Benchmarks for QDyn

All equation and calculation are in atomic units.

In[1]:=
```
ℏ = 1;
me = 1;
```

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[3]:=
```
ω = 0.1;
m = 1;
V = 1 / 2 * m * ω ^ 2 * x ^ 2
```

Out[5]= $0.005\,x^2$

Energies for benchmark

In[6]:=
```
Table[{n, ℏ * ω * (1 / 2 + n)}, {n, 0, 9}] // TableForm
```

Out[6]//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[7]:=
```
Clear[ω, m, V]
```

Harmonic oscillator 2D - symmetric

Harmonic oscillator with potential in form:

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

Exact energies correspond to the following formula:

$$E_n = \hbar\omega(n_x + n_y + 1), \quad n_x, n_y = 0, 1, 2, \ldots$$

In[8]:=
```
ωx = 0.1; ωy = 0.1;
m = 1;
V = 1 / 2 * m * ωx ^ 2 * x ^ 2 + 1 / 2 * m * ωy ^ 2 * y ^ 2
```

Out[10]=

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

Energies for benchmark

In[11]:=
```
data = Table[{nx, ny, ℏ * (ωx * (1 / 2 + nx) + ωy * (1 / 2 + ny))}, {nx, 0, 4}, {ny, 0, 4}]
```

Out[11]=
```
{{{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[12]:=
```
Sort[ArrayReshape[data[[ ;; , ;; , 3]], 5 * 5]][[ ;; 10]] // TableForm
```

Out[12]//TableForm=
```
0.1
0.2
0.2
0.3
0.3
0.3
0.4
0.4
0.4
0.4
```

In[13]:=
```
Clear[m, ωx, ωy, V, data]
```

Harmonic oscillator 2D - asymmetric

Harmonic oscillator with potential in form:

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

Exact energies correspond to the following formula:

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

In[14]:=
```
ωx = 0.1; ωy = 0.15;
m = 1;
V = 1 / 2 * m * ωx ^ 2 * x ^ 2 + 1 / 2 * m * ωy ^ 2 * y ^ 2
```

Out[16]=

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

Energies for benchmark

In[17]:=
```
data = Table[{nx, ny, ℏ * (ωx * (1 / 2 + nx) + ωy * (1 / 2 + ny))}, {nx, 0, 4}, {ny, 0, 4}]
```

Out[17]=
```
{{{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[18]:=
```
Sort[ArrayReshape[data[[ ;; , ;; , 3]], 5 * 5]][[ ;; 10]] // TableForm
```

Out[18]//TableForm=
```
0.125
0.225
0.275
0.325
0.375
0.425
0.425
0.475
0.525
0.525
```

In[19]:=
```
Clear[m, ωx, ωy, V, data]
```