QUANTUM MECHANICS I

PHYS 516

Solutions to Problem Set # 3

1. Thermal Expectation Value: A harmonic oscillator with energy spacing $\Delta E = \hbar\omega$ is in thermal equilibrium with a bath at temperature T. Compute the mean energy of the oscillator, not forgetting to include the zero point energy.

Solution:

$$Z = \sum_{n=0} e^{-\beta\hbar\omega(n+\frac{1}{2})} = \frac{e^{-\beta\hbar\omega/2}}{1-e^{-\beta\hbar\omega}}, \quad \langle E\rangle = -\frac{\partial}{\partial\beta}\log Z = (\overline{n}+\frac{1}{2})\hbar\omega, \quad \overline{n} = \frac{1}{1-e^{-\beta\hbar\omega}}$$

2. Linear Chain: In one dimension, n particles, each of mass m, are coupled to each other by springs of spring constant k. The two masses at the ends are coupled to brick walls with similar springs.

a. Draw picture.

b. Compute the energy dispersion relation for the n modes.

c. What is the mean thermal energy in each mode?

d. What is the mean thermal energy in all modes taken together?

e. Set $T = 0$. What is the zero-point energy?

Solution:

a. See class notes.

b. In the mth mode the displacement of the jth atom is $\sin\left(\frac{mj\pi}{n+1}\right)$, from which we find $m\omega^2 = 2k - 2k\cos\left(\frac{m\pi}{n+1}\right)$, which translates into $\omega(m) = 2\omega_0|\sin\left(\frac{m\pi/2}{n+1}\right)|$.

c. $\langle E\rangle_m = (\overline{n(m)} + \frac{1}{2})\hbar\omega(m), \qquad \overline{n(m)} = \frac{1}{1-e^{-\beta\hbar\omega(m)}}$

d. $\langle E\rangle = \sum_{m=1}^{n} \langle E\rangle_m$. There does not seem to be a closed form expression for this sum.

e. $\langle E\rangle_{Z.Pt.En.} = \frac{1}{2}\hbar\sum_{m=1}^{n} 2\omega_0 \sin\left(\frac{\pi m/2}{n+1}\right)$. The sum can be carried out either by hand or by Maple:

$$\frac{\langle E\rangle_{Z.Pt.En.}}{\hbar\omega_0} = \frac{1}{2}\,\frac{\sin x + \cos x - 1}{1-\cos x} \qquad x = \frac{\pi/2}{n+1}$$

For future convenience we expand this using (with $x = \frac{\pi/2}{n+1}$)

$$ZP(n) = \frac{1}{x} - \frac{1}{2} - \frac{x}{12} - \frac{x^3}{720} - \frac{x^5}{30240} - \frac{x^7}{1209600} - \cdots$$

If we search for the series: $2, 12, 720, 30240, 1209600$ on the web the first hit is A060055 in the Online Encylcopedia of Integer Sequences. It dates back from a long time ago.

Note that this energy diverges *linearly* as $n \to \infty$. For problems in D dimensions the divergence goes like n^D.

3. Quantum Surprise: Continuing the problem above ...

f. Place your finger on the mass at the kth position. What is the zero point energy in the subchain with masses $1, 2, \cdots k-1$? What is the zero point energy in the subchain with masses $k+1, ...n$?

g. Remove your finger and place it on the mass at position $k+1$. What is the zero point energy in the two subchains now?

h. Assume that the equilibrium spacing of the masses is a. What is the force on your finger when it is placed on the kth mass? And which direction is it in?

Solution: **(f)** If I place my finger on the mass at position k there are $k-1$ masses oscillating to the left and $n-k$ oscillating to the right. The energy $V(k)/\hbar\omega_0$ is $V(k) = ZP(k-1) + ZP(n-k)$ and the energy difference between the state with a 'finger on the scale' and without is

$$\Delta E = ZP(k-1) + ZP(n-k) - Z(n) = -\frac{1}{2} - \frac{\pi}{24}\left(\frac{1}{k} + \frac{1}{n-k+1} - \frac{1}{n+1}\right)$$

If the spacing between the brick walls is fixed at L and n is very large, then the spacing between masses is aabout $a = L/n$ and the expression above becomes

$$\Delta E = -\frac{1}{2} - \frac{\pi a}{24}\left(\frac{1}{x} + \frac{1}{L-x} - \frac{1}{L}\right)$$

The graph of this is shown in Fig. 1. Note that the slope is positive for $0 < x < L/2$, meaning that the force is to the left.

