Computational Physics HW4

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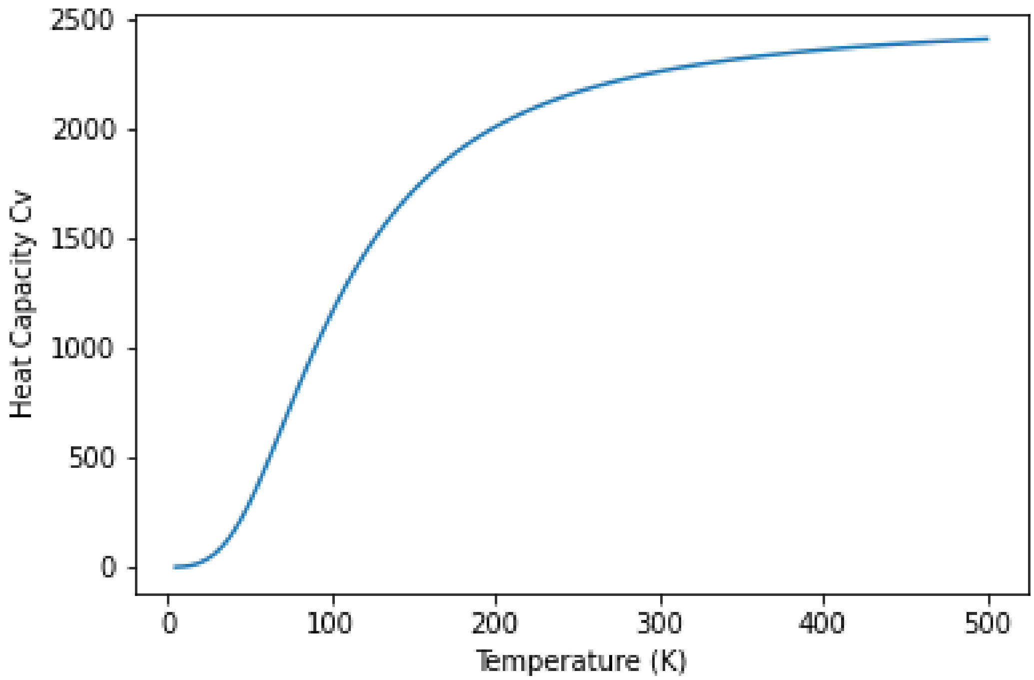

Figure 1: **P1: Heat Capacity of a solid** Use given equation of heat capacity and given conditions, we find the Heat Capacity of $1000cm^3$ Al as a function of Temperature as plotted. To do the integral of capacity equation, we notice that there is no singularity point within the range of integration; thus we could simply use the built-in function fixed_quad of SciPy to do the Gaussian quadrature. We applied the number of sample points $N = 50$ in this plot.

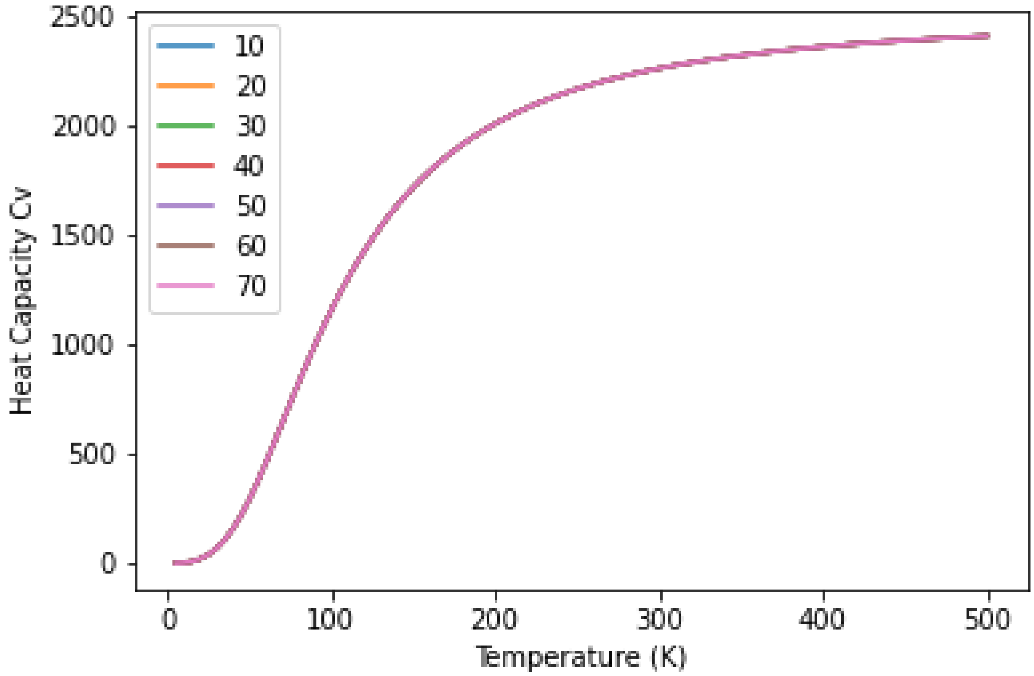

Figure 2: **P1(c): Convergence of integral for N=10,20,30,40,50,60,70** Requiring different order of fixed_quad, we find that the integration results converge rapidly for $N \geq 10$. As shown in the figure, these plots fit perfectly. Read the data of Cv_M in the code, we see the exact data are approximately the same.

