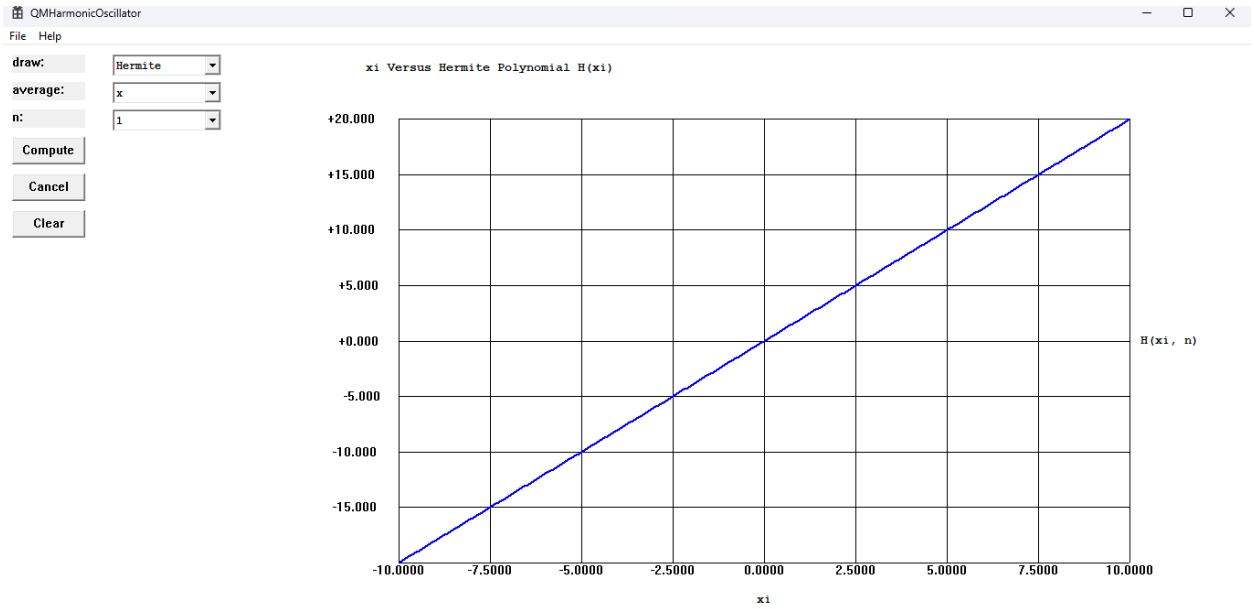
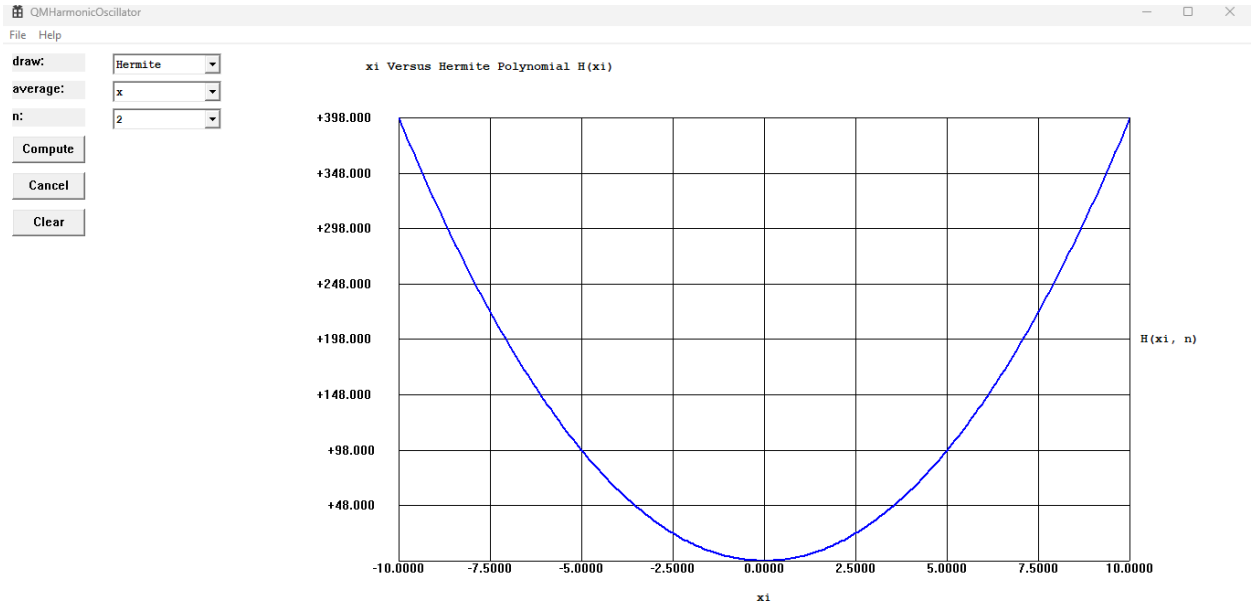
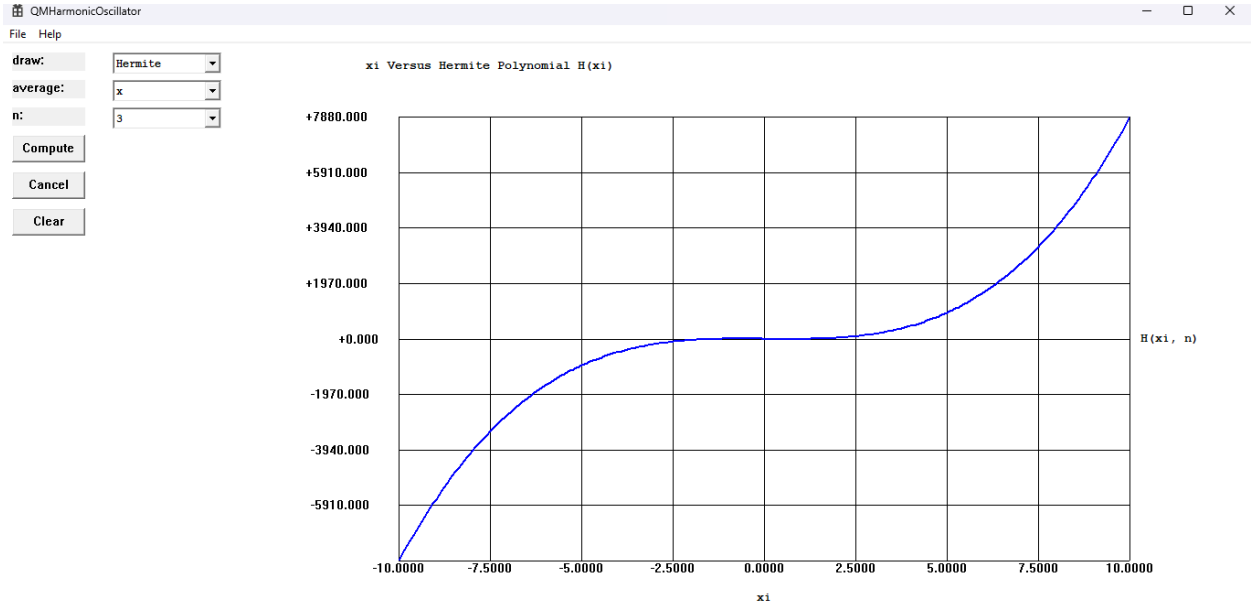
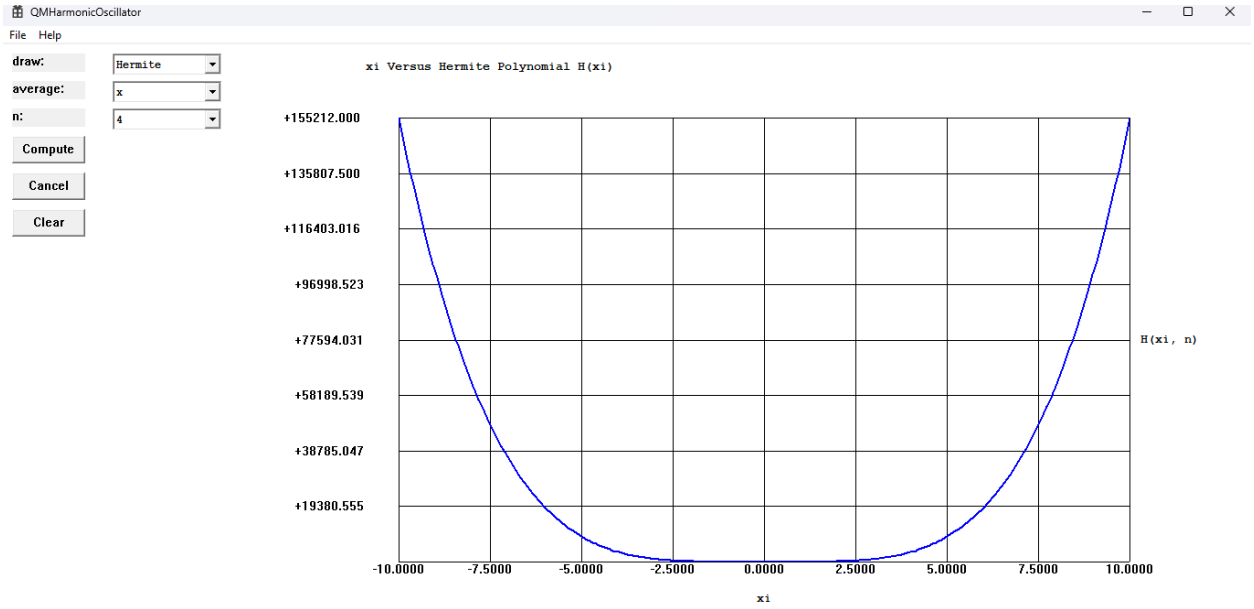
Blog Entry © Thursday, October 30, 2025, by James Pate Williams, Jr. Quantum Mechanical Harmonic Oscillator See ***Introduction to Quantum Mechanics with Applications to Chemistry*** by Linus Pauling and E. Bright Wilson, Jr. Chapter III

