Benchmarks for QDyn

All equations and calculations are in atomic units.

In[69]:=
```
ℏ = 1;
me = 1;
e = 1;
ϵ0 = 1 / 4 / Pi;
```

Imaginary - time dynamics

Harmonic oscillator 1D

Harmonic oscillator with potential in form:

$$V(x) = \frac{1}{2} m\, \omega^2 x^2$$

Exact energies correspond to the following formula:

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right), \quad n = 0, 1, 2, \ldots$$

In[73]:=
```
ω = 0.1;
m = 1;
V = 1 / 2 * m * ω^2 * x^2
```

Out[75]=

$0.005\, x^2$

Energies for benchmark

In[76]:=
```
Table[{n, ℏ * ω * (1 / 2 + n)}, {n, 0, 9}] // TableForm
```

Out[76]//TableForm=

0	0.05
1	0.15
2	0.25
3	0.35
4	0.45
5	0.55
6	0.65
7	0.75
8	0.85
9	0.95

In[77]:=
```
Clear[ω, m, V]
```

Morse potential 1D

Harmonic oscillator with potential in form:

$$V(x) = D_e\left(1 - e^{-a(r-r_e)}\right)^2 - D_e$$

Exact energies correspond to the following formula:

$$E_n = h\nu_0\left(n + \frac{1}{2}\right) - \frac{\left[h\nu_0\left(n+\frac{1}{2}\right)\right]^2}{4D_e}, \quad n = 0, 1, 2, \ldots \lambda - \frac{1}{2}$$

[Solution according to https://en.wikipedia.org/wiki/Morse_potential]

This Morse potential should correspond to one of the states of the N2 molecule.

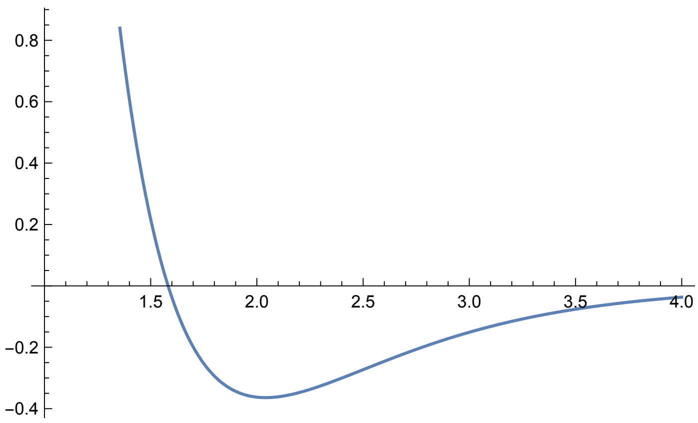
In[78]:=
```
h = ℏ * 2 * Pi;
De = 0.364;
re = 2.041;
a = 1.51;
m = 1834 * 28;
ν0 = a / 2 / Pi * Sqrt[2 * De / m];
V[r_] = De * (1 - Exp[-a * (r - re)]) ^ 2 - De
```

Out[84]=

$$-0.364 + 0.364\left(1 - e^{-1.51(-2.041+r)}\right)^2$$

In[85]:=
```
Plot[V[x], {x, 1, 4}]
```

Out[85]=



Energies for benchmark

```
In[86]:= Table[{n, h * ν0 * (1 / 2 + n) - (h * ν0 * (1 / 2 + n)) ^ 2 / (4 * De) - De}, {n, 0, 9}] //
  TableForm
```

Out[86]//TableForm=

0	-0.361163
1	-0.355522
2	-0.349925
3	-0.344373
4	-0.338865
5	-0.333402
6	-0.327983
7	-0.322608
8	-0.317278
9	-0.311992

```
In[87]:= Clear[ν0, m, V, a, re, De, h]
```

