

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. Hydrogenic atoms have eigenfunctions $\psi_{nlm} = R_{nl}(r)Y_{lm}(\theta, \varphi)$. Using the COLLECTION OF FORMULAE we find

$$\begin{aligned}\psi_{100}(\mathbf{r}) &= \left(\frac{Z^3}{\pi a_0^3}\right)^{1/2} e^{-Zr/a_0} \\ \psi_{200}(\mathbf{r}) &= \left(\frac{Z^3}{8\pi a_0^3}\right)^{1/2} \left(1 - \frac{Zr}{2a_0}\right) e^{-Zr/2a_0} \\ \psi_{210}(\mathbf{r}) &= \left(\frac{Z^3}{32\pi a_0^3}\right)^{1/2} \frac{Zr}{a_0} \cos\theta e^{-Zr/2a_0} \\ \psi_{21\pm 1}(\mathbf{r}) &= \left(\frac{Z^3}{\pi a_0^3}\right)^{1/2} \frac{Zr}{8a_0} \sin\theta e^{\pm i\varphi} e^{-Zr/2a_0}\end{aligned}$$

where a_0 is the Bohr radius. The β -decay instantaneously changes $Z = 1 \rightarrow Z = 2$. According to the expansion theorem, it is possible to express the wave function $u_i(\mathbf{r})$ before the decay as a linear combination of eigenfunctions $v_j(\mathbf{r})$ after the decay as

$$u_i(\mathbf{r}) = \sum_j a_j v_j(\mathbf{r})$$

where

$$a_j = \int v_j^*(\mathbf{r}) u_i(\mathbf{r}) d^3r.$$

The probability to find the electron in state j is given by $|a_j|^2$.

- (a) Here $u_i = \psi_{100}(Z = 1)$ and $v_j = \psi_{200}(Z = 2)$. This gives

$$\begin{aligned}a &= \left(\frac{1}{\pi a_0^3}\right)^{1/2} \left(\frac{2^3}{8\pi a_0^3}\right)^{1/2} \int_0^\infty e^{-r/a_0} \left(1 - \frac{2r}{2a_0}\right) e^{-2r/2a_0} 4\pi r^2 dr \\ &= \frac{4}{a_0^3} \int_0^\infty e^{-2r/a_0} \left(r^2 - \frac{r^3}{a_0}\right) dr = \frac{4}{a_0^3} \left[2 \left(\frac{a_0}{2}\right)^3 - \frac{6}{a_0} \left(\frac{a_0}{2}\right)^4\right] = -\frac{1}{2}.\end{aligned}$$

Thus, the probability is $1/4 = 0.25$.

- (b) For $u_i = \psi_{100}(Z = 1)$ and $v_j = \psi_{210}(Z = 2)$ the θ -integral is

$$\int_0^\pi \cos\theta \sin\theta d\theta = \frac{1}{2} \int_0^\pi \sin 2\theta d\theta = \left[-\frac{\cos 2\theta}{4}\right]_0^\pi = 0.$$

For $u_i = \psi_{100}(Z = 1)$ and $v_j = \psi_{21\pm 1}(Z = 2)$ the φ -integral is

$$\int_0^{2\pi} e^{\pm i\varphi} d\varphi = 0.$$

Thus, the probability to find the electron in a 2p state is zero.

(c) Here $u_i = \psi_{100}(Z = 1)$ and $v_j = \psi_{100}(Z = 2)$. This gives

$$\begin{aligned} a &= \left(\frac{1}{\pi a_0^3}\right)^{1/2} \left(\frac{2^3}{\pi a_0^3}\right)^{1/2} \int_0^\infty e^{-r/a_0} e^{-2r/a_0} 4\pi r^2 dr = \frac{8\sqrt{2}}{a_0^3} \int_0^\infty e^{-3r/a_0} r^2 dr \\ &= \frac{8\sqrt{2}}{a_0^3} \frac{a_0^3}{3^3} \int_0^\infty e^{-x} x^2 dx = \frac{8\sqrt{2}}{27} \int_0^\infty e^{-x} x^2 dx = \frac{8\sqrt{2}}{27} \int_0^\infty 2e^{-x} dx = \frac{16\sqrt{2}}{27} \end{aligned}$$

Thus, the probability is $512/729 \approx 0.70233$.