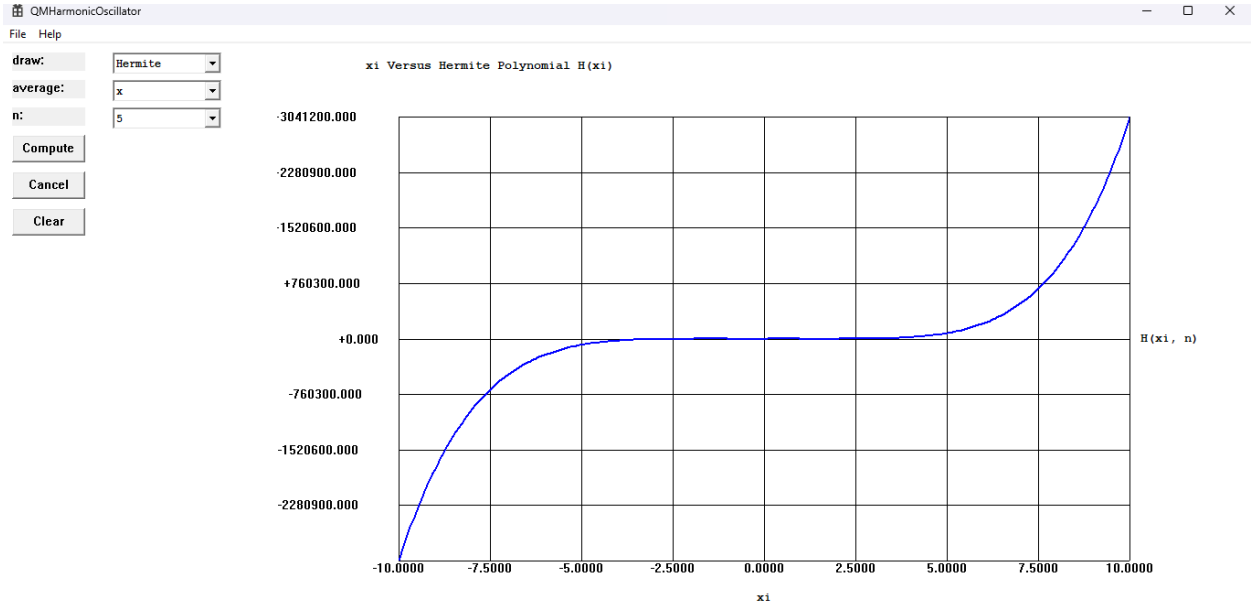
$$\psi_n(\xi) = \sqrt{\frac{\alpha}{\sqrt{\pi}}\frac{1}{2^n n!}}e^{-\xi^2/2}H_n(\xi), \xi = \alpha x, \alpha = 1$$

