Chart, line chart

Description automatically generated

(Matrix-matrix multiplication is O(N3))

Chart, line chart

Description automatically generated

(Vector-vector multiplication is O(N1))

Chart, line chart

Description automatically generated

(Matrix-vector multiplication is O(N2))

Chart, scatter chart

Description automatically generated

Ground state energy as a function of basis set size, for V(x) = mx, m = 1

Chart, scatter chart

Description automatically generated

Ground state energy as a function of basis set size, for V(x) = 10x, m = 1

Chart

Description automatically generated with medium confidence

Ground state wavefunctions for three different potential and mass conditions.

The addition of the potential from V = mx to V = 10x shifts the wavefunction amplitude to the left (x --> 0). This is sensible; both V = x and V = 10x are sloping potentials that increase as x-->L, and the steeper potential (V = 10x) will favor a greater probability densities towards x-->0. Using V = mx and setting m to 10 creates a drastically different wavefunction reminiscent of the Morse potential (or perhaps an Airy function?) Increasing m decreases the magnitude of the kinetic energy throughout the entire range of x; the potential energy will more strongly determine the shape of the wavefunction. This can be observed in the coefficients for the three wavefunctions; for the other two wavefunctions, nearly all of the “character” of the composite wavefunction comes from the ground state of the unperturbed particle in a box and the contributions from higher states drop off rapidly, while for V = mx, m = 10, the first excited state contributes nearly as much as the ground state (the contribution from the first excited state may be why the left half of the wavefunction looks almost identical to a sine curve that’s antisymmetric about x = 0.5)

Table: coefficients of the first four basis set functions for the above wavefunctions

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **Φ1** | **Φ2** | **Φ3** | **Φ4** |
| V = mx, m = 1 | 0.999926 | 0.012165 | 0.000061 | 0.000195 |
| V = 10x, m = 1 | 0.992776 | 0.119818 | 0.005978 | 0.002093 |
| V = mx, m = 10 | -0.746506 | -0.613818 | -0.245723 | -0.071525 |