Benchmarks for QDyn

All equations and calculations are in atomic units.

In[1]:=
```
ℏ = 1;
me = 1;
```

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

Out[ ]=

$0.005\, x^2$

Energies for benchmark

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

Out[ ]//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[ ]:=
```
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:

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

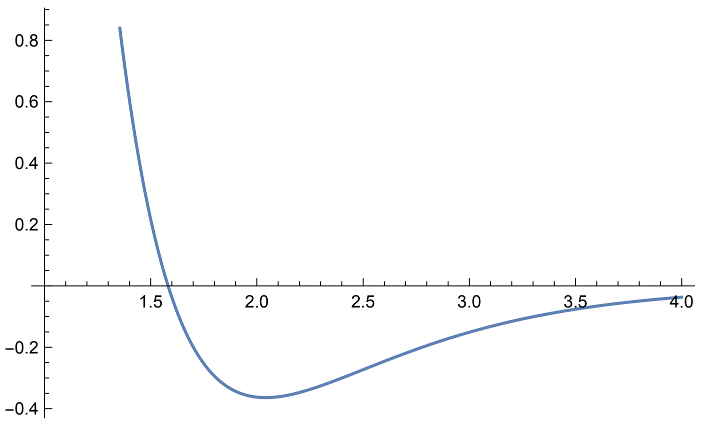
[Solution according to https://en.wikipedia.org/wiki/Morse_potential]

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

In[◦]:=
```
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[◦]=

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

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



Energies for benchmark

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

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

Out[ ]=

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

Energies for benchmark

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

Out[ ]=
```
{{{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[•]:= Sort[ArrayReshape[data⟦ ;; ,  ;; , 3⟧, 5 * 5]]⟦ ;; 10⟧ // TableForm
Out[•]//TableForm=
0.1
0.2
0.2
0.3
0.3
0.3
0.4
0.4
0.4
0.4
```

```
In[•]:= 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[•]:= ωx = 0.1; ωy = 0.15;
m = 1;
V = 1 / 2 * m * ωx ^ 2 * x ^ 2 + 1 / 2 * m * ωy ^ 2 * y ^ 2
Out[•]=
```

$0.005\, x^2 + 0.01125\, y^2$

Energies for benchmark

```
In[•]:= data = Table[{nx, ny, ℏ * (ωx * (1 / 2 + nx) + ωy * (1 / 2 + ny))}, {nx, 0, 4}, {ny, 0, 4}]
Out[•]=
{{{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[ ]:=
```
Sort[ArrayReshape[data[[ ;; , ;; , 3]], 5 * 5]][[ ;; 10]] // TableForm
```
Out[ ]//TableForm=
```
0.125
0.225
0.275
0.325
0.375
0.425
0.425
0.475
0.525
0.525
```

In[ ]:=
```
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[ ]:=
```
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[ ]=

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

Energies for benchmark

In[ ]:=
```
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[ ]:=
```
Sort[ArrayReshape[data[[ ;; , ;; , ;; , 4]], 5 * 5 * 5]][[ ;; 10]] // TableForm
```
Out[ ]//TableForm=
```
0.15
0.25
0.25
0.25
0.35
0.35
0.35
0.35
0.35
0.35
```

In[ ]:=
```
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[ ]:=
```
ωx = 0.1; ωy = 0.07; ωz = 0.13;
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[ ]=

$0.005\, x^2 + 0.00245\, y^2 + 0.00845\, z^2$

Energies for benchmark

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

Out[ ]//TableForm=

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

In[ ]:=
```
Clear[m, ωx, ωy, ωz, 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[2]:=
```
ω = 0.25;
m = 10;
V = 1 / 2 * m * ω ^ 2 * x ^ 2
```

Out[4]= $0.3125\, x^2$