpos.Fdg // N;

(* equation 18: (P.P+X.X)/2 would give the exact result, instead we use  *)
Idtil = Adg.A - A.Adg;
HhoPos = ((Xpos.Xpos // N) + (Ppos.Ppos // N)) / 2 // Chop;
HhoPosE = Eigenvalues[HhoPos];
ordP = Ordering[HhoPosE];
HhoPosE = HhoPosE[[ordP]];

(* equation 13: exact theoretical values *)
HhoExactE = ParallelTable[i + 0.5, {i, 0, 2^n - 1, 1}];

(* compare *)
ListPlot[{HhoPosE, HhoEnergyE, HhoExactE},
 PlotLegends → {"Position", "Energy", "Exact"},
 Joined → True, AxesLabel → {"Eigenvalue", "Energy"},
 PlotLabel → "Fig 1 QHO Comparison, Matrix Size = 32 x 32"]
```

Out[181]=

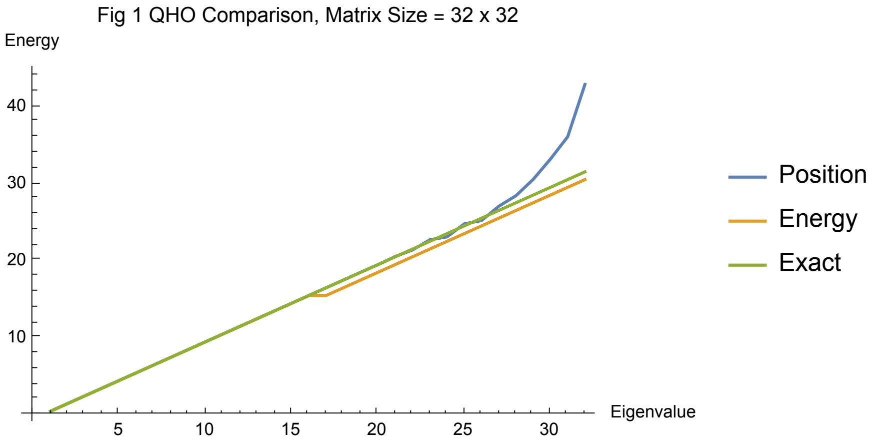


Fig 1 QHO Comparison, Matrix Size = 32 x 32
Energy
40
30
20
10
5
10
15
20
25
30
Eigenvalue
Position
Energy
Exact

Figures 3 and 4

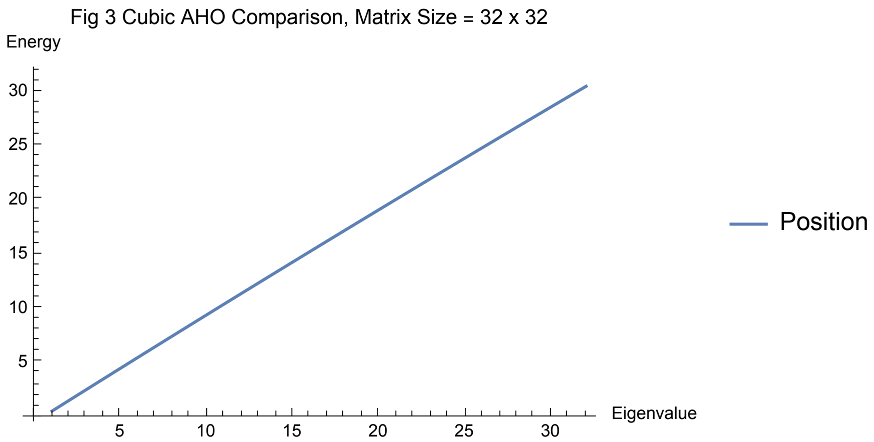
In[21]:=
```
(*   *)
Clear[n, A, Adg, Id, Idtil, HhoEnergy,
 HhoPos, HhoEnergyE, X, P, Xpos, Ppos, F, Fdg, λ]

n = 5;
λ = 0.05;
HcubExactE = ParallelTable[(i + 0.5) - (5 λ^2)/12 (i^2 + i + 11/30), {i, 0, 2^n - 1, 1}];
HquaExactE = ParallelTable[(i + 0.5) + (3 λ)/8 (i^2 + i + 1/2) -
    (λ^2)/64 (17 i^3 + 51/2 i^2 + 59/2 i + 21/2), {i, 0, 2^n - 1, 1}];


ListPlot[{HcubExactE}, PlotLegends → {"Position", "Energy", "Exact"},
 Joined → True, AxesLabel → {"Eigenvalue", "Energy"},
 PlotLabel → "Fig 3 Cubic AHO Comparison, Matrix Size = 32 x 32"]

(* equation 22 does not seem to reproduce figure 4*)
ListPlot[{HquaExactE}, PlotLegends → {"Position", "Energy", "Exact"},
 Joined → True, AxesLabel → {"Eigenvalue", "Energy"},
 PlotLabel → "Fig 4 Quartic AHO Comparison, Matrix Size = 32 x 32"]
```

Out[26]=



Out[27]=

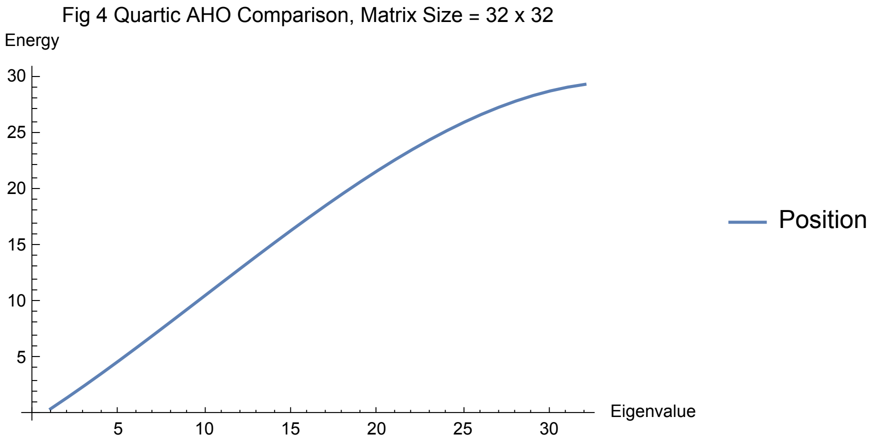


Fig 4 Quartic AHO Comparison, Matrix Size = 32 x 32
Energy
30
25
20
15
10
5
5
10
15
20
25
30
Eigenvalue
Position