

Solution to written exam in QUANTUM PHYSICS AND STATISTICAL PHYSICS  
F0018T / MTF131

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Note solutions are more detailed compared to previous solutions, earlier than October 2007.

## 1. a

The spinor is not normalised and we need to do this first:

$$1 = \chi^* \chi = |A|^2 (2 - 5i, 3 + i) \begin{pmatrix} 2 + 5i \\ 3 - i \end{pmatrix} = |A|^2 |2 + 5i|^2 |3 - i|^2 \rightarrow A = \frac{1}{\sqrt{39}}$$

Note an expectation value is always a real number, never a complex one! Even if you had taken  $A$  to be a complex number like  $A = \frac{i}{\sqrt{39}}$  it would not change the expectation value as the expectation value below only involves  $|A|^2$ .

$$\langle S_x \rangle = \frac{1}{39} (2 - 5i, 3 + i) \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 2 + 5i \\ 3 - i \end{pmatrix} = \frac{1}{39} \hbar$$

$$\langle S_y \rangle = \frac{1}{39} (2 - 5i, 3 + i) \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 2 + 5i \\ 3 - i \end{pmatrix} = -\frac{17}{39} \hbar$$

$$\langle S_z \rangle = \frac{1}{39} (2 - 5i, 3 + i) \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 2 + 5i \\ 3 - i \end{pmatrix} = \frac{19}{78} \hbar$$

## b

Measurement along the  $x$  direction means:  $S = (1, 0, 0) \cdot (S_x, S_y, S_z) = S_x$ . The idea is to expand the initial spinor  $\chi$  into the eigenspinors of  $S_x$ . So we start to calculate the eigenvalues and eigenspinors to  $S_x$ . The spin operator  $S_x$  is

$$S_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

we find the eigenvalues from the following equation

$$S_x \chi = \lambda \chi \Leftrightarrow \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \lambda \begin{pmatrix} a \\ b \end{pmatrix} \quad (1)$$

We find the eigenvalues from the equation

$$\begin{vmatrix} -\lambda & \frac{\hbar}{2} \\ \frac{\hbar}{2} & -\lambda \end{vmatrix} = 0 \Rightarrow \lambda = \pm \frac{\hbar}{2}$$

The eigenspinors to  $S_x$  corresponding to the  $+\frac{\hbar}{2}$  we get from

$$\frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = +\frac{\hbar}{2} \begin{pmatrix} a \\ b \end{pmatrix}$$

The two equations above are linearly dependent and one of them is

$$a = b \Leftrightarrow \text{let } b = 1 \text{ and hence } a = 1$$

This gives the unnormalised spinor

$$\begin{pmatrix} 1 \\ 1 \end{pmatrix} \text{ and after normalisation we have } \chi_{x+} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

The other eigenspinor  $\chi_{x-}$  has to be orthogonal to  $\chi_{x+}$ . An appropriate choice is:

$$\chi_{x-} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

Now we can expand the initial spinor  $\chi$  in these eigenspinors to  $S_x$ . the second eigenspinor you can get from orthogonality to the first one.

$$\chi = \frac{1}{\sqrt{39}} \begin{pmatrix} 2 + 5i \\ 3 - i \end{pmatrix} = b_+ \chi_{x+} + b_- \chi_{x-}$$

The coefficient  $b_+$  is given by

$$b_+ = \chi_{x+}^* \chi = \frac{1}{\sqrt{78}} (1 \ 1) * \begin{pmatrix} 2 + 5i \\ 3 - i \end{pmatrix} = \frac{1}{\sqrt{78}} (2 + 5i + 3 - i) = \frac{1}{\sqrt{78}} (5 + 4i)$$

A similar calculation gives  $b_-$  :

$$b_- = \chi_{x-}^* \chi = \frac{1}{\sqrt{78}} (1 \ -1) * \begin{pmatrix} 2 + 5i \\ 3 - i \end{pmatrix} = \frac{1}{\sqrt{78}} (2 + 5i - 3 + i) = \frac{1}{\sqrt{78}} (-1 + 6i)$$

We may now check that  $|b_+|^2 + |b_-|^2 = 1$

$$|b_+|^2 + |b_-|^2 = \frac{1}{78} (25 + 16 + 1 + 36) = 1 \quad \text{ok}$$

The probability (to get  $+\frac{\hbar}{2}$ ) is given by  $|b_+|^2$ .

$$|b_+|^2 = \frac{1}{78} (25 + 16) = \frac{41}{78} \approx \mathbf{0.526}$$

and (to get  $-\frac{\hbar}{2}$ ) is given by  $|b_-|^2$ .

$$|b_-|^2 = \frac{1}{78} (1 + 36) = \frac{37}{78} \approx \mathbf{0.474}$$

You may make the following check for consistency:

$$\langle S_x \rangle = \left( \frac{41}{78} \left( \frac{\hbar}{2} \right) + \frac{37}{78} \left( -\frac{\hbar}{2} \right) \right) = \frac{1}{39} \hbar$$

The same result as in part **a**.

