Problem Set 4

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October 2, 2024

GitHub link

https://github.com/dariolop76/phys-ga2000

1 Problem 1

Exercise 5.9 asks us to write a code for the computation of the heat capacity of a solid at temperature T according to Debye's theory of solids, which is given by the following integral:

$$C_V = 9V\rho k_B\Big(\frac{T}{\theta_D}\Big)^3\int_0^{\theta_D/T}\frac{x^4e^x}{(e^x-1)^2}dx, \tag{1}$$

where V is the volume of the solid, ρ is the number density, $k_B = 1.38$ x $10^{-23}J/K$ is the Boltzmann's constant and θ_D is the Debye temperature. In our case, we have $\rho = 6.022$ x $10^{28}m^{-3} =$ 6.022 x $10^{22}cm^{-3}$, $V = 1000cm^3$ and $\theta_D = 428K$. The integral has been performed using the method `numpy.polynomial.legendre.leggauss`, which computes the sample points and weights for Gauss-Legendre quadrature. In the code `prob_1.py`, the nodes and weights for the interval $[-1, 1]$, characteristic of this method, are mapped to the integration interval $[a, b] = [0, \theta_D/T]$ as follows:

$$\text{nodes} \to \frac{b-a}{2}\text{nodes} + \frac{b+a}{2} \tag{2}$$

$$\text{weights} \to \frac{b-a}{2}\text{weights} \tag{3}$$

Using Gaussian quadrature with $N = 50$ sample points, we evaluated the integral for a given (arbitrary) temperature $T^* = 50K$, obtaining:

$$C_V(T^*) = 289.21\ J/K. \tag{4}$$

Then, we performed the integration for values of the temperature in the range $T \in [5, 500]K$. The obtained heat capacity as a function of the temperature is given in Figure 1.

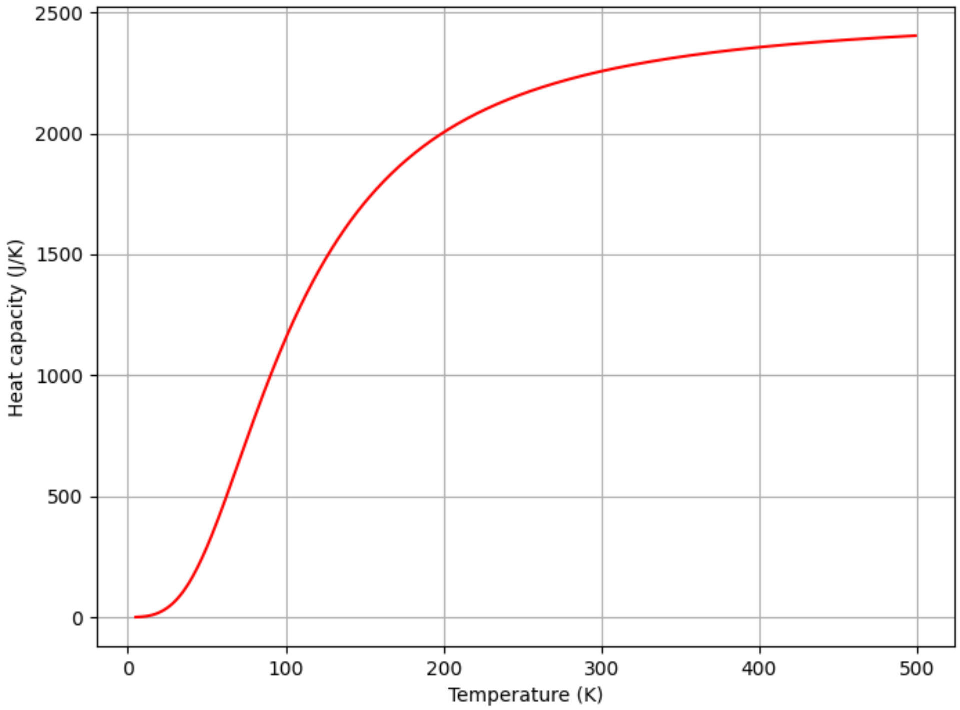

Figure 1: Heat capacity C_V as a function of the temperature T in the range $[5, 500]k$.