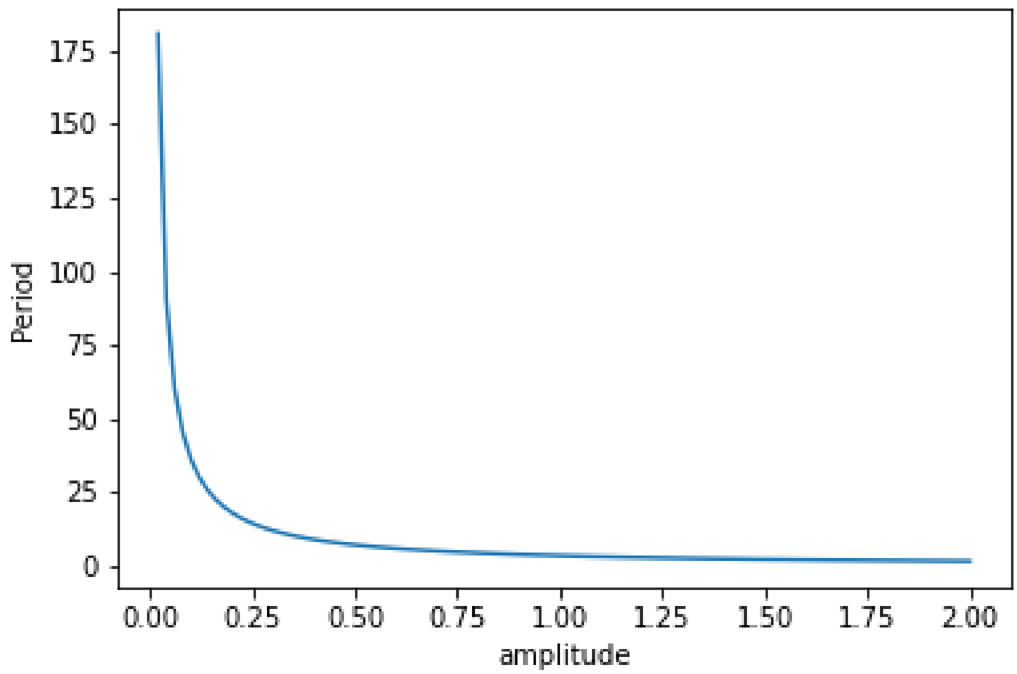

Figure 3: **P2: Period of an anharmonic oscillator** Given the initial condition, t=0, x=a, $\frac{dx}{dt} = 0$, we obtain that E=V(a). Plug into the energy equation then we get $V(a) = \frac{1}{2}m(\frac{dx}{dt})^2 + V(x)$. Use the separation of variable, we rearrange the equation to be $dt = \sqrt{\frac{m}{2}}\frac{dx}{\sqrt{V(a)-V(x)}}$. Then integrate both side for time t=0 to t=$\frac{1}{4}$T and position x=a to x=0. The time for this process is $\frac{1}{4}$T is by the symmetry of potential V(x). Then we can get the equation of period in part a. Integrating this equation with fixed_quad for different amplitude a, we get the plot as above. Notice that the period decreases as amplitude increases. This is because as amplitude increases, the magnitude of restoring force by potential also increases, and it increases by the order of x^3. The period diverges as $a = 0$. As amplitude approaches zero, the force is also zero and will not accelerate velocity; so it takes infinite time for the object to move for a period. $V(x) = x^2$ is a special order that the change of restoring force perfectly compensates the change of amplitude. There is a plot p2_harmonic.png in the folder that shows the period is a fixed value with changing amplitude.