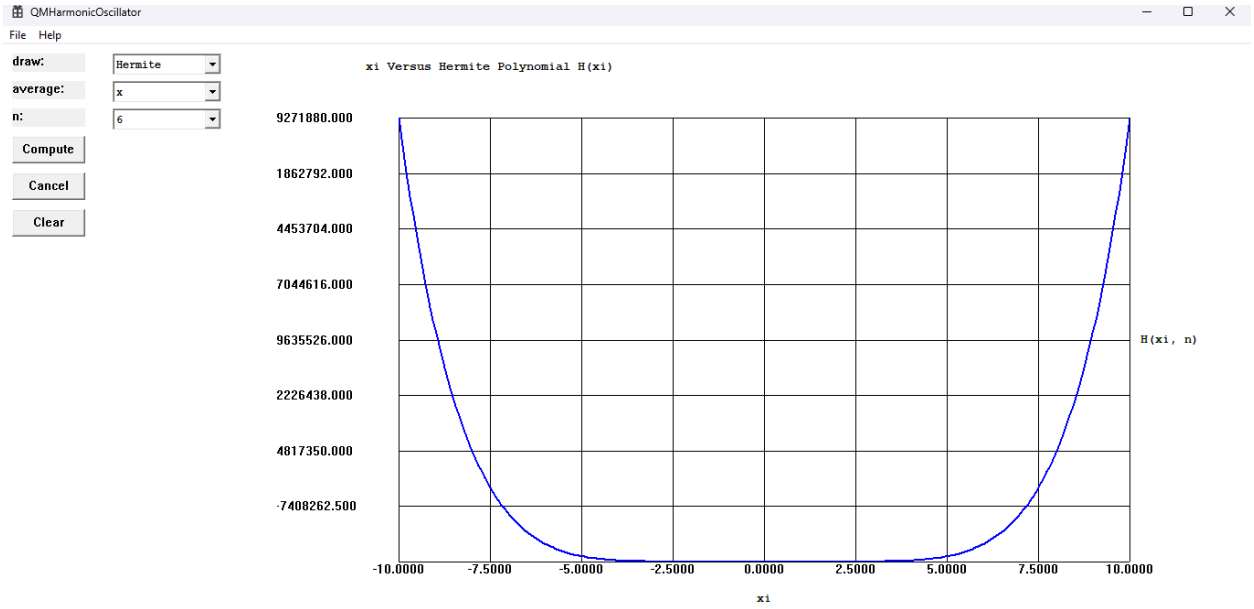


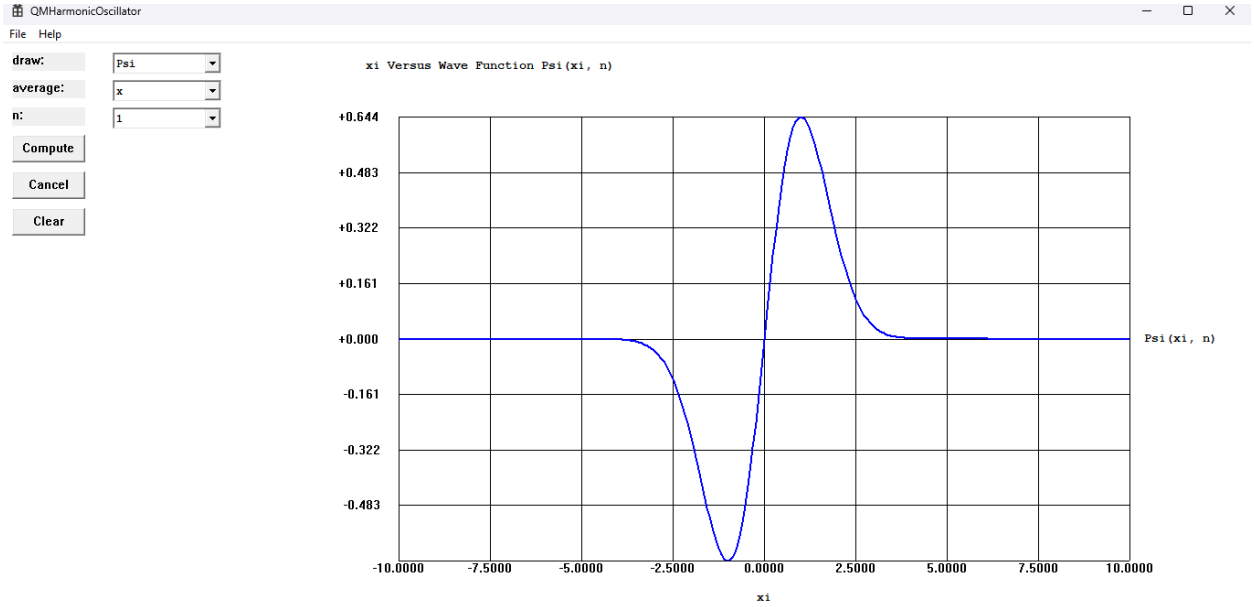


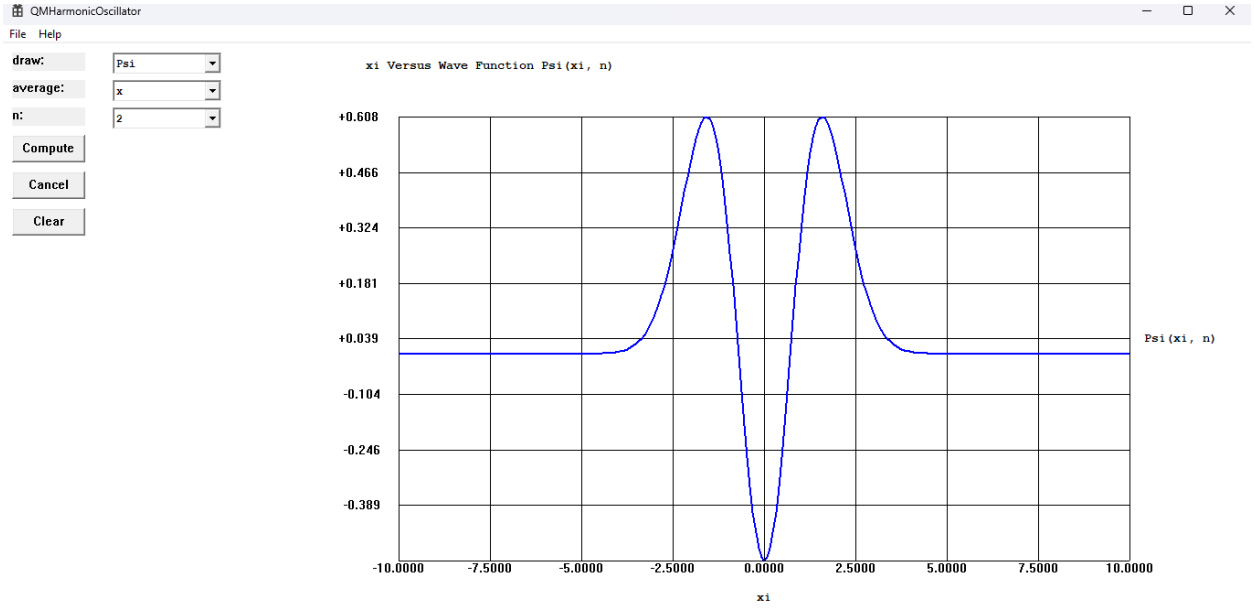

QMHarmonicOscillator
File Help
draw: Hermite
average: x
n: 3
Compute
Cancel
Clear
xi Versus Hermite Polynomial H(xi)
+7880.000
+5910.000
+3940.000
+1970.000
+0.000
-1970.000
-3940.000
-5910.000
H(xi, n)
-10.0000 -7.5000 -5.0000 -2.5000 0.0000 2.5000 5.0000 7.5000 10.0000
xi

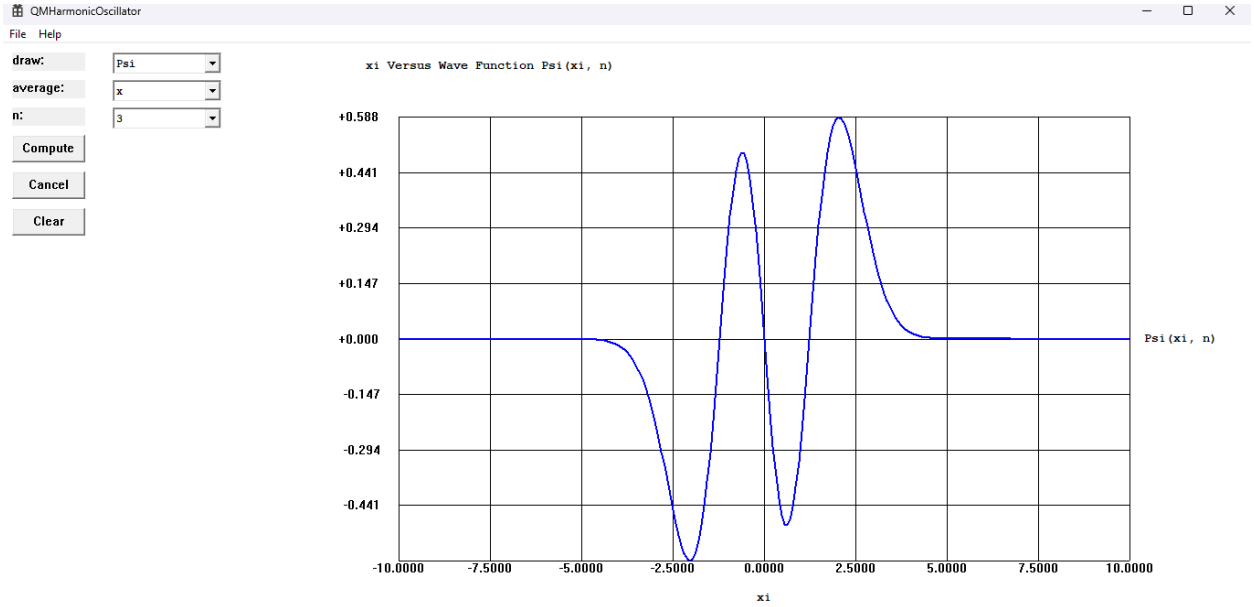

QMHarmonicOscillator
File Help
draw: Hermite
average: x
n: 4
Compute
Cancel
Clear
xi Versus Hermite Polynomial H(xi)
+155212.000
+135807.500
+116403.016
+96998.523
+77594.031
+58189.539
+38785.047
+19380.555
H(xi, n)
-10.0000 -7.5000 -5.0000 -2.5000 0.0000 2.5000 5.0000 7.5000 10.0000
xi