Finally, we tested the convergence by evaluating the integral for $T = T^*$ using different sample points, for $N \in [10, 20, 30, 40, 50, 60, 70]$. The result is shown in Figure 2

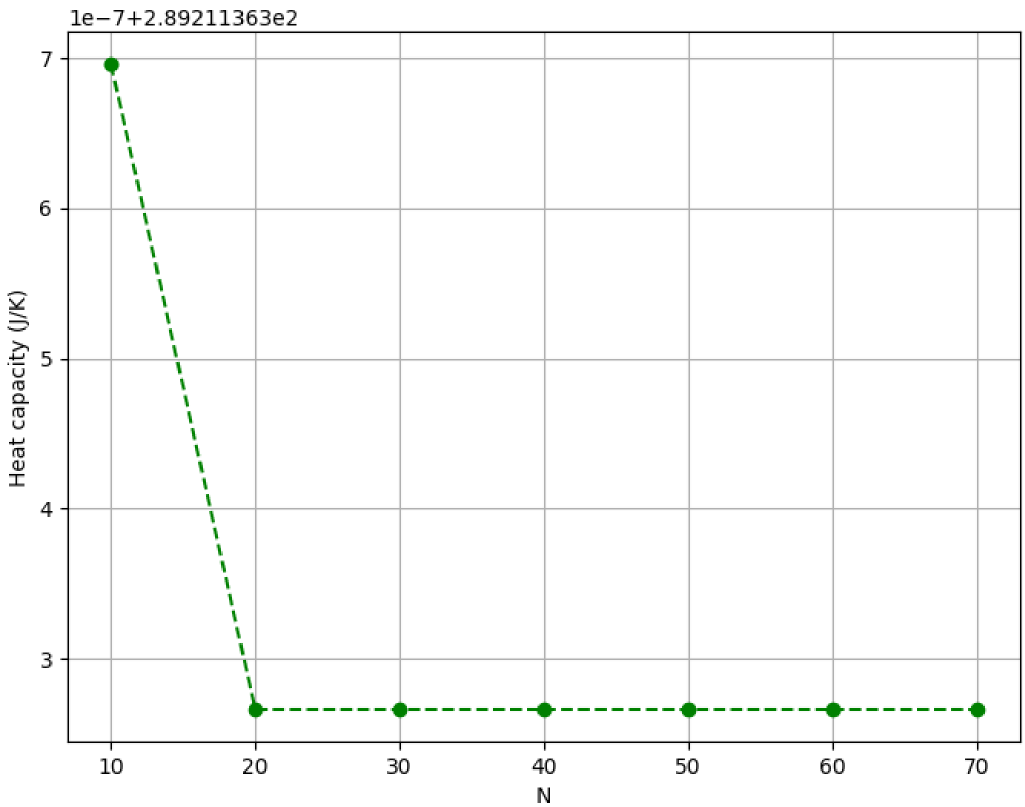

Figure 2: Heat capacity C_V as a function of the number of sample points N. On the y axis, the value is given by +289.211363 K, while the difference between the values is of order 10^{-7} K.

As we can see, the value of the heat capacities for $N = 10$ is the only one that differs from those obtained with higher sample points, but this difference is very small, being $\mathcal{O}(10^{-7}K)$.

2 Problem 2

In Exercise 5.10, we deal with an anharmonic oscillator. The energy of the particle is given by

$$E = \frac{1}{2}m\dot{x}^2 + V(x), \tag{5}$$

where the total energy of the particle is obtained by noticing that the particle has zero velocity ($\dot{x} = 0$) at $x = A$, where A is the amplitude of oscillation, namely $E = V(A)$.

