Problem Set 1

1. Partial derivatives

(a) $w = xy$, $x = yz$

$$\Downarrow$$

$$y = \frac{x}{z} \implies w = x \cdot \frac{x}{z} = \frac{x^2}{z}$$

also: $$w = \underbrace{(yz)}_{x} \cdot y = y^2 z$$

Thus: $w = \frac{x^2}{z}$ and $w = y^2 z$

(b)
$$\left(\frac{\partial w}{\partial x}\right)_y = \left(\frac{\partial (xy)}{\partial x}\right)_y = y$$

$$\left(\frac{\partial w}{\partial x}\right)_z = \left(\frac{\partial \left(\frac{x^2}{z}\right)}{\partial x}\right)_z = \frac{2x}{z}$$

(c)
$$\left(\frac{\partial w}{\partial y}\right)_x = \left(\frac{\partial (xy)}{\partial y}\right)_x = x$$

$$\left(\frac{\partial w}{\partial y}\right)_z = \left(\frac{\partial (y^2 z)}{\partial y}\right)_z = 2yz$$

$$\left(\frac{\partial w}{\partial z}\right)_x = \left(\frac{\partial \left(\frac{x^2}{z}\right)}{\partial z}\right)_x = -\frac{x^2}{z^2}$$

$$\left(\frac{\partial w}{\partial z}\right)_y = \left(\frac{\partial (y^2 z)}{\partial z}\right)_y = y^2$$

(2.) Two harmonic oscillators

Change notation from q (used in the problem formulation) to j (used here in the solution).

(a) The total energy of the composed system, U_1, equals to the sum of the energies of the two harmonic oscillators, E_{j1} and E_{j2}. Each of these are given by:

$$E_{j_1} = j_1 \hbar\omega \,, \quad \text{where} \quad j_1 = 0, 1, 2, 3, \ldots$$

and

$$E_{j_2} = j_2 \hbar\omega \,, \quad \text{where} \quad j_2 = 0, 1, 2, 3, \ldots$$

Therefore

$$U_1 = E_{j_1} + E_{j_2} = (j_1 + j_2)\hbar\omega$$

On the other hand, the problem states (requires) that

$$U_1 = n_1 \hbar\omega \,, \quad \text{where} \quad n_1 = 0, 1, 2, 3, \ldots$$

Therefore we must have

$$(j_1 + j_2)\cancel{\hbar\omega} = n_1 \cancel{\hbar\omega}$$

i.e. for any given n_1, j_1 and j_2 must satisfy

$$j_1 + j_2 = n_1$$

So the question of "how many microstates are available to the system" is reduced to finding the number of ways that a pair of non-negative integers j_1 and j_2 can result in the given value of n_1 (which in turn runs $n_1 = 0, 1, 2, \ldots$; i.e. for each n_1, have to find the respective multiplicity)

$$n_1 = j_1 + j_2$$

Consider, for example $n_1 = 3$. This can be obtained in the following ways (from pairs of non-negative j_1 and j_2)

$$\left.\begin{array}{l} j_1 = 0, \ j_2 = 3 \\ j_1 = 1, \ j_2 = 2 \\ j_1 = 2, \ j_1 = 1 \\ j_1 = 3, \ j_2 = 0 \end{array}\right\}$$

4 ways (microstates)

$\Rightarrow$ the multiplicity of $n_1 = 3$:

$$g(n_1 = 3) = 4$$

How about other possible value of n_1, or rather <u>all</u> possible values of n_1?