4. Mathematical Tricks: Like all the special functions of Mathematical Physics, the Hermite polynomials satisfy Recursion Relations, Differential Relations, and have Generating Functions:

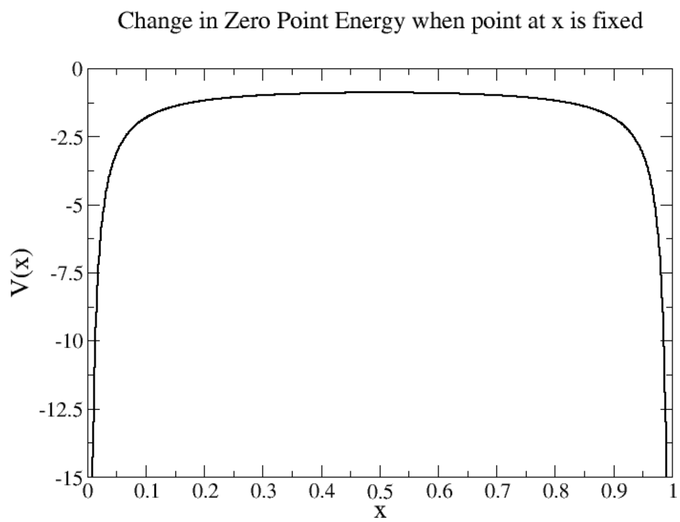

Figure 1: Change in the zero point energy for a string with n particles separated by a distance a, with $na = L$ and L scaled to 1. The force is to the left for $x < 1/2$ and to the right for $x > 1/2$. The force is due to the zero point energy and is a quantum phenomenon.

Recursion Relations :	$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x)$	**22.7**
Differential Relations :	$\frac{d}{dx}H_n(x) = 2nH_{n-1}(x)$	**22.8**
Generating Function :	$e^{2zx-z^2} = \sum \frac{1}{n!}H_n(x)z^n$	**22.9**

Use the connection between these classical polynomials and the harmonic oscillator wavefunctions

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

to construct Recursion Relations, Differential Relations, and Generating Functions for the harmonic oscillator wavefunctions.

Boldface points to tables in Abramowitz and Stegun.

Solution:

$$2x\psi_n = \frac{e^{-x^2/2}}{\sqrt{2^n n!\sqrt{\pi}}}(2xH_n) = \frac{e^{-x^2/2}}{\sqrt{2^n n!\sqrt{\pi}}}(H_{n+1}+2nH_{n-1}) = \sqrt{2}\sqrt{n+1}\psi_{n+1}+\sqrt{2}\sqrt{n}\psi_{n-1}$$

$$\frac{d}{dx}\frac{e^{-x^2/2}}{\sqrt{2^n n!\sqrt{\pi}}}H_n = \frac{e^{-x^2/2}}{\sqrt{2^n n!\sqrt{\pi}}}\left(\frac{dH_n}{dx} - xH_n\right) = \frac{e^{-x^2/2}}{\sqrt{2^n n!\sqrt{\pi}}}\left(2nH_{n-1} - xH_n\right) =$$

$$\sqrt{2n}\psi_{n-1} - \frac{1}{2}\left(\sqrt{2}\sqrt{n+1}\psi_{n+1} + \sqrt{2}\sqrt{n}\psi_{n-1}\right) = \frac{1}{2}\left(-\sqrt{2}\sqrt{n+1}\psi_{n+1} + \sqrt{2}\sqrt{n}\psi_{n-1}\right)$$

5. Modify the code you wrote for Problem # 2 in Problem Set # 2 to compute the energy eigenvalues of the bimodal potential $V(x) = \frac{1}{4}x^4 - \frac{5}{2}x^2$. Print the six lowest eigenvalues and plot the corresponding eigenvectors. Discuss the results.

Solution: See Fig. 2.

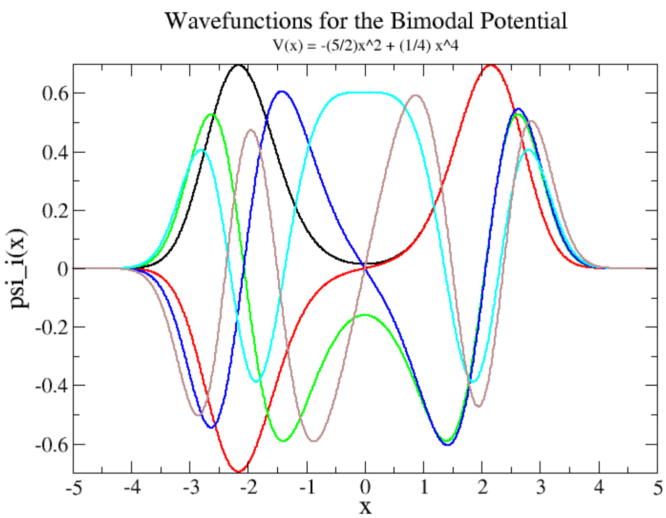

Figure 2: Six lowest eigenfunctions for the bimodal potential $V(x) = -\frac{5}{2}x^2 + \frac{1}{4}x^4$, normalized to one. The corresponding energy eigenvalues are: $-4.723518, -4.722843, -1.960872, -1.919549, -0.006859, 0.634634$. $black = \psi_0; red = \psi_1; green = \psi_2; blue = \psi_3; cyan = \psi_4; brown = \psi_5$. Notice the symmetries of the wavefunctions.