2.1 Part a

Given Equation 5, we can obtain an expression for the period T of oscillation:

$$
\begin{aligned}
V(A) &= \frac{1}{2}m\dot{x}^2 + V(x), && (6)\\
\dot{x}^2 &= \frac{2}{m}\Big(V(A) - V(x)\Big) && (7)\\
\dot{x} = \frac{dx}{dt} &= \sqrt{\frac{2}{m}}\sqrt{V(A) - V(x)} && (8)\\
\int_0^A \sqrt{\frac{m}{2}}\frac{dx}{\sqrt{V(A) - V(x)}} &= \int_0^{T/4} = \frac{T}{4} && (9)\\
T &= \sqrt{8m}\int_0^A \frac{dx}{\sqrt{V(A) - V(x)}}. && (10)
\end{aligned}
$$

2.2 Part b

Now we set $m = 1$ and use the following form for the potential:

$$V(x) = x^4. \tag{11}$$

The period of oscillation can be then obtained as a function of the amplitude A by performing the integral in Equation 10. This has been implemented in the code `prob_2.py`, again by using the method `numpy.polynomial.legendre.leggauss`, with $N = 20$ sample points. Figure 3 shows the period as a function of the amplitude for $A \in [0, 2]$.

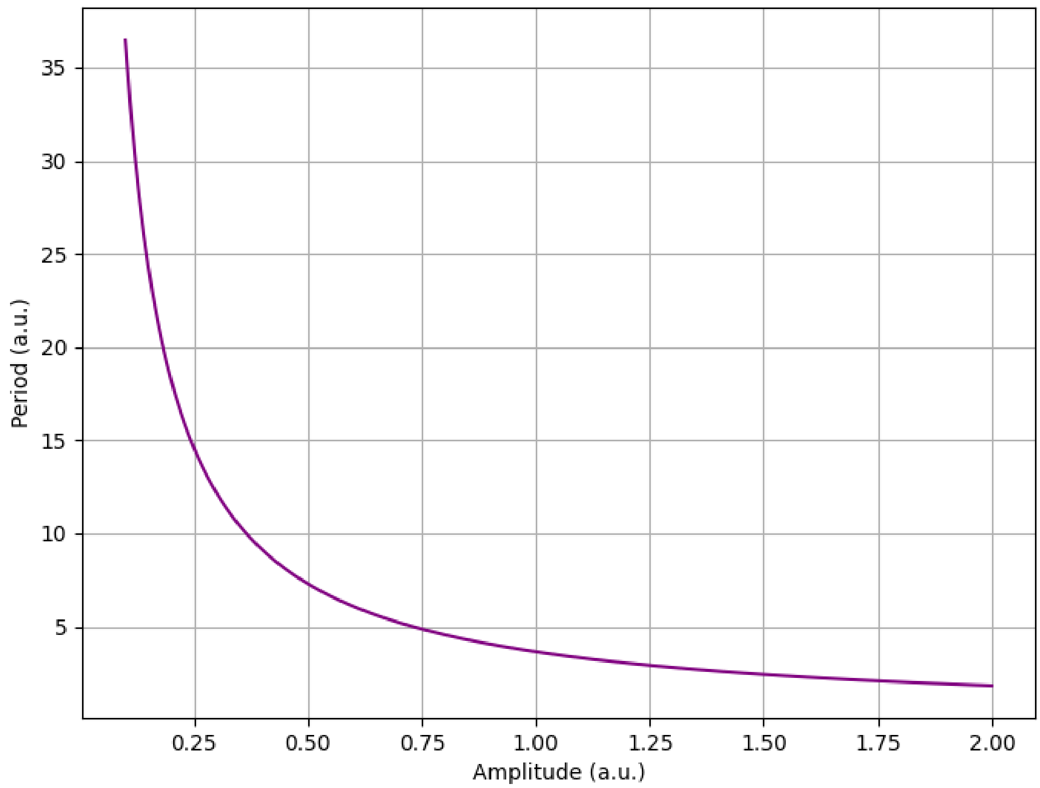

Figure 3: Period as a function of the amplitude.

As we can see, the period of oscillation decreases as the amplitude increases.