2. The specific heat at low temperatures is given by

$$C_v = \gamma T + AT^3 = \frac{\pi^2 N_e k_B^2}{2\epsilon_F} T + \frac{12\pi^4}{5} N k_B \left( \frac{T}{\Theta_D} \right)^3$$

where  $\gamma T$  is the contribution from the electrons valid for temperatures from zero to a bit below the Fermi temperature  $T_F = 3.66 \cdot 10^4 \text{K}$ . The second term  $AT^3$  is the contribution (Debye  $T^3$  law) from the phonons valid for temperatures from zero to a bit below the Debye temperature  $\Theta_D = 160 \text{K}$ . At room temperature the specific heat is dominated by the phonons and given the two different powers there has to be a low temperature  $T_l$  (above absolute zero) at which the two contributions are equal.

The Fermi energy relates to the Fermi temperature by  $\epsilon_F = k_B T_F$ . As each Sodium atom contributes with one electron to the Fermi system the number of atoms  $N$  equals the number of free electrons  $N_e$ . We arrive at the following equation for the temperature  $T_l$ .

$$\frac{\pi^2 N_e k_B^2}{2k_B T_F} T_l = \frac{12\pi^4}{5} N k_B \left( \frac{T_l}{\Theta_D} \right)^3$$

Which solves for

$$T_l^2 = \frac{5}{24\pi^2} \cdot \frac{\Theta_D^3}{T_F} = \frac{5}{24\pi^2} \frac{160^3}{3.66 \cdot 10^4} = 2.3623 \text{ K}^2 \text{ and hence } T_l \approx 1.5 \text{ K}.$$

Other numbers that might come in handy. Atomic weight  $m = 22.99u$ , molar weight  $22.99 \text{ g/mole}$ , density  $\rho = 971 \text{ kgm}^{-3}$ . The density of atoms in Sodium  $n = 971 * 6.022 \cdot 10^{23} / 0.02299 = 2.543 \cdot 10^{28} \text{ m}^{-3}$ .

3. Rewrite the wave function in terms of spherical harmonics: (polar coordinates:  $x = r \sin \theta \sin \phi$ ,  $z = r \cos \theta$  and hence  $zx = r^2 \cos \theta \sin \theta (e^{i\phi} + e^{-i\phi})/2$  using the Euler relations) the appropriate spherical harmonics can now be identified and we arrive at

$$\psi(\mathbf{r}) = \psi(x, y, z) = N(zx)e^{-r/3a_0} = N \frac{r^2}{2} \sqrt{\frac{8\pi}{15}} (-Y_{2,1} + Y_{2,-1}) e^{-r/3a_0}. \quad (2)$$

As all the involved  $Y_{l,m}$  have  $l = 2$  the probability to get  $\mathbf{L}^2 = 2(2+1)\hbar^2 = 6\hbar^2$  is one. For the operator  $L_z$  we note the two spherical harmonics have the same pre factor (one has -1 and the other has +1 but the absolute value square is the same) ie they will have the same probability. The probability to find  $m = 2\hbar$  is 0, for  $m = 1\hbar$  is  $\frac{1}{2}$ , for  $m = 0\hbar$  is 0 for  $m = -1\hbar$  is  $\frac{1}{2}$ , and for  $m = -2\hbar$  is 0. As all the involved  $Y_{l,m}$  have  $l = 2$  the probability to get  $\mathbf{L}^2 = 2(2+1)\hbar^2 = 6\hbar^2$  is one.