Harmonic oscillator 2D - symmetric

Harmonic oscillator with potential in form:

$$V(x, y) = \frac{1}{2} m\, \omega_x^2 x^2 + \frac{1}{2} m\, \omega_y^2 y^2$$

Exact energies correspond to the following formula:

$$E_{n_x,n_y} = \hbar\omega \left(n_x + n_y + 1\right), \quad n_x, n_y = 0, 1, 2, \ldots$$

```
In[88]:= ωx = 0.1; ωy = 0.1;
m = 1;
V = 1 / 2 * m * ωx ^ 2 * x ^ 2 + 1 / 2 * m * ωy ^ 2 * y ^ 2
```

Out[90]=

$0.005\, x^2 + 0.005\, y^2$

Energies for benchmark

```
In[91]:= data = Table[{nx, ny, ℏ * (ωx * (1 / 2 + nx) + ωy * (1 / 2 + ny))}, {nx, 0, 4}, {ny, 0, 4}]
```

Out[91]=

```
{{{0, 0, 0.1}, {0, 1, 0.2}, {0, 2, 0.3}, {0, 3, 0.4}, {0, 4, 0.5}},
 {{1, 0, 0.2}, {1, 1, 0.3}, {1, 2, 0.4}, {1, 3, 0.5}, {1, 4, 0.6}},
 {{2, 0, 0.3}, {2, 1, 0.4}, {2, 2, 0.5}, {2, 3, 0.6}, {2, 4, 0.7}},
 {{3, 0, 0.4}, {3, 1, 0.5}, {3, 2, 0.6}, {3, 3, 0.7}, {3, 4, 0.8}},
 {{4, 0, 0.5}, {4, 1, 0.6}, {4, 2, 0.7}, {4, 3, 0.8}, {4, 4, 0.9}}}
```

In[92]:=
```
Sort[ArrayReshape[data[[ ;; , ;; , 3]], 5 * 5]][[ ;; 10]] // TableForm
```
Out[92]//TableForm=
```
0.1
0.2
0.2
0.3
0.3
0.3
0.4
0.4
0.4
0.4
```

In[93]:=
```
Clear[m, ωx, ωy, V, data]
```

Harmonic oscillator 2D - asymmetric

Harmonic oscillator with potential in form:

$$V(x, y) = \frac{1}{2} m \omega_x^2 x^2 + \frac{1}{2} m \omega_y^2 y^2$$

Exact energies correspond to the following formula:

$$E_{n_x, n_y} = \hbar \left[\omega_x \left(n_x + \frac{1}{2}\right) + \omega_y \left(n_y + \frac{1}{2}\right)\right], \quad n_x, n_y = 0, 1, 2, \ldots$$

In[94]:=
```
ωx = 0.1; ωy = 0.15;
mx = 1; my = 2;
V = 1 / 2 * mx * ωx ^ 2 * x ^ 2 + 1 / 2 * my * ωy ^ 2 * y ^ 2
```
Out[96]=

$0.005\, x^2 + 0.0225\, y^2$

Energies for benchmark

In[97]:=
```
data = Table[{nx, ny, ℏ * (ωx * (1 / 2 + nx) + ωy * (1 / 2 + ny))}, {nx, 0, 4}, {ny, 0, 4}]
```
Out[97]=
```
{{{0, 0, 0.125}, {0, 1, 0.275}, {0, 2, 0.425}, {0, 3, 0.575}, {0, 4, 0.725}},
 {{1, 0, 0.225}, {1, 1, 0.375}, {1, 2, 0.525}, {1, 3, 0.675}, {1, 4, 0.825}},
 {{2, 0, 0.325}, {2, 1, 0.475}, {2, 2, 0.625}, {2, 3, 0.775}, {2, 4, 0.925}},
 {{3, 0, 0.425}, {3, 1, 0.575}, {3, 2, 0.725}, {3, 3, 0.875}, {3, 4, 1.025}},
 {{4, 0, 0.525}, {4, 1, 0.675}, {4, 2, 0.825}, {4, 3, 0.975}, {4, 4, 1.125}}}
```

In[98]:=
```
Sort[ArrayReshape[data[[ ;; , ;; , 3]], 5 * 5]][[ ;; 10]] // TableForm
```

Out[98]//TableForm=
```
0.125
0.225
0.275
0.325
0.375
0.425
0.425
0.475
0.525
0.525
```