2.3 Part c

The period of oscillation for an anharmonic oscillator depends generally on the amplitude because the restoring force $F(x) = -\frac{dV}{dx}$ is not linear in x. In particular, for the potential in Equation 11, the restoring force is

$$F(x) = -4x^3. \tag{12}$$

So, the force does not increase linearly with the displacement, but more rapidly for greater displacements, leading to higher kinetic energy. This explains why the period decreases when the amplitude of the motion increases. Instead, when the amplitudes goes to zero, we find that the period diverges. This is still due to the non linearity of the problem, since a small displacement from equilibrium corresponds to a very small restoring force. This indicates that the closer the particle starts oscillating from the equilibrium position, the smaller the restoring force it will receive, hence the smaller kinetic energy it will have. Therefore, it takes longer time to complete an oscillation. In the limit of $A \to 0$, we have $T \to \infty$.

3 Problem 3

In Exercise 5.13, we are asked to define a function `H(n,x)` that calculate the n^{th} order Hermite polynomial, which satisfies the following recursive relation:

$$H_n(x) = 2xH_{n-1} - 2(n-1)H_{n-2}(x). \tag{13}$$

Given that $H_0(x) = 1$ and $H_1(x) = 2x$, we can use Equation 13 to obtain the value of $H_n(x)$ for a given $n \geq 0$ at x. Then we can use this to obtain the wavefunction of the harmonic oscillator in quantum mechanics, which is given by

$$\psi_n(x) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} e^{-\frac{x^2}{2}} H_n(x). \tag{14}$$

The functions `H(n,x)` and `psi(n,x)` have been implemented in the module `hermite.py`.

3.1 Part a

Figure 4 shows the wavefucntions $\psi_n(x)$ for $n = 0, 1, 2, 3$ and $-4 \leq x \leq 4$.

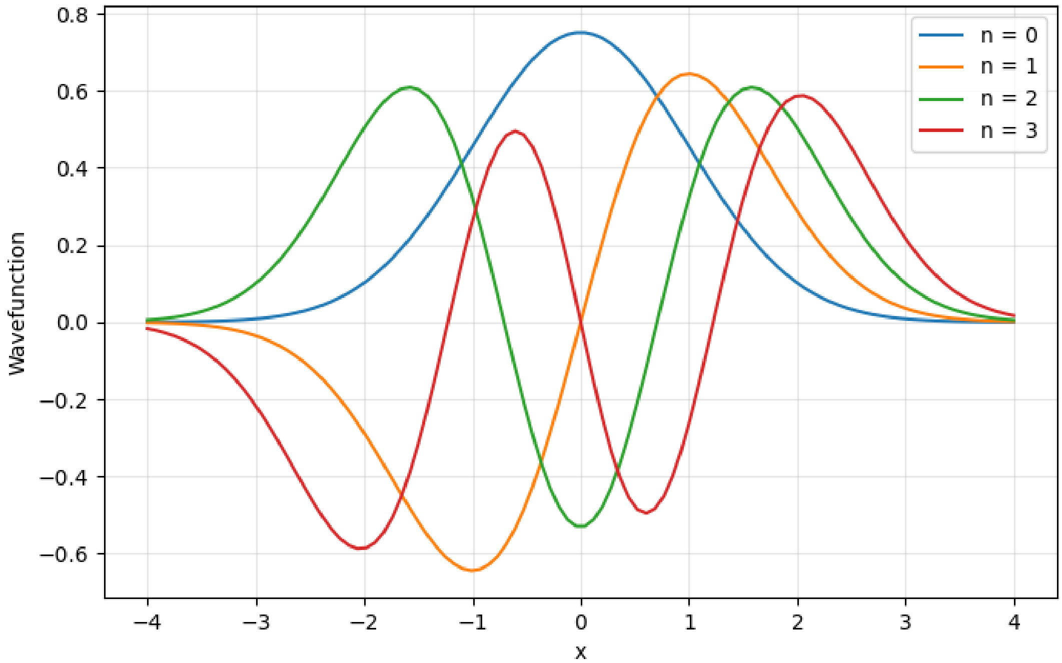

Figure 4: Wavefunctions ψ_0, ψ_1, ψ_2 and ψ_3 in the range $-4 \leq x \leq 4$.

3.2 Part b

Figure 5 shows the wavefucntion $\psi_{30}(x)$ in the range $-10 \leq x \leq 10$.