**b.** To calculate the expectation value  $\langle r \rangle$  we need to normalise the given wave function if we wish to do the integral. In order to achieve this in a simple way is to identify the radial wave function. As  $l$  is equal to 2 we know that  $n$  cannot be equal to 1 or 2 it has to be **larger or equal** to 3. By inspection of eq (2) and 2 we find  $n = 3$  this function has the correct exponential and the correct power of  $r$  ( $r^2$ ) and hence  $R_{3,2}(r) = \frac{2\sqrt{2}}{27\sqrt{5}} \left( \frac{z}{3a_0} \right)^{3/2} \left( \frac{zr}{a_0} \right)^2 e^{-Zr/3a_0}$ . We also note that  $Y_{2,1}$  and  $Y_{2,-1}$  are normalised but the sum  $(-Y_{2,1} + Y_{2,-1})$  is not normalised. The sum has to be changed to  $(-\frac{1}{\sqrt{2}}Y_{2,1} + \frac{1}{\sqrt{2}}Y_{2,-1})$  in order to be normalised. Note that  $R_{3,2}(r)$  contains an  $r^2$  term as also a  $e^{-r/3a_0}$  term. The wave function can now be completed to the following

normalized wave function (note that we do not need to calculate the constant  $N$  as all separate parts of  $\psi(r)$  are normalised by them selves)

$$\psi(\mathbf{r}) = \psi(x, y, z) = N(zx)e^{-r/3a_0} = R_{3,2}(r)\left(-\frac{1}{\sqrt{2}}Y_{2,1} + \frac{1}{\sqrt{2}}Y_{2,-1}\right)e^{-r/3a_0}$$

From physics handbook page 292 you find

$$\langle r \rangle = \frac{1}{2} [3n^2 - l(l+1)] \left(\frac{a_0}{Z}\right) = \frac{1}{2} [3 \cdot 3^2 - 2(2+1)] \left(\frac{a_0}{1}\right) = \frac{21}{2} a_0 = 10.5 \cdot 0.5292 \text{ \AA} = 5.56 \text{ \AA}.$$

You may also do the integral directly like this:

$$\langle r \rangle = \int_0^\infty \int_0^\pi \int_0^{2\pi} d\phi d\theta dr r^2 \sin(\theta) r |R_{3,2}(r)|^2 \left(-\frac{1}{\sqrt{2}}Y_{2,1} + \frac{1}{\sqrt{2}}Y_{2,-1}\right)^2 e^{-2r/3a_0} = \int_0^\infty dr r^3 |R_{3,2}(r)|^2 e^{-2r/3a_0} = \frac{21}{2} a_0 = 10.5 \cdot 0.5292 \text{ \AA} = 5.56 \text{ \AA}.$$

4. This is a 2 dimensional problem with a Schrödinger equation (where  $V(x, y) = 0$ ) like

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi(x, y) - \frac{\hbar^2}{2m} \frac{d^2}{dy^2} \Psi(x, y) = E \Psi(x, y)$$

This equation is separable and the ansatz  $\Psi(x, y) = \psi(x) * \psi(y)$  gives the following result

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi_x(x) - \frac{\hbar^2}{2m} \frac{d^2}{dy^2} \psi_y(y) = E_x \psi_x(x) + E_y \psi_y(y)$$

ie two independent one dimensional Schrödinger equations one for the variable  $x$  and one for  $y$ . We therefor solve the one dimensional problem first and after that we construct the two dimensional solution.

To find the eigenfunctions we need to solve the Schrödinger equation which is (in the region where  $V(x)$  is zero)

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi = E \Psi \rightarrow \frac{d^2}{dx^2} \Psi + k^2 \Psi = 0 \text{ where } k^2 = \frac{2mE}{\hbar^2}$$

Solutions are of the kind:

$$\Psi(x) = A \cos kx + B \sin kx$$

Now we need to take the boundary conditions for the wave function  $\Psi$  ( $\Psi(-\frac{a}{2}) = \Psi(\frac{a}{2}) = 0$ ) into account.

$$A \cos\left(-\frac{ka}{2}\right) + B \sin\left(-\frac{ka}{2}\right) = 0 \text{ and } A \cos\left(\frac{ka}{2}\right) + B \sin\left(\frac{ka}{2}\right) = 0$$

Adding the two conditions gives:  $\cos\left(\frac{ka}{2}\right) = 0$  and subtracting them gives  $\sin\left(\frac{ka}{2}\right) = 0$ . These two conditions cannot be fulfilled at the same time, so either  $A$  or  $B$  has to be zero. We start with  $A = 0$  and we get the following solution: The normalising constant  $B = \sqrt{\frac{2}{a}}$  you get from the

condition  $\int_{-a/2}^{a/2} |\Psi|^2 dx = 1$ . The condition  $\sin(\frac{ka}{2}) = 0$  gives  $\frac{ka}{2} = \frac{\pi}{2} * (\text{even} - \text{integer})$ . The solution is:

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \text{ with eigenenergys } E_n = \frac{n^2\pi^2\hbar^2}{2Ma^2} \text{ where } n = 2, 4, 6, \dots \quad (3)$$

In a similar way the other function is analysed ( $A = 0$ ) which gives: The condition  $\cos(\frac{ka}{2}) = 0$  gives  $\frac{ka}{2} = \frac{\pi}{2} * (\text{odd} - \text{integer})$ . The solution is:

$$\psi_n(x) = \sqrt{\frac{2}{a}} \cos\left(\frac{n\pi x}{a}\right) \text{ with eigenenergys } E_n = \frac{n^2\pi^2\hbar^2}{2Ma^2} \text{ where } n = 1, 3, 5, \dots \quad (4)$$

The eigenfunctions in the  $y$  direction are the same as for the  $x$  direction as the potential is similar for this direction. Now we have the eigenfunctions of the one dimensional and the solution to the 2 dimensional problem is readily produced. The eigenfunctions are:

$$\Psi_{n,m}(x, y) = \psi_n(x) \cdot \psi_m(y) \text{ eigenenergys } E_{n,m} = E_n + E_m \text{ where } n = 1, 2, \dots \text{ and } m = 1, 2, \dots \quad (5)$$

In the area where the potential is infinite the wave function is equal to zero.

An **alternative route** taken by many has been to present a calculation with the following boundary conditions:  $\Psi$  ( $\Psi(0) = \Psi(a) = 0$ ) into account. In this case the solution is for these boundary conditions:

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \text{ with eigenenergys } E_n = \frac{n^2\pi^2\hbar^2}{2Ma^2} \text{ where } n = 1, 2, 3, \dots \quad (6)$$

This solution has to be adapted to the boundary conditions related to this exam problem:

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}\left(x + \frac{a}{2}\right)\right) \text{ with eigenenergys } E_n = \frac{n^2\pi^2\hbar^2}{2Ma^2} \text{ where } n = 1, 2, 3, \dots \quad (7)$$

$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a} + \frac{n\pi}{2}\right) = \sqrt{\frac{2}{a}} \left(\sin\left(\frac{n\pi x}{a}\right) \cdot \cos\left(\frac{n\pi}{2}\right) + \cos\left(\frac{n\pi x}{a}\right) \cdot \sin\left(\frac{n\pi}{2}\right)\right)$ . We see that we recover the solution in eq (3), (4) and (5) as we let  $n$  run from 1 to  $\infty$ .

**b)** Now we turn to the question of **parity**, ie whether the wave function is *odd* or *even* under a change of coordinates from  $(x, y)$  to  $(-x, -y)$ . The one dimensional eigenfunctions in eq (3) and (4) have a definite parity. The functions in (3) are odd whereas the functions in (4) are even. As the eigenstates for the 2 dimensional system are formed from eq (5) ie products of functions that are even or odd the total function itself will be either even or odd as well.

The four lowest eigenenergies are given by

$$E_{n,m} = \frac{\pi^2\hbar^2}{2Ma^2}(n^2 + m^2), \text{ where the 4 lowest are } (n^2 + m^2) = 2, 5, 8, 10.$$

When we form the eigenstates we need to keep track of the parity of the  $\psi_n(x)$  and  $\psi_m(y)$ . It is therefore necessary to have the functions in the form like in eq (3) and (4) to identify the parity as odd or even. This is difficult if you try with functions like eq (7) even though it is a correct eigenstate it is hard to identify their parity.

$$E_{1,1} = \text{one state } (n^2 + m^2 = 2) \quad \text{odd} * \text{odd} = \text{even}$$

$$\begin{aligned}
E_{1,2} = E_{2,1} &= \text{two states } (n^2 + m^2 = 5) && \text{odd} * \text{even} = \text{odd} \\
E_{2,2} &= \text{one state } (n^2 + m^2 = 8) && \text{even} * \text{even} = \text{even} \\
E_{1,3} = E_{3,1} &= \text{two states } (n^2 + m^2 = 10) && \text{odd} * \text{odd} = \text{even}
\end{aligned}$$

So of the four states only one is even and three where odd.