In[99]:=
```
Clear[m, ωx, ωy, V, data]
```

Harmonic oscillator 3D - symmetric

Harmonic oscillator with potential in form:

$$V(x, y, z) = \frac{1}{2} m\, \omega_x^2 x^2 + \frac{1}{2} m\, \omega_y^2 y^2 + \frac{1}{2} m\, \omega_z^2 z^2$$

Exact energies correspond to the following formula:

$$E_{n_x, n_y, n_z} = \hbar\omega\left(n_x + n_y + n_z + \frac{3}{2}\right), \quad n_x, n_y, n_z = 0, 1, 2, \ldots$$

In[100]:=
```
ωx = 0.1; ωy = 0.1; ωz = 0.1;
m = 1;
V = 1 / 2 * m * ωx ^ 2 * x ^ 2 + 1 / 2 * m * ωy ^ 2 * y ^ 2 + 1 / 2 * m * ωz ^ 2 * z ^ 2
```

Out[102]=

$0.005\, x^2 + 0.005\, y^2 + 0.005\, z^2$

Energies for benchmark

In[103]:=
```
data = Table[{nx, ny, nz, ℏ * (ωx * (1 / 2 + nx) + ωy * (1 / 2 + ny) + ωz * (1 / 2 + nz))},
   {nx, 0, 4}, {ny, 0, 4}, {nz, 0, 4}];
```

In[104]:=

```
Sort[ArrayReshape[data⟦ ;; , ;; , ;; , 4⟧, 5 * 5 * 5]]⟦ ;; 10⟧ // TableForm
```

Out[104]//TableForm=

```
0.15
0.25
0.25
0.25
0.35
0.35
0.35
0.35
0.35
0.35
```

In[105]:=

```
Clear[m, ωx, ωy, ωz, V, data]
```

Harmonic oscillator 3D - asymmetric

Harmonic oscillator with potential in form:

$$V(x, y, z) = \frac{1}{2} m\,\omega_x^2 x^2 + \frac{1}{2} m\,\omega_y^2 y^2 + \frac{1}{2} m\,\omega_z^2 z^2$$

Exact energies correspond to the following formula:

$$E_{n_x,n_y,n_z} = \hbar\left[\omega_x\left(n_x + \frac{1}{2}\right) + \omega_y\left(n_y + \frac{1}{2}\right) + \omega_z\left(n_z + \frac{1}{2}\right)\right], \quad n_x, n_y, n_z = 0, 1, 2, \ldots$$

In[106]:=

```
ωx = 0.1; ωy = 0.07; ωz = 0.13;
mx  = 1; my  = 2; mz  = 3;
V = 1 / 2 * mx * ωx ^ 2 * x ^ 2 + 1 / 2 * my * ωy ^ 2 * y ^ 2 + 1 / 2 * mz * ωz ^ 2 * z ^ 2
```

Out[108]=

$0.005\,x^2 + 0.0049\,y^2 + 0.02535\,z^2$

Energies for benchmark

In[109]:=

```
data = Table[{nx, ny, nz, ℏ * (ωx * (1 / 2 + nx) + ωy * (1 / 2 + ny) + ωz * (1 / 2 + nz))},
   {nx, 0, 4}, {ny, 0, 4}, {nz, 0, 4}];
```

In[110]:=

```
Sort[ArrayReshape[data[[ ;; , ;; , ;; , 4]], 5 * 5 * 5]][[ ;; 10]] // TableForm
```

Out[110]//TableForm=

```
0.15
0.22
0.25
0.28
0.29
0.32
0.35
0.35
0.36
0.38
```

In[111]:=

```
Clear[m, ωx, ωy, ωz, V, data]
```

Harmonic oscillator 3D - spherical

The purpose of this test is to probe the ability of the code to deal with spherical harmonics and their degeneracy. The spherical harmonic oscillator has energies depending on both the radial quantum number and also the angular quantum number. Further more, it is degenerate by the magnetic quantum number.