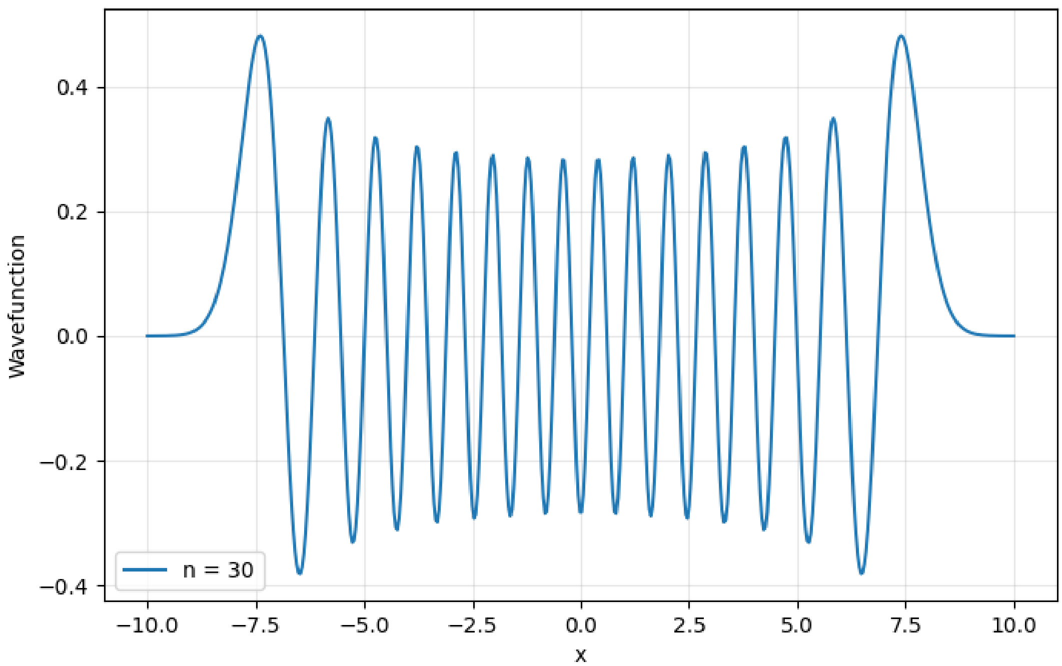

Figure 5: Wavefunction $\psi_{30}(x)$ in the range $-10 \leq x \leq 10$.

3.3 Part c

The code `prob_3c.py` performs the evaluation of the integral which returns the quantum uncertainty in the position of a particle in the n^{th} level, which is given by

$$< x^2 >= \int_{-\infty}^{+\infty} x^2 \left|\psi_n(x)\right|^2 dx. \tag{15}$$

To perform this integral using the method `numpy.polynomial.legendre.leggauss` (with $N = 100$ sample points), we used the change of variable

$$x = tan\Big(\frac{\pi y}{2}\Big), \tag{16}$$

in order to map the integration interval from $[-1, 1]$ to $[-\infty, +\infty]$. The obtained value for the root-mean-square position $\sqrt{< x^2 >}$ for $n = 5$ is:

$$\sqrt{< x^2 >} \sim 2.3452. \tag{17}$$

Given that

$$< x^2 >= \int_{-\infty}^{+\infty} x^2 \left|\psi_5(x)\right|^2 dx = \frac{11}{2}. \tag{18}$$

we compared our numerical result with the analytical one, obtaining a difference of $\mathcal{O}(10^{-10})$

3.4 Part d

We performed the same integration of the previous section, but this time using the method `numpy.polynomial.hermite.hermgauss`, which computes the sample points and weights for Gauss-Hermite quadrature. In particular, it allows to perform integrals of the form

$$\int_{-\infty}^{+\infty} f(x)e^{-x^2}. \tag{19}$$

In our case the function $f(x)$ corresponds to the part in front of the exponential in Equation 14. Given that this method correctly integrates polynomials of order $2n-1$, we can choose $N = 2*5-1 = 9$ to obtain a result which should be very close to the exact one, namely to $\sqrt{11/2}$. Indeed, the obtained difference is now of $\mathcal{O}(10^{-16})$.