(The probability to find the electron in $\psi_{100}(Z = 2)$ is $512/729 = 0.702$. Therefore, the electron is found with 95% probability in one of the states 1s or 2s.)

(d) No l has to be less than n .

2. The energies of the states are given by $\epsilon_j = (j + \frac{1}{2})\hbar\omega$. Note that we can treat the oscillators as independent from each other. To find the fraction of oscillators in a particular state is the same as to ask for the probability of a oscillator to be in that particular state. In order to find the probabilities (fractions) we need to calculate the partition function for the system consisting of a single oscillator $Z = \sum e^{-(j+\frac{1}{2})\hbar\omega/\tau} = e^{-\frac{\hbar\omega}{2\tau}} \sum_{n=0}^\infty e^{-n\hbar\omega/\tau} = e^{-\frac{\hbar\omega}{2\tau}} \frac{1}{1-e^{-\hbar\omega/\tau}}$. Note the partition function is a geometric sum. At the characteristic temperature given by $\tau_{ch} = \hbar\omega$ the partition function is $Z = e^{-\frac{1}{2}} \frac{1}{1-e^{-1}} = \frac{1}{e^{1/2}-e^{-1/2}}$.

The fraction of oscillators in the ground state ($j = 0$) is given by

$$f_0 = \frac{e^{-\epsilon_0/\tau}}{Z} = e^{-\frac{1}{2}}(e^{1/2} - e^{-1/2}) = (1 - e^{-1}) = 0.632.$$

The next states ($j = 1$) fraction is given by $f_1 = \frac{e^{-\epsilon_1/\tau}}{Z} = e^{-\frac{3}{2}}(e^{1/2} - e^{-1/2}) = (e^{-1} - e^{-2}) = 0.233$.

The next states ($j = 2$) fraction is given by

$$f_2 = \frac{e^{-\epsilon_2/\tau}}{Z} = e^{-\frac{5}{2}}(e^{1/2} - e^{-1/2}) = (e^{-2} - e^{-3}) = 0.0855.$$

The next states ($j = 3$) fraction is given by

$$f_3 = \frac{e^{-\epsilon_3/\tau}}{Z} = e^{-\frac{7}{2}}(e^{1/2} - e^{-1/2}) = (e^{-3} - e^{-4}) = 0.0315.$$

3. Same as problem 4.4 in Bransden & Joachain. In the region where the potential is zero ($x < 0$) the solutions are of the traveling wave form e^{ikx} and e^{-ikx} , where $k^2 = 2mE/\hbar^2$. A plane wave $\psi(x) = Ae^{i(kx-\omega t)}$ describes a particle moving from $x = -\infty$ towards $x = \infty$. The probability current associated with this plane wave is

$$j = \frac{\hbar}{2mi} |A|^2 (e^{-ikx} \frac{\partial}{\partial x} e^{+ikx} - e^{+ikx} \frac{\partial}{\partial x} e^{-ikx}) = |A|^2 \frac{\hbar}{m} k = |A|^2 v$$

A plane wave $\psi(x) = Be^{i(-kx-\omega t)}$ describes a particle moving the opposite direction from $x = \infty$ towards $x = -\infty$. The probability current associated with this plane wave is

$$j = \frac{\hbar}{2mi} |B|^2 (e^{+ikx} \frac{\partial}{\partial x} e^{-ikx} - e^{-ikx} \frac{\partial}{\partial x} e^{+ikx}) = -|B|^2 \frac{\hbar}{m} k = -|B|^2 v$$

- (a) Solution for the region $x > 0$ where the potential is $V_0 = 5.0\text{eV}$. The potential step is larger than the kinetic energy 2.5 eV of the incident beam. The particle may therefore **not** enter this region classically. It will be totally reflected. In quantum mechanics we perform the following calculation: The two solutions for the two regions are:

$$\Psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & \text{for } x < 0 \text{ where } k^2 = 2mE/\hbar^2 \\ Ce^{\kappa x} + De^{-\kappa x} & \text{for } x > 0 \text{ where } \kappa^2 = 2m(V_0 - E)/\hbar^2 \end{cases}$$

we can put $C = 0$ as this part of the solution would diverge, and is hence not physical, as x approaches ∞ . At $x = 0$ both the wavefunction and its derivative have to be continuous functions. The derivative is:

$$\frac{\partial \Psi(x)}{\partial x} = \begin{cases} Aike^{ikx} - Bike^{-ikx} \\ -D\kappa e^{-\kappa x} \end{cases}$$