5. As the temperature raises the ground state gets de populated and excited states get populated. The ground state has all the  $n_i = 0$  and has an energy  $\frac{3}{2}\hbar\omega$  there is only one state with this energy. The next excited state has one of the  $n_i = 1$  and the other two are equal to zero ((1,0,0) or (0,1,0) or (0,0,1)) the degeneracy of this state is hence equal to 3 the energy of it is  $\frac{5}{2}\hbar\omega$ .

a) There is one state of the lower energy and three states with the higher energy. The probability to find the oscillator in a state of energy is proportional to the Boltzmann factor we arrive at the following equation.  $1e^{-1.5\hbar\omega/k_B T} = 3e^{-2.5\hbar\omega/k_B T}$  and  $e^{1\hbar\omega/k_B T} = 3$  which evaluates to  $T = \frac{1\hbar\omega}{k_B \ln 3}$  or if you prefer  $\tau$ ,  $\tau = \frac{1\hbar\omega}{\ln 3}$ , which is equally correct.

b) The partition sum is given by:  $Z = \sum_{n_1=0, n_2=0, n_3=0}^{\infty} e^{-(n_1+n_2+n_3+1.5)\hbar\omega/k_B T} = \sum_{n=0}^{\infty} g(n)e^{-(n+1.5)\hbar\omega/k_B T}$ , where  $g(n)$  is the degeneracy of the energy levels and  $n = n_1 + n_2 + n_3$ . There are two ways to evaluate this sum. One simple and one more elaborate. First we do the simple solution. The sum for  $Z$  can be done as a product of three separate geometric sums.  $Z = \sum_{n_1=0, n_2=0, n_3=0}^{\infty} e^{-(n_1+n_2+n_3+1.5)\hbar\omega/k_B T} = \sum_{n_1=0}^{\infty} e^{-(n_1+0.5)\hbar\omega/k_B T} \cdot \sum_{n_2=0}^{\infty} e^{-(n_2+0.5)\hbar\omega/k_B T} \cdot \sum_{n_3=0}^{\infty} e^{-(n_3+0.5)\hbar\omega/k_B T} = \left(\sum_{n=0}^{\infty} e^{-(n+0.5)\hbar\omega/k_B T}\right)^3 = e^{-3/2\hbar\omega/k_B T} \left(\sum_{n=0}^{\infty} e^{-n\hbar\omega/k_B T}\right)^3 = e^{-3/2\hbar\omega/k_B T} \left(\frac{1}{1-e^{-\hbar\omega/k_B T}}\right)^3 = \left(\frac{1}{e^{+\hbar\omega/2k_B T} - e^{-\hbar\omega/2k_B T}}\right)^3$ . With  $k_B T = \tau = \frac{1\hbar\omega}{\ln 3}$  we get arrive at the following

$$Z = \left(\frac{1}{e^{+\frac{\ln 3}{2}} - e^{-\frac{\ln 3}{2}}}\right)^3 = \left(\frac{1}{\sqrt{3} - \frac{1}{\sqrt{3}}}\right)^3$$

The solution continues after the following alternative calculation for  $Z$ .

Now we turn our attention to the more complicated calculation for the partition function  $Z$ : One can make a geometric construction in three dimensions as well  $g(n)$  will be the number of points in the plane that cuts through the coordinates: ((n,0,0) or (0,n,0) or (0,0,n)). We can set up the following table for the degeneracy  $g(n)$ . The first values you get from inspecting the different possibility's for the  $n_x, n_y, n_z$ .

$n$	0	1	2	3	4	5	...	$n$
$g(n)$	1	3	6	10	15	21	...	$\frac{(n+1)(n+2)}{2}$
$\Delta$	1	2	3	4	5	6	7	

The result for  $g(n) = \frac{(n+1)(n+2)}{2}$  is reached by inspection. You can use the fact that the degenerate values form a triangle with a base length of  $n + 1$  and a height in the range of  $n$ . The lower line of the table is the difference between two consecutive  $g(n)$ .

The sum we have to calculate is  $Z = \sum_{n=0}^{\infty} \frac{(n+1)(n+2)}{2} e^{-(n+1.5)\hbar\omega/k_B T}$ . This sum breaks down into three separate geometric sums, one with pre factor  $n^2$  one with  $n$  and one with a constant.  $Z = e^{-1.5\hbar\omega/k_B T} \sum_{n=0}^{\infty} (n^2/2 + 3n/2 + 1)e^{-n\hbar\omega/k_B T}$ .