Harmonic oscillator with potential in form:

$$V(x, y, z) = \frac{1}{2} m\, \omega^2 \left(x^2 + y^2 + z^2\right)$$

Exact energies correspond to the following formula:

$$E_n = \hbar\omega\left(n + \frac{3}{2}\right); \qquad n = 0, 1, 2, \ldots$$

with degeneracy of the n-th level is $\frac{(n+1)(n+2)}{2}$.

Other way to write the formula is

$$E_{v,l} = \hbar\omega\left(2\, v + l + \frac{3}{2}\right); \qquad v, l = 0, 1, 2, \ldots$$

where v is the quantum number for the radial part of Ψ and l is the quantum number of the angular part of Ψ. Note that each of these energy levels is also degenerate by m_l quantum number which goes from $-l$ to l.

In[112]:=

```
ω = 0.1
m = 2
V = 1 / 2 * m * ω ^ 2 * (x ^ 2 + y ^ 2 + z ^ 2)
```

Out[112]=

0.1

Out[113]=

2

Out[114]=

$0.01\left(x^2+y^2+z^2\right)$

Energies for benchmark

In[115]:=

```
data = Table[{nu, l, ml, ℏ * ω * (3 / 2 + 2 * nu + l)}, {nu, 0, 4}, {l, 0, 4}, {ml, -l, l}];
```

In[116]:=

```
Sort[ArrayReshape[data⟦ ;; , ;; , ;; , 4⟧, 5 * 5 * 5]]⟦ ;; 12⟧ // TableForm
```

Out[116]//TableForm=

```
0.15
0.25
0.25
0.25
0.35
0.35
0.35
0.35
0.35
0.35
0.45
0.45
```

In[117]:=

```
Clear[m, ω, V, data]
```

Hydrogen atom 3D

Hydrogen atom potential has form:

$$V(x, y, z) = -\frac{e^2}{4\pi\epsilon_0 r}$$

Exact energies correspond to the following formula:

$$E_n = \frac{m_e e^4}{2(4\pi\epsilon_0)^2 (h/2\pi)^2}\frac{1}{n^2}; \qquad n = 1, 2, 3, \ldots$$

In[118]:=

```
V = - (e^2) / (4 * Pi * ϵ0 * (x^2 + y^2 + z^2) ^0.5)
```

Out[118]=

$$-\frac{1}{\left(x^2+y^2+z^2\right)^{0.5}}$$

Energies for benchmark

In[119]:=

```
data = Table[{n, l, ml, -me * e^4 / ( 2 * (4 * Pi * ϵ0) ^2 * ℏ^2) / n^2},
   {n, 1, 5}, {l, 0, n - 1}, {ml, -l, l}];
```

In[120]:=

```
Sort[ArrayReshape[data⟦ ;; , ;; , ;; , 4⟧, Sum[n^2, {n, 1, 5}]]]⟦ ;; 15⟧ //
 TableForm
```

Out[120]//TableForm=

$-\frac{1}{2}$
$-\frac{1}{8}$
$-\frac{1}{8}$
$-\frac{1}{8}$
$-\frac{1}{8}$
$-\frac{1}{18}$
$-\frac{1}{18}$
$-\frac{1}{18}$
$-\frac{1}{18}$
$-\frac{1}{18}$
$-\frac{1}{18}$
$-\frac{1}{18}$
$-\frac{1}{18}$
$-\frac{1}{18}$
$-\frac{1}{32}$

In[121]:=

```
Clear[m, ω, V, data]
```

Real - time dynamics

Harmonic oscillator 1D

Harmonic oscillator with potential in form:

$$V(x) = \frac{1}{2} m\, \omega^2 x^2$$

The initial wave function is considered as a gaussian function, for which the average position and momenta evolve according to Newton’s equations

$$\frac{\mathrm{d}<x>}{\mathrm{d}t} = \frac{<p>}{m}$$
$$\frac{\mathrm{d}<p>}{\mathrm{d}t} = -m\,\omega^2 <x>^2$$

The result is a harmonic motion $x(t) = \cos(\omega t)$.

In[122]:=

```
ω = 0.25;
m = 10;
V = 1 / 2 * m * ω ^ 2 * x ^ 2
```

Out[124]=

$0.3125\,x^2$