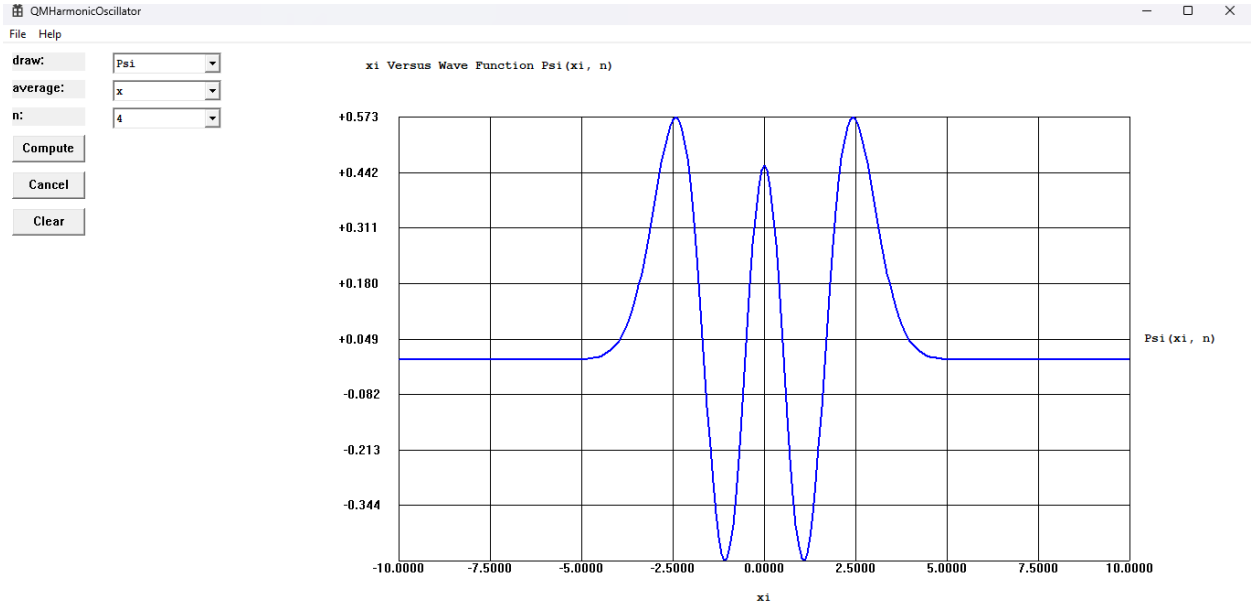

QMHarmonicOscillator
File Help
draw: Hermite
average: x
n: 5
Compute
Cancel
Clear
xi Versus Hermite Polynomial H(xi)
3041200.000
2280900.000
1520600.000
+760300.000
+0.000
-760300.000
-1520600.000
-2280900.000
-10.0000 -7.5000 -5.0000 -2.5000 0.0000 2.5000 5.0000 7.5000 10.0000
xi
H(xi, n)

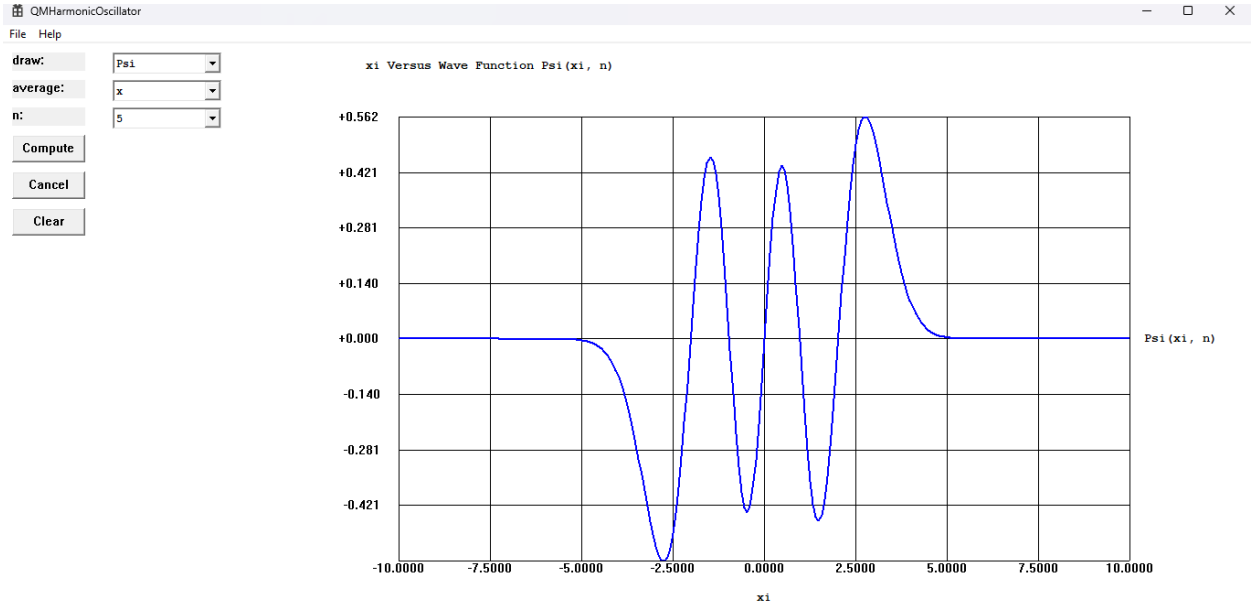

QMHarmonicOscillator
File Help
draw: Hermite
average: x
n: 6
Compute
Cancel
Clear
xi Versus Hermite Polynomial H(xi)
9271880.000
1862792.000
4453704.000
7044616.000
9635526.000
2226438.000
4817350.000
7408262.500
-10.0000 -7.5000 -5.0000 -2.5000 0.0000 2.5000 5.0000 7.5000 10.0000
xi
H(xi, n)

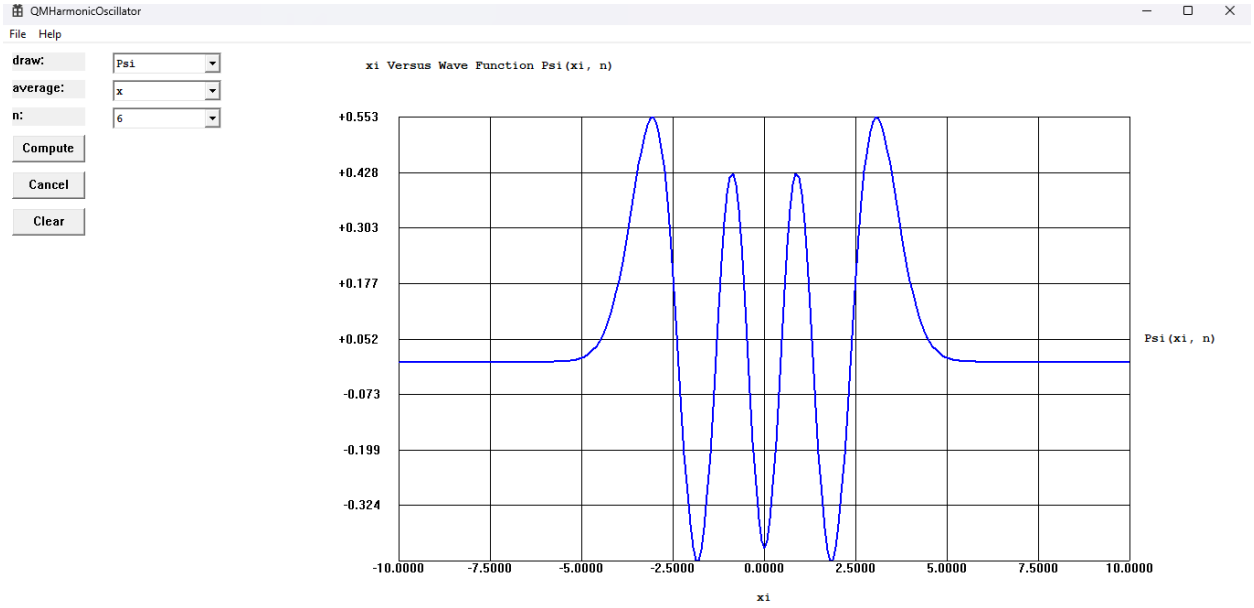

QMHarmonicOscillator
File Help
draw: Psi
average: x
n: 1
Compute
Cancel
Clear
xi Versus Wave Function Psi(xi, n)
+0.644
+0.483
+0.322
+0.161
+0.000
-0.161
-0.322
-0.483
-10.0000
-7.5000
-5.0000
-2.5000
0.0000
2.5000
5.0000
7.5000
10.0000
xi
Psi(xi, n)