[general solution]

Can draw a table:

n_1	j_1	j_2	g_1
0	0	0	1
1	0 1	1 0 } 2	2
2	0 2 1	2 0 1 } 3	3
3	0 1 2 3	3 2 1 0 } 4	4
n_1	0 1 2 ⋮ n_1	n_1 $n_1 - 1$ $n_1 - 2$ 0	$n_1 + 1$

Thus, for any n_1,

$$\boxed{g(n_1) = n_1 + 1}$$

The definition of entropy is:

$$S = k_B \log_e(g) \qquad [\log_e \equiv \ln]$$

So, in this example

$$S_1 = k_B \log(g_1) = k_B \log(n_1 + 1)$$

Usually we want to know the dependence of the entropy on the total energy of the system, $S_1(U_1)$. In the present example $U_1 = n_1 \hbar\omega \implies n_1 = \frac{U_1}{\hbar\omega}$

$$\implies \boxed{S_1 = k_B \log\left(\frac{U_1}{\hbar\omega} + 1\right)}$$

(b) Second system (we'll use index "2"):

We now have $E_{j_1} = j_1 \hbar(2\omega) = 2 j_1 \hbar\omega$

and $E_{j_2} = j_2 \hbar(2\hbar) = 2 j_2 \hbar\omega$

$$U_2 = E_{j_1} + E_{j_2}$$

$$n_2 \hbar\omega = 2j_1\hbar\omega + 2j_2\hbar\omega$$

$$\implies \boxed{n_2 = 2(j_1 + j_2)}$$

[$j_1 = 0, 1, 2, \ldots$ and $j_2 = 0, 1, 2, \ldots$ as before]

Then, our multiplicity table would look like:

n_2	j_1	j_2	g_2	$U_2 = n_2\hbar\omega = 2(j_1+j_2)\hbar\omega$
0	0	0	1	0
2	0 1	1 0	2 microstates	$2\hbar\omega$
4	0 1 2	2 1 0	3 microstates	$4\hbar\omega$
6	0 1 2 3	3 2 1 0	4	$6\hbar\omega$
$\vdots$				
n_2	0 1 2 $\vdots$ $\frac{n_2}{2}$	$\frac{n_2}{2}$ $\frac{n_2}{2}-1$ $\vdots$ 0	$\frac{n_2}{2}+1$	$n_2\hbar\omega$

Thus, for any given value of n_2 of the combined system, or equivalently for any given total energy of the combined system $U_2 = n_2\hbar\omega$, the respective multiplicity is

$$g_2(n_2) = \frac{n_2}{2} + 1$$

or

$$g_2(U_2) = \frac{n_2}{2} + 1$$

Accordingly, the entropy $S = k_B \log(g)$ is now given by

$$S_2 = k_B \log\left(\frac{n_2}{2} + 1\right) =$$

$$= k_B \log\left(\frac{U_2}{2\hbar\omega} + 1\right)$$

(c) For the system composed of the two previous systems ~~two~~, taking into account their independence,

$$g_{total} = g_1 \cdot g_2$$

$$\Longrightarrow S_{total} = k_B \log(g_{total}) = k_B \log(g_1 \cdot g_2)$$

$$= k_B \log(g_1) + k_B \log(g_2) = S_1 + S_2$$

$$= \log\left(\frac{U_1}{\hbar\omega} + 1\right) + \log\left(\frac{U_2}{2\hbar\omega} + 1\right)$$

$$= \log\left[\left(\frac{U_1}{\hbar\omega} + 1\right)\left(\frac{U_2}{2\hbar\omega} + 2\right)\right]$$

3. Properties of a Gaussian function

$$f(x) = f(0)\, e^{-x^2/2\sigma^2}$$

(a).

$$1 = \int_{-\infty}^{+\infty} dx\; f(x) = f(0) \int_{-\infty}^{+\infty} dx\; \underbrace{e^{-x^2/2\sigma^2}}_{\text{even function of } x,\ f(-x)=f(x)}$$

$$= 2 f(0) \int_{0}^{+\infty} dx\; e^{-x^2/2\sigma^2} = 2 f(0) \frac{\sqrt{\pi}}{2\left(\frac{1}{\sqrt{2}\,\sigma}\right)}$$

$$= \sqrt{2\pi}\,\sigma\, f(0)$$

$$\therefore \quad f(0) = \frac{1}{\sqrt{2\pi}\,\sigma} \qquad (\sigma > 0)$$

(b)

$$\langle x \rangle = \int_{-\infty}^{+\infty} dx\; x\, f(x) = 0 \quad \text{since}$$