At $x = 0$ we arrive at the following two equations:

$$\left\{ \begin{array}{l} A + B = D \\ iAk - iBk = -D\kappa \end{array} \right. \text{ solving for } \left\{ \begin{array}{l} \frac{D}{A} = \frac{2k}{k+\kappa} \\ \frac{B}{A} = \frac{k-i\kappa}{k+i\kappa} \end{array} \right. \text{ solving for } \left\{ \begin{array}{l} \frac{D}{A} = \frac{2}{1+i\sqrt{V_0/E-1}} \\ \frac{B}{A} = \frac{1-i\sqrt{V_0/E-1}}{1+i\sqrt{V_0/E-1}} \end{array} \right.$$

We can now calculate the coefficient of reflection, R . The coefficients represent the following amplitudes: A is the incident beam, B is the reflected beam and C is the transmitted beam. The associated probability currents are denoted j_A, j_B and j_C . Conservation yields $j_A = j_B + j_C$. Hence we can define the coefficient of reflection as the fraction of reflected flux $R = \frac{|j_B|}{|j_A|}$ and the coefficient of transmission as $T = \frac{|j_C|}{|j_A|}$

$$\left\{ R = \frac{|j_B|}{|j_A|} = \frac{B^2 k}{A^2 k} = 1 \right.$$

This is easily seen from the ratio B/A being the ratio of two complex number where one is the complex conjugate of the other and therefore having the same absolute value.

Immediately follows that $T = 0$ as the currents have to be conserved.

- (b) This case can be seen as either the limiting case of a) or c). Both give the same answer $R = 1$ and $T = 0$.
- (c) Solution for the region $x > 0$ where the potential is $V_0 = 5.0\text{eV}$. The potential step is smaller than the kinetic energy 7.5eV of the incident beam. The particle may therefore enter this region classically. It will however lose some of its kinetic energy. In quantum mechanics there is a probability for the wave to be reflected as well. The two solutions for the two regions are:

$$\Psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & \text{for } x < 0 \text{ where } k^2 = 2mE/\hbar^2 \\ Ce^{ik'x} + De^{-ik'x} & \text{for } x > 0 \text{ where } k'^2 = 2m(E - V_0)/\hbar^2 \end{cases}$$

we can put $D = 0$ as there cannot be an incident beam from $x = \infty$. At $x = 0$ both the wavefunction and its derivative have to be continuous functions. The derivative is:

$$\frac{\partial \Psi(x)}{\partial x} = \begin{cases} Aike^{ikx} - Bike^{-ikx} \\ C ik' e^{ik'x} \end{cases}$$

At $x = 0$ we arrive at the following two equations:

$$\left\{ \begin{array}{l} A + B = C \\ Ak - Bk = Ck' \end{array} \right. \text{ solving for } \left\{ \begin{array}{l} \frac{C}{A} = \frac{2k}{k+k'} \\ \frac{B}{A} = \frac{k-k'}{k+k'} \end{array} \right. \text{ solving for } \left\{ \begin{array}{l} \frac{C}{A} = \frac{2\sqrt{E}}{\sqrt{E} + \sqrt{E-V_0}} \\ \frac{B}{A} = \frac{\sqrt{E} - \sqrt{E-V_0}}{\sqrt{E} + \sqrt{E-V_0}} \end{array} \right.$$