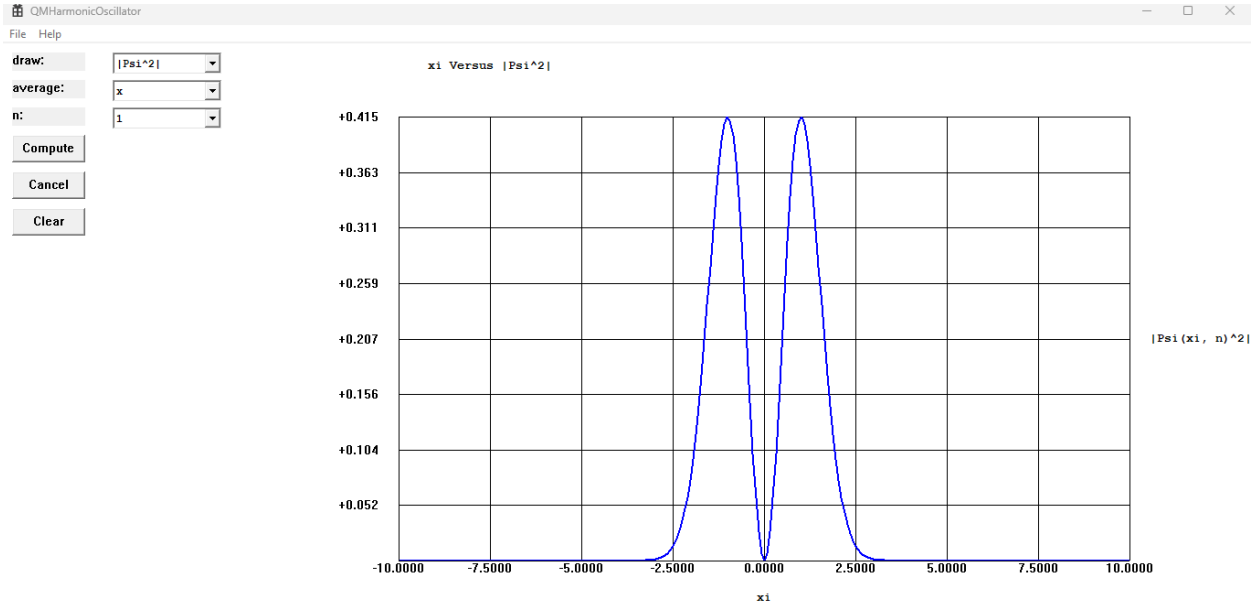

QMHarmonicOscillator
File Help
draw: Psi
average: x
n: 2
Compute
Cancel
Clear
xi Versus Wave Function Psi(xi, n)
+0.608
+0.466
+0.324
+0.181
+0.039
-0.104
-0.246
-0.389
-10.0000
-7.5000
-5.0000
-2.5000
0.0000
2.5000
5.0000
7.5000
10.0000
xi
Psi(xi, n)

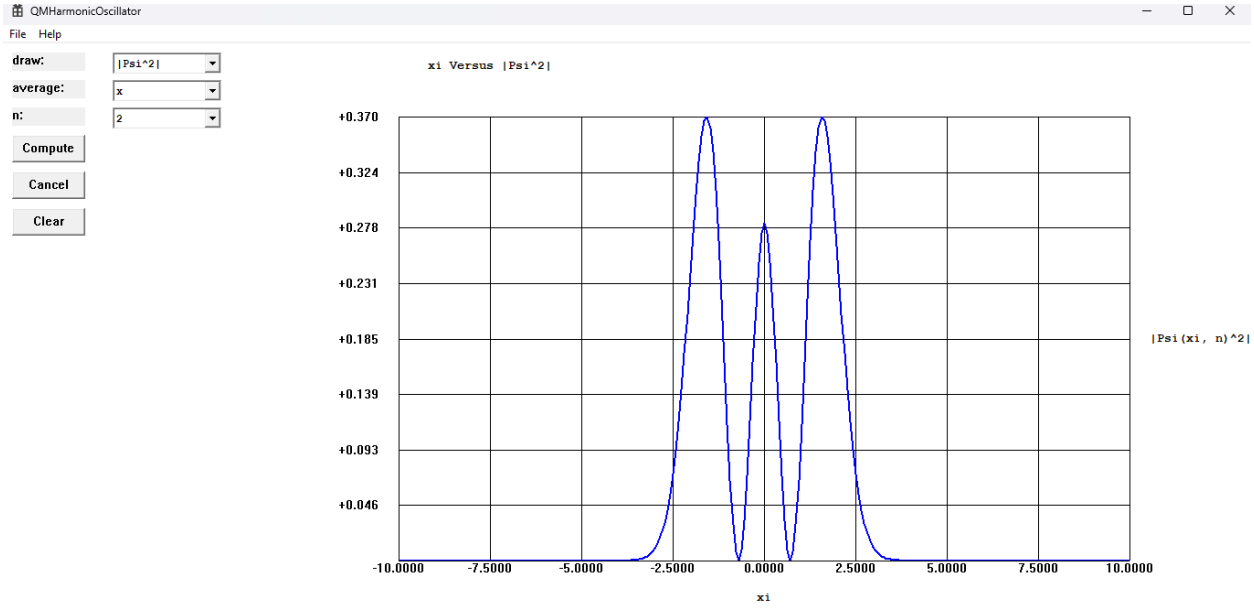

QMHarmonicOscillator
File Help
draw: Psi
average: x
n: 3
Compute
Cancel
Clear
xi Versus Wave Function Psi(xi, n)
+0.588
+0.441
+0.294
+0.147
+0.000
-0.147
-0.294
-0.441
-10.0000
-7.5000
-5.0000
-2.5000
0.0000
2.5000
5.0000
7.5000
10.0000
xi
Psi(xi, n)