$g(x) \equiv x\, f(x)$ — is an odd function of x, i.e. $g(-x) = -g(x)$

$$\int_{-\infty}^{+\infty} dx\, g(x) = \underbrace{\int_{-\infty}^{0} dx\, g(x)}_{\text{change of variables: } x \to -y} + \int_{0}^{+\infty} dx\, g(x)$$

$$= \int_{\substack{x=-\infty \\ (y=+\infty)}}^{0} d(-y)\, g(-y) + \int_{0}^{+\infty} dx\, g(x)$$

$$= \int_{+\infty}^{0} dy\, g(y) + \int_{0}^{+\infty} dx\, g(x) = -\int_{0}^{+\infty} dy\, g(y) + \int_{0}^{+\infty} dx\, g(x) = 0$$

(c). $$\langle x^2 \rangle = \int_{-\infty}^{+\infty} dx \; \underbrace{x^2 f(x)}_{\text{even function}} =$$

$$= f(0) \cdot 2 \int_0^{\infty} dx \; x^2 e^{-x^2/2\sigma^2} =$$

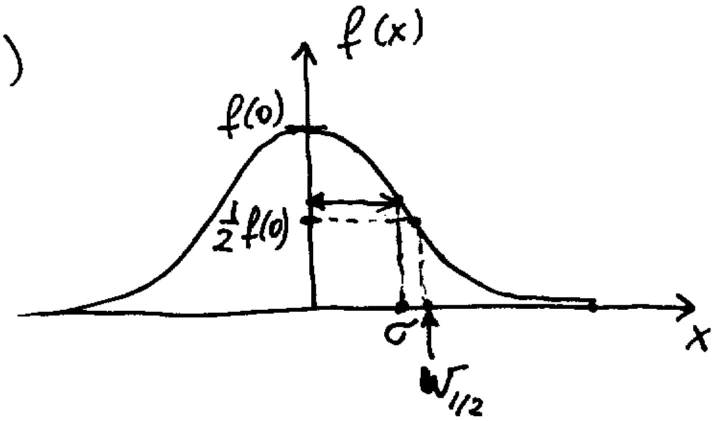
$$= 2 f(0) \cdot \frac{\sqrt{\pi}}{4 \left(\frac{1}{\sqrt{2}\sigma}\right)^3} = \cancel{2} \underbrace{f(0)}_{= \frac{1}{\sqrt{2\pi}\sigma}} \frac{\cancel{2} \sqrt{2\pi}\, \sigma^3}{\cancel{4}}$$

$$= \sigma^2$$

(d) $$W_{rms} = \left(\langle x^2 \rangle - \langle x \rangle^2 \right)^{1/2} = \left(\sigma^2 - 0 \right)^{1/2} = \sigma$$

σ in the Gaussian function of the form $f(x) = f(0)\, e^{-x^2/2\sigma^2}$ has the meaning of the rms width.

(e)



$$f(\sigma) > \frac{1}{2} f(0)$$

$$\left[f(\sigma) = f(0)\, e^{-1/2} = \frac{f(0)}{\sqrt{e}} = \simeq 0.6\, f(0) \right]$$

(f) $$f(W_{1/2}) = \frac{1}{2} f(0) \quad , \quad W_{1/2} - ?$$

$$f(W_{1/2}) = f(0)\, e^{-W_{1/2}^2/2\sigma^2} = \frac{1}{2} f(0)$$

$$\therefore \; e^{W_{1/2}^2/2\sigma^2} = 2$$

$$e^{\omega_{1/2}^2/2\sigma^2} = 2 \implies \omega_{1/2}^{\,2} = 2\sigma^2 \ln 2 = \sigma^2 \ln 4$$

$$\implies \omega_{1/2} = \sigma \sqrt{\ln 4} \simeq \sigma \cdot 1.18$$

$$(\ln 4 > 1 \implies \sqrt{\ln 4} > 1$$

$$\implies \boxed{\omega_{1/2} > \sigma}$$

$$\omega_{1/2} \simeq 1.2\ \sigma$$