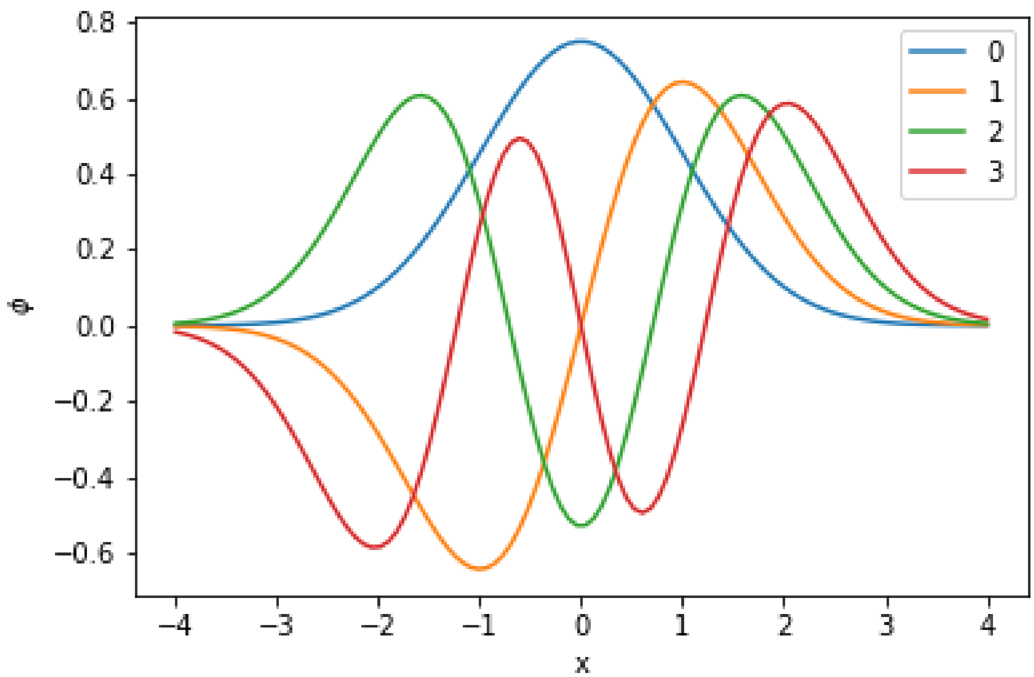

Figure 4: **P3(a): Wavefunctions for Energy level n=0,1,2,3** Given the first two Hermite polynomials and the recurring relationships, use recursion to generate the Hermite polynomials of any order. Plug into the wavefunction equation to get the wavefunctions.

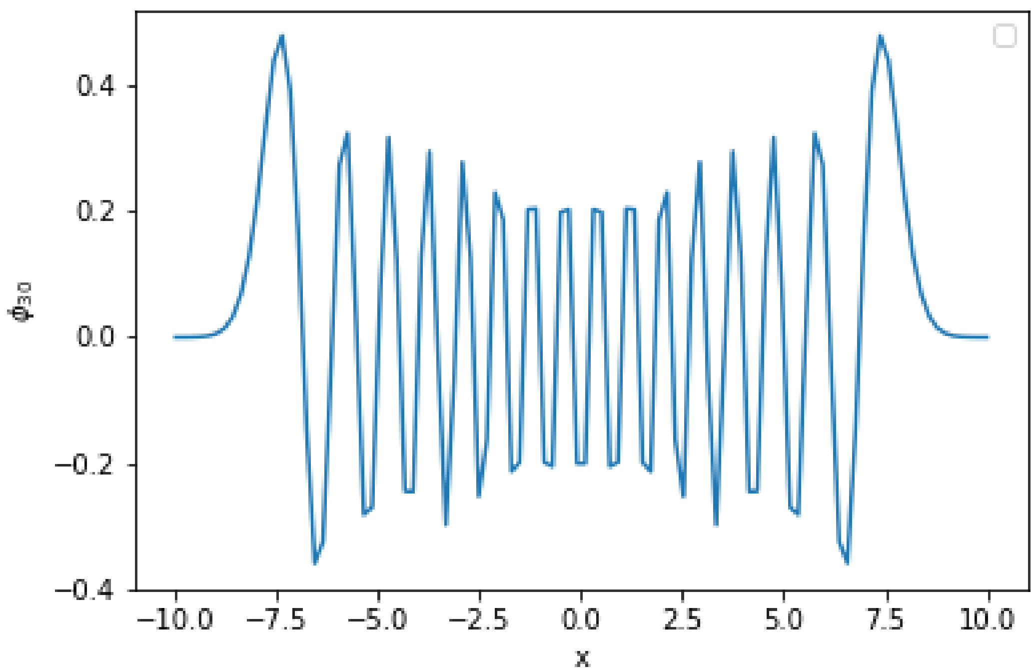

Figure 5: **P3(b): Wavefunctions for Energy level n=30** This is the wavefunction for n=30. Just plugin n=30 and the range of position wanted to the program of p3_a to obtain this figure.

P3(c): To calculate the integral, notice that the bounds are infinites. We need to first map the integral to a finite range. We apply the method in lecture notes "Integration" equation 20 to rescale the function. Notice from P3(a),(b) that the wavefunction is either symmetric or antisymmetric about origin, therefore $\phi_n(x)^2$ in the integral is symmetric. Applying equation 20, we use fixed_quad with bounds at ± 1 to calculate the original integral from 0 to infinity, then times 2 to get the integral we want. Take square-root, we get the uncertainty to be 2.3452078799117158.

P3(d): Similarly, we can use Gauss-Hermite polynomials to do the integral instead. We do the mapping to finite bounds and use Gauss-Hermite polynomials to give the roots and weights. Gauss-Hermite polynomials can give exact integration as we can always find a complete basis set of polynomals that are orthogonal to use the procedure analogue to Gaussian quadrature.