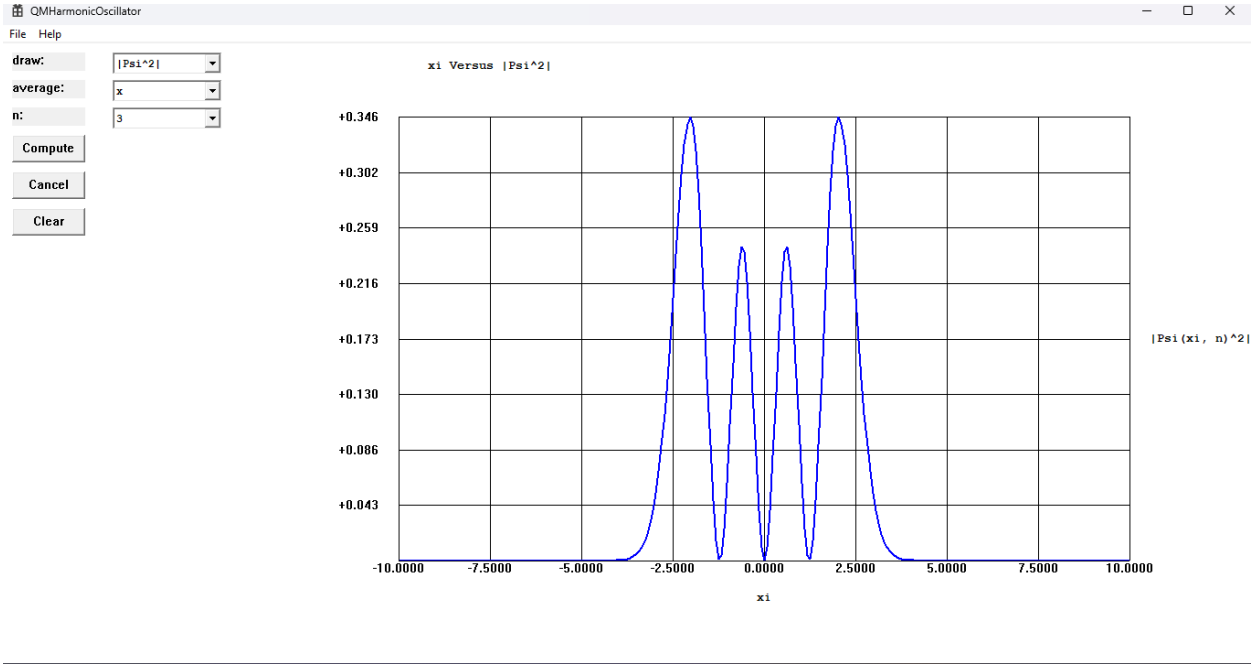

QMHarmonicOscillator
File Help
draw: Psi
average: x
n: 4
Compute
Cancel
Clear
xi Versus Wave Function Psi(xi, n)
+0.573
+0.442
+0.311
+0.180
+0.049
-0.082
-0.213
-0.344
-10.0000
-7.5000
-5.0000
-2.5000
0.0000
2.5000
5.0000
7.5000
10.0000
xi
Psi(xi, n)

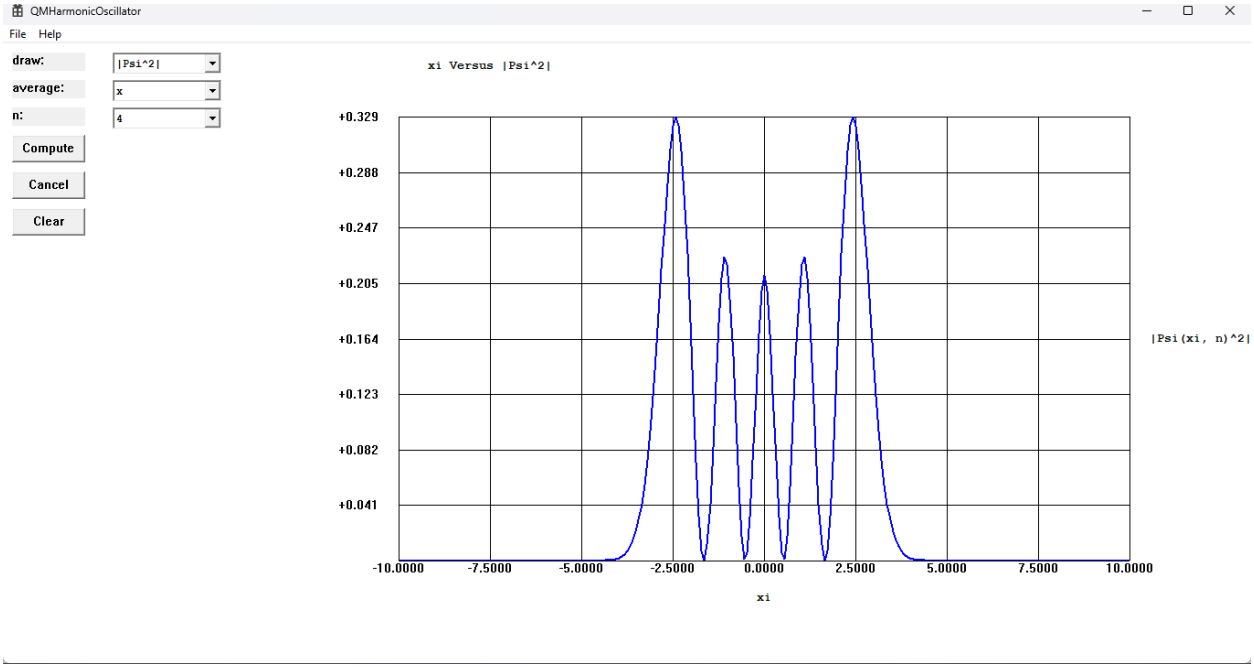

QMHarmonicOscillator
File Help
draw: Psi
average: x
n: 5
Compute
Cancel
Clear
xi Versus Wave Function Psi(xi, n)
+0.562
+0.421
+0.281
+0.140
+0.000
-0.140
-0.281
-0.421
-10.0000
-7.5000
-5.0000
-2.5000
0.0000
2.5000
5.0000
7.5000
10.0000
xi
Psi(xi, n)

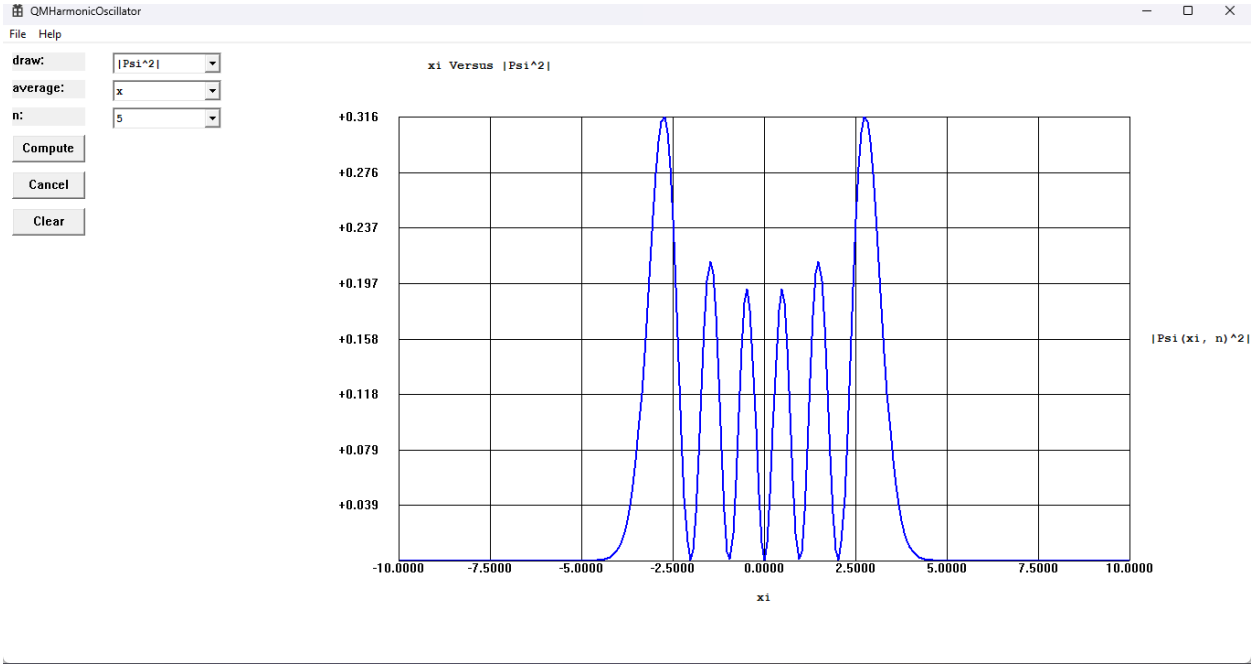

QMHarmonicOscillator
File Help
draw: Psi
average: x
n: 6
Compute
Cancel
Clear
xi Versus Wave Function Psi(xi, n)
+0.553
+0.428
+0.303
+0.177
+0.052
-0.073
-0.199
-0.324
-10.0000
-7.5000
-5.0000
-2.5000
0.0000
2.5000
5.0000
7.5000
10.0000
xi
Psi(xi, n)