The coefficients represent the following amplitudes: A is the incident beam, B is the reflected beam and C is the transmitted beam. The associated probability currents are denoted j_A, j_B and j_C . Conservation yields $j_A = j_B + j_C$. Hence we can define the coefficient of reflection as the fraction of reflected flux $R = \frac{|j_B|}{|j_A|}$ and the coefficient of transmission as $T = \frac{|j_C|}{|j_A|}$

$$\left\{ \begin{array}{l} R = \frac{|j_B|}{|j_A|} = \frac{B^2 k}{A^2 k} = \left(\frac{B}{A}\right)^2 = \left(\frac{\sqrt{E} - \sqrt{E-V_0}}{\sqrt{E} + \sqrt{E-V_0}}\right)^2 = \left(\frac{\sqrt{7.5} - \sqrt{2.5}}{\sqrt{7.5} + \sqrt{2.5}}\right)^2 = 0.071797 \\ T = \frac{|j_C|}{|j_A|} = \frac{C^2 k'}{A^2 k} = \left(\frac{C}{A}\right)^2 \frac{\sqrt{E-V_0}}{\sqrt{E}} = \left(\frac{2\sqrt{E}}{\sqrt{E} + \sqrt{E-V_0}}\right)^2 \frac{\sqrt{E-V_0}}{\sqrt{E}} = \left(\frac{2\sqrt{7.5}}{\sqrt{7.5} + \sqrt{2.5}}\right)^2 \frac{\sqrt{2.5}}{\sqrt{7.5}} = 0.928203 \end{array} \right.$$

The last result could also be reached by $T + R = 1$.

4. Count the states in a box of size L . After some steps one reaches at (eq 7 page 185 KK)

$\tau_F = (3\pi^2 n)^{2/3} \frac{\hbar^2}{2m}$ this gives $T_F = k_B \tau_F = 5.0\text{K}$ which much less than $T = 0.5\text{K}$ so the approximation of the Fermi-Dirac distribution function as a step function will be fairly good. Calculate U (along lines according to eq 27 page 189 KK) after some steps $C_v = \frac{1}{2}\pi^2 N k_B T/T_F$ is reached. Evaluating the fermi contribution gives $C_v = 0.196 N k_B = 1.64 \text{ J/mole/K}$ at $T = 0.2\text{K}$.

5. The overall strategy is as follows. The specific heat we get from the entropy which we get from the free energy and to reach the free energy we need to calculate the partition function.

The partition function of the rotor is (approximation for the low temperature limit, in this limit the rotor will spend most of its time in the ground state and little time in the lowest excited state and negligible time in higher excited states)

$Z_{\text{rot}} = \sum_{j=0}^{\infty} (2j+1) e^{-j(j+1) \frac{\hbar^2}{2I\tau}} \approx 1 + 3e^{-\frac{\hbar^2}{I\tau}} = 1 + 3e^{-x}$ where $x = \frac{\hbar^2}{I\tau} \gg 1$ in the low temperature limit. For N identical molecules $Z_{\text{rot}}^{(N)} = \frac{1}{N!} Z_{\text{rot}}^N$, and hence the free energy is $F_{\text{rot}} = -N\tau \ln Z_{\text{rot}} + \tau \ln N! = -N\tau \ln(1 + 3e^{-x}) + \tau \ln N! \approx -3N\tau e^{-x} + \tau \ln N! = -3N\tau e^{-\frac{\hbar^2}{I\tau}} + \tau \ln N!$. The entropy is: $\sigma_{\text{rot}} = -\left(\frac{\partial F}{\partial \tau}\right)_v \approx$

$3N(1+x)e^{-x} + \ln N! = 3N\left(1 + \frac{\hbar^2}{I\tau}\right)e^{-\frac{\hbar^2}{I\tau}} + \ln N!$ and the specific heat in the low temperature limit is: $(C_v)_{\text{rot}} = \tau \left(\frac{\partial \sigma}{\partial \tau}\right)_v \approx 3Nx^2 e^{-x} = 3N \left(\frac{\hbar^2}{I\tau}\right)^2 e^{-\frac{\hbar^2}{I\tau}}$.

An alternative route is as follows. You can also calculate the inner energy

$U = -\tau^2 \left(\frac{\partial}{\partial \tau} \frac{F}{\tau}\right)_{v,N} = 3N \left(\frac{\hbar^2}{I\tau}\right) e^{-\frac{\hbar^2}{I\tau}}$. From this you reach the specific heat as well.