The standard geometric sum is given by  $1 + x + x^2 + x^3 + x^4 \dots = \frac{1}{1-x}$  and the next one is  $x + 2x^2 + 3x^3 + 4x^4 \dots = \frac{x}{(1-x)^2}$  (you get this one by taking the derivative of the previous one and multiplying with an appropriate factor of  $x$ , or you get it from Beta page 188). The third sum with the  $n^2$  factor is reached in a similar way:

$$x + 4x^2 + 9x^3 + 16x^4 \dots = \frac{x}{(1-x)^2} + \frac{2x^2}{(1-x)^3}$$

(you get this one by taking the The first one you get by taking another derivative.

$$\begin{aligned} Z &= e^{-1.5\hbar\omega/k_B T} \sum_{n=0}^{\infty} (n^2/2 + 3n/2 + 1)e^{-n\hbar\omega/k_B T} \\ Z &= e^{-\frac{3\hbar\omega}{2k_B T}} \left( \frac{1}{1 - e^{-\frac{\hbar\omega}{\tau}}} + \frac{3e^{-\frac{\hbar\omega}{\tau}}}{2(1 - e^{-\frac{\hbar\omega}{\tau}})^2} + \frac{1e^{-\frac{\hbar\omega}{\tau}}}{2(1 - e^{-\frac{\hbar\omega}{\tau}})^2} + \frac{2e^{-\frac{2\hbar\omega}{\tau}}}{2(1 - e^{-\frac{\hbar\omega}{\tau}})^3} \right) = \\ &= e^{-\frac{3\hbar\omega}{2k_B T}} \left( \frac{1}{1 - e^{-\frac{\hbar\omega}{\tau}}} + \frac{2e^{-\frac{\hbar\omega}{\tau}}}{(1 - e^{-\frac{\hbar\omega}{\tau}})^2} + \frac{e^{-\frac{2\hbar\omega}{\tau}}}{(1 - e^{-\frac{\hbar\omega}{\tau}})^3} \right) = \\ &= e^{-\frac{3\hbar\omega}{2k_B T}} \left( \frac{(1 - e^{-\frac{\hbar\omega}{\tau}})^2}{(1 - e^{-\frac{\hbar\omega}{\tau}})^3} + \frac{(1 - e^{-\frac{\hbar\omega}{\tau}})2e^{-\frac{\hbar\omega}{\tau}}}{(1 - e^{-\frac{\hbar\omega}{\tau}})^3} + \frac{e^{-\frac{2\hbar\omega}{\tau}}}{(1 - e^{-\frac{\hbar\omega}{\tau}})^3} \right) = \\ &= e^{-\frac{3\hbar\omega}{2k_B T}} \left( \frac{1 - 2e^{-\frac{\hbar\omega}{\tau}} + e^{-2\frac{\hbar\omega}{\tau}} + 2e^{-\frac{\hbar\omega}{\tau}} - 2e^{-2\frac{\hbar\omega}{\tau}} + e^{-2\frac{\hbar\omega}{\tau}}}{(1 - e^{-\frac{\hbar\omega}{\tau}})^3} \right) = \\ &= e^{-\frac{3\hbar\omega}{2k_B T}} \left( \frac{1}{(1 - e^{-\frac{\hbar\omega}{\tau}})^3} \right) = \left( \frac{1}{(e^{+\frac{\hbar\omega}{2\tau}} - e^{-\frac{\hbar\omega}{2\tau}})^3} \right) = \end{aligned}$$

With  $k_B T = \tau = \frac{1\hbar\omega}{\ln 3}$  we arrive at the following:

$$Z = \left( \frac{1}{(e^{+\frac{\ln 3}{2}} - e^{-\frac{\ln 3}{2}})^3} \right) = \left( \frac{1}{\sqrt{3} - \frac{1}{\sqrt{3}}} \right)^3$$

After these two alternative calculations for  $Z$  we may continue with the calculation of the probability: (we may choose any of the two energies as their probabilities will be equal:  $1e^{-1.5\hbar\omega/k_B T} = 3e^{-2.5\hbar\omega/k_B T}$ )

$$\begin{aligned} P &= e^{-3\hbar\omega/2k_B T} / \left( \frac{1}{\sqrt{3} - \frac{1}{\sqrt{3}}} \right)^3 = 3^{-3/2} \left( \sqrt{3} - \frac{1}{\sqrt{3}} \right)^3 = \left( \frac{1}{\sqrt{3}} \right)^3 \left( \sqrt{3} - \frac{1}{\sqrt{3}} \right)^3 = \\ &= \left( 1 - \frac{1}{3} \right)^3 = \frac{8}{27} \approx 0.296 \end{aligned}$$

The probability to be in one of these energies is  $P = \frac{8}{27} \approx 0.296$