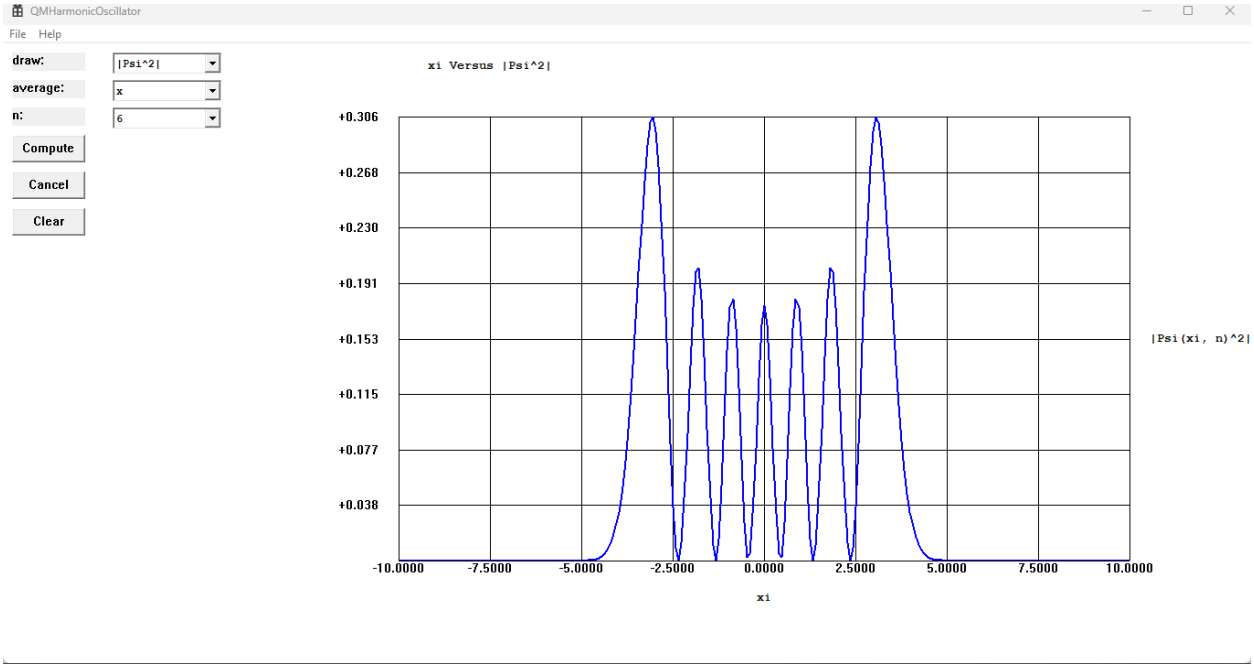

QMHarmonicOscillator
File Help
draw: |Psi^2|
average: x
n: 1
Compute
Cancel
Clear
xi Versus |Psi^2|
+0.415
+0.363
+0.311
+0.259
+0.207
+0.156
+0.104
+0.052
-10.0000 -7.5000 -5.0000 -2.5000 0.0000 2.5000 5.0000 7.5000 10.0000
xi
|Psi(xi, n)^2|

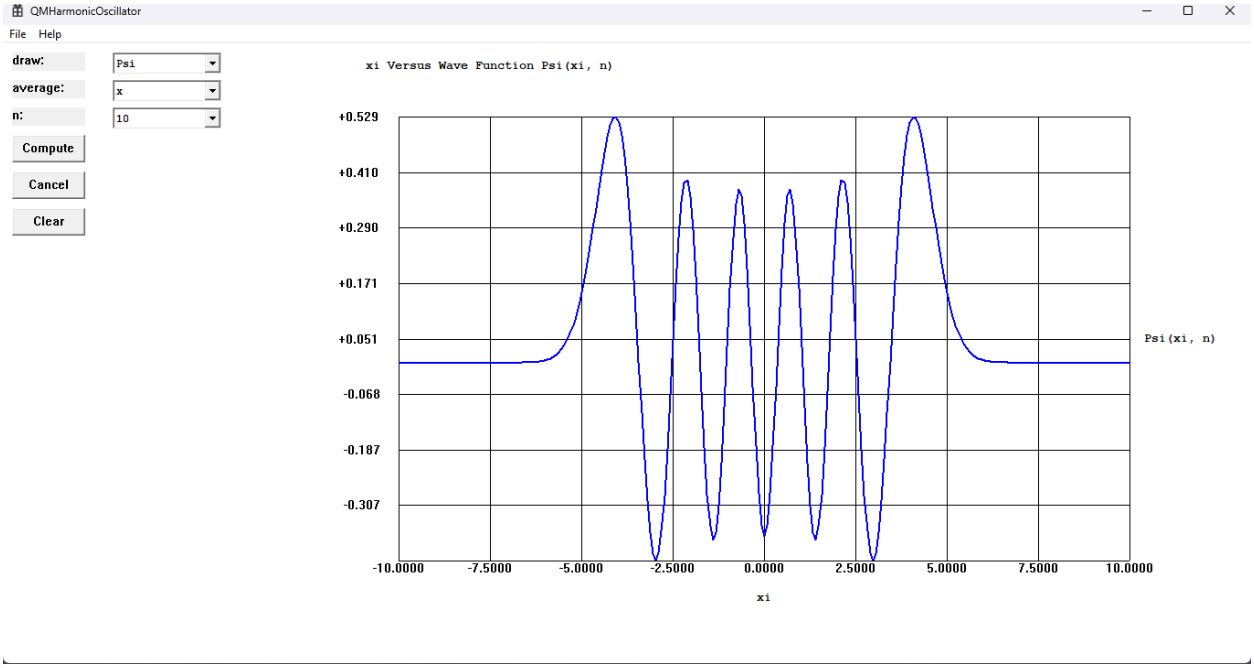

QMHarmonicOscillator
File Help
draw: |Psi^2|
average: x
n: 2
Compute
Cancel
Clear
xi Versus |Psi^2|
+0.370
+0.324
+0.278
+0.231
+0.185
+0.139
+0.093
+0.046
-10.0000 -7.5000 -5.0000 -2.5000 0.0000 2.5000 5.0000 7.5000 10.0000
xi
|Psi(xi, n)^2|

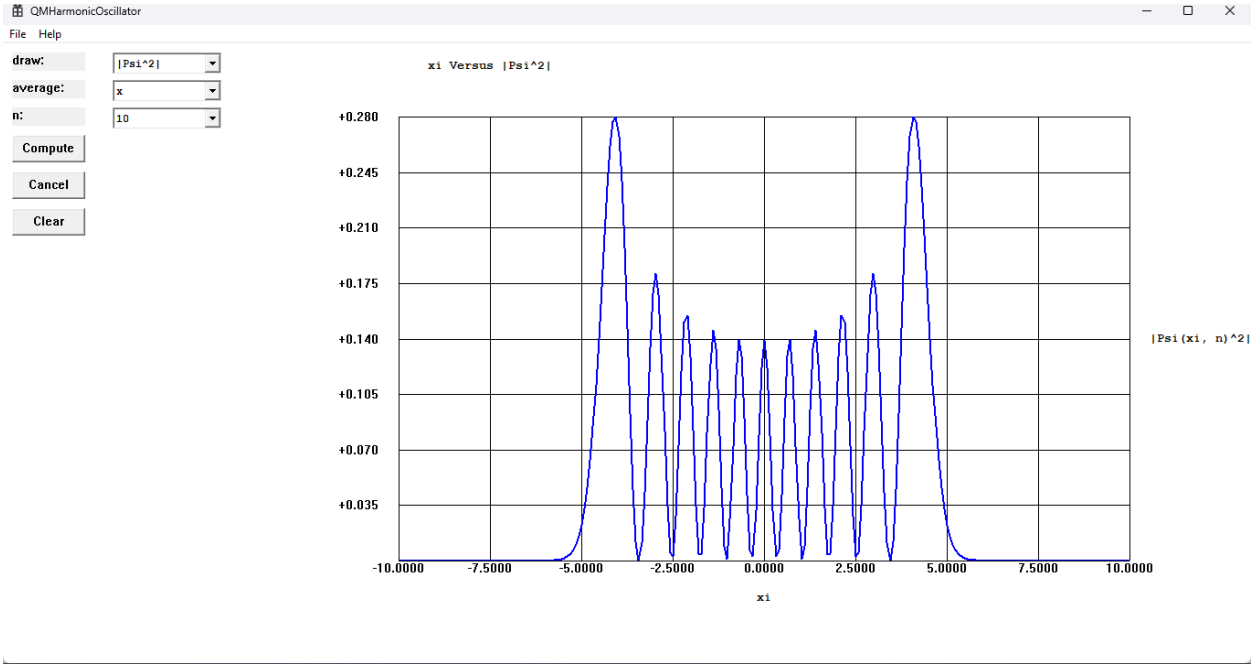

QMHarmonicOscillator
File Help
draw: |Psi^2|
average: x
n: 3
Compute
Cancel
Clear
xi Versus |Psi^2|
+0.346
+0.302
+0.259
+0.216
+0.173
+0.130
+0.086
+0.043
-10.0000 -7.5000 -5.0000 -2.5000 0.0000 2.5000 5.0000 7.5000 10.0000
xi
|Psi(xi, n)^2|


QMHarmonicOscillator
File Help
draw: |Psi^2|
average: x
n: 4
Compute
Cancel
Clear
xi Versus |Psi^2|
+0.329
+0.288
+0.247
+0.205
+0.164
+0.123
+0.082
+0.041
-10.0000 -7.5000 -5.0000 -2.5000 0.0000 2.5000 5.0000 7.5000 10.0000
xi
|Psi(xi, n)^2|


QMHarmonicOscillator
File Help
draw: |Psi^2|
average: x
n: 5
Compute
Cancel
Clear
xi Versus |Psi^2|
+0.316
+0.276
+0.237
+0.197
+0.158
+0.118
+0.079
+0.039
-10.0000 -7.5000 -5.0000 -2.5000 0.0000 2.5000 5.0000 7.5000 10.0000
xi
|Psi(xi, n)^2|


QMHarmonicOscillator
File Help
draw: |Psi^2|
average: x
n: 6
Compute
Cancel
Clear
xi Versus |Psi^2|
+0.306
+0.268
+0.230
+0.191
+0.153
+0.115
+0.077
+0.038
-10.0000 -7.5000 -5.0000 -2.5000 0.0000 2.5000 5.0000 7.5000 10.0000
xi
|Psi(xi, n)^2|


QMHarmonicOscillator
File Help
draw: Psi
average: x
n: 10
Compute
Cancel
Clear
xi Versus Wave Function Psi(xi, n)
+0.529
+0.410
+0.290
+0.171
+0.051
-0.068
-0.187
-0.307
-10.0000
-7.5000
-5.0000
-2.5000
0.0000
2.5000
5.0000
7.5000
10.0000
xi
Psi(xi, n)

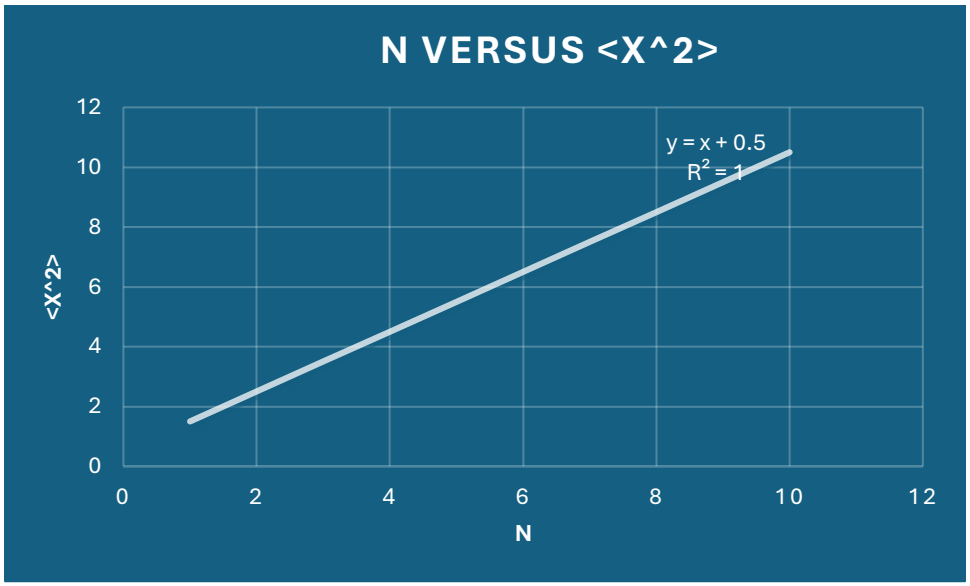

QMHarmonicOscillator
File Help
draw: |Psi^2|
average: x
n: 10
Compute
Cancel
Clear
xi Versus |Psi^2|
+0.280
+0.245
+0.210
+0.175
+0.140
+0.105
+0.070
+0.035
-10.0000
-7.5000
-5.0000
-2.5000
0.0000
2.5000
5.0000
7.5000
10.0000
xi
|Psi(xi, n)^2|

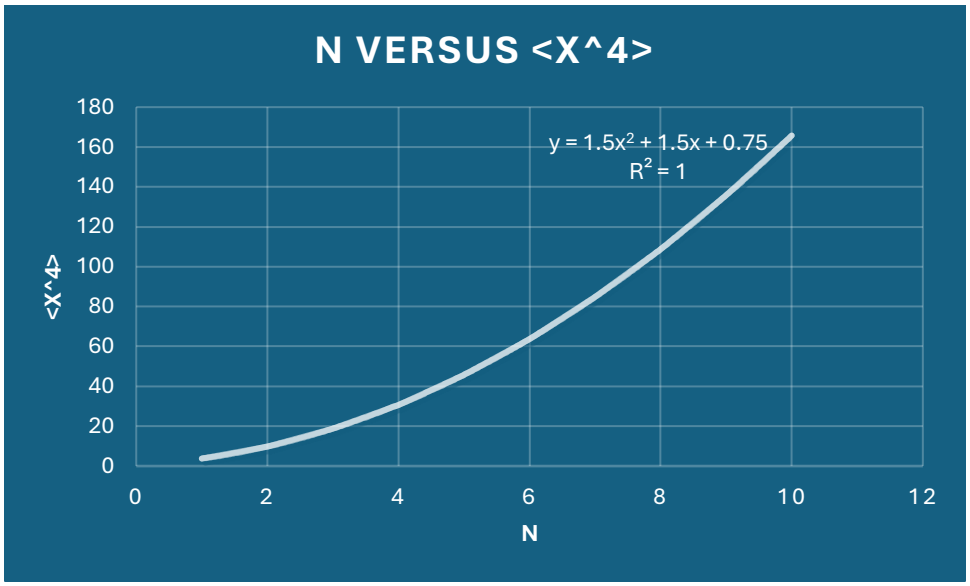
n	x	x^2	x^3	x^4
1	0	1.5	0	3.75
2	0	2.5	0	9.75
3	0	3.5	0	18.75
4	0	4.5	0	30.75
5	0	5.5	0	45.75
6	0	6.5	0	63.75
7	0	7.5	0	84.75
8	0	8.5	0	108.75
9	0	9.5	0	135.75
10	0	10.5	0	165.75

Moments of the Harmonic Oscillator

$$< x^m >= \int_{-\infty}^{\infty} \psi_n(x) x^m \psi_n(x)\, dx$$

We used Simpson's Rule for the integrations with 1024 steps. Also, the endpoints were -10 to 10.




N VERSUS <X^4>
y = 1.5x² + 1.5x + 0.75
R² = 1
<X^4>
N
180
160
140
120
100
80
60
40
20
0
0
2
4
6
8
10
12