# 2

# Old Quantum Theory

**Spectroscopy and fundamental constants; Compton effect; Bohr–Sommerfeld quantization; specific heats; de Broglie waves.**

***Note.*** *The problems in this chapter are based on what is known as Old Quantum Theory: Bohr and de Broglie quantization rules. Those situations are treated in which the results will substantially be confirmed by quantum mechanics and some problems of statistical mechanics are proposed where the effects of quantization are emphasized.*

**2.1** The visible part of the electromagnetic spectrum is conventionally thus divided:

4000 Å    4680 4860    5390    5900    6200    7500

violet    blue    green    yellow    orange    red

wavelengths being given in Å .

a) Convert the above wavelengths into the energies of the associated photons, expressed in eV.

**2.2** The dimensionless *fine structure constant* is defined as $\alpha \equiv e^2/\hbar c$ .

a) Show that the Rydberg constant $R_\infty \equiv m_{\rm e} e^4/4\pi\hbar^3 c$ may be written as $R_\infty = \alpha^2/2\lambda_c$ ($\lambda_c \equiv h/m_{\rm e} c$ is the Compton electron wavelength) and the ionization energy of the hydrogen atom (in the approximation of infinite proton mass) as $E_{\rm I} = \frac{1}{2}\alpha^2 m_{\rm e} c^2$.

According to the present day (2016) available data in the field of spectroscopy one has:

$$R_\infty = 109\,737.315\,685\,08(65)\,\mathrm{cm}^{-1}\,; \qquad \alpha = 7.297\,352\,5664(17)\times 10^{-3}$$
$$m_{\rm e} = 0.910\,938\,356(11)\times 10^{-27}\,\mathrm{g}\,; \qquad \frac{m_{\rm e}}{m_{\rm p}} = 5.446\,170\,213\,52(52)\times 10^{-4}$$

and in addition, by definition, $c = 299\,792\,458\,\mathrm{m/s}$ .



E. d'Emilio and L.E. Picasso, *Problems in Quantum Mechanics*,
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b) Calculate the relative standard uncertainties for the values of $R_\infty$, $\alpha$, $m_e$.

The Rydberg constant $R_H$ for the hydrogen differs from $R_\infty$ because of the finite proton mass.

c) Calculate $R_H$ and the Planck constant $h$ with the correct number of significant figures; also give the relative standard uncertainties of the results.

**2.3** The frequency of an absorption transition from the $n = 2$ level of hydrogen was measured in a high precision spectroscopy experiments. The measured frequency was $\nu_H = 799\,191\,727\,409\,\mathrm{kHz}$.
Owing to relativistic corrections and other minor effects, the energy levels of hydrogen are not exactly those given by the Bohr theory. Nonetheless:

a) Find the value of $n$ for the final level.

In deuterium (the isotope of hydrogen with $A = 2$) the same transition gives rise to an absorption line whose frequency is $\nu_D = 799\,409\,184\,973\,\mathrm{kHz}$.

b) Assuming the difference between $\nu_D$ and $\nu_H$ is mainly due to the different masses of the nuclei, calculate (with no more than three or four significant figures) the value of the ratio between the deuterium nuclear mass and the electron mass. (Use the numerical data given in Problem 2.2.)

**2.4** Positronium is a system consisting of an electron and a positron (equal masses, opposite charges) bound together by the Coulomb force.

a) Calculate the value of positronium binding energy $E_b$ (i.e. the opposite of the energy of the ground state).

One of the decay channels of positronium is the annihilation into two photons: $e^+ + e^- \to 2\gamma$ (the lifetime for this channel being $\tau_{2\gamma} \simeq 1.25 \times 10^{-10}\,\mathrm{s}$).

b) Compute the energy and wavelength of each of the two photons in the center-of-mass reference frame of positronium.

The decay photons are revealed by means of the Compton effect on electrons.

c) Calculate the maximum energy a photon can give to an electron at rest.
d) Assume the electrons are in a uniform magnetic field $B = 10^3\,\mathrm{G}$ with the energy found in the previous question. Calculate the radius of curvature of the trajectories described by the electrons.

**2.5** Muonium is an atom consisting of a proton and a $\mu^-$ meson. It is formed via radiative capture: the proton (at rest) captures a meson (at rest) and this reaches the ground state by emitting one or more photons while effecting transitions to levels with lower energy (radiative cascade).

a) Calculate the mass of the $\mu^-$ meson, given that the maximum energy of the photons emitted in the radiative cascade is 2.5 keV.

b) Calculate the characteristic dimension of muonium in its ground state.

c) Say what is the resolving power $\Delta\nu/\nu$ necessary to distinguish – by measuring the frequency of the photons emitted during the radiative cascade – whether the $\mu^-$ has been captured by a proton or by a deuteron (the latter being the nucleus of deuterium: the bound state of a proton and a neutron).

**2.6** The purpose of this problem is to show that any quantum state (i.e. in the present case: any energy level), relative to a one-dimensional system quantized according to the Bohr rule, occupies a (two-dimensional) volume $h$ in phase space.

Consider a one-dimensional harmonic oscillator quantized according to the Bohr rule.

a) Compute the volume of phase space bounded by the surface of energy $E_n = n\,\hbar\,\omega$ and that of energy $E_{n-1}$.

Consider now a particle constrained to move on a segment of length $a$; its energy levels $E_n$ are obtained by means of the Bohr quantization rule.

b) Compute the volume of phase space bounded by the two surfaces of energy $E_n$ and $E_{n-1}$.

c) Show that the same result obtains for any one-dimensional system with energy levels $E_n$ obtained through the Bohr rule. (Hint: use Stokes' theorem.)

Consider now an isotropic three-dimensional harmonic oscillator.

d) Use the Bohr quantization rule in the form $\sum_i \oint p_i\,\mathrm{d}q_i = n\,h$ to show that the energy levels still read $E_n = n\,\hbar\,\omega$ and that the (six-dimensional) volume of phase space bounded by the surface of energy $E_n$ has magnitude $n^3h^3/6$.

**2.7** When a system with several degrees of freedom enjoys the possibility of the *separation of variables* – i.e. there exists a choice of $q$'s and $p$'s such that the Hamiltonian takes the form $H = H_1(q_1, p_1) + H_2(q_2, p_2)\ \cdots$ – it is possible to use the Bohr–Sommerfeld quantization rules $\oint p_i\,\mathrm{d}q_i = n_i h$ for all $i = 1, \cdots$ relative to the individual degrees of freedom.

a) Find the energy levels $E(n_1, n_2, n_3)$ of an *anisotropic* three-dimensional harmonic oscillator. Exploit the fact that its Hamiltonian can be written in the form:

$$H = \frac{p_1^2}{2m} + \frac{1}{2}m\omega_1^2\,q_1^2 + \frac{p_2^2}{2m} + \frac{1}{2}m\omega_2^2\,q_2^2 + \frac{p_3^2}{2m} + \frac{1}{2}m\omega_3^2\,q_3^2\ .$$

Consider now an *isotropic* three-dimensional harmonic oscillator. The number of states corresponding to a given energy level $E_n = n\,\hbar\omega$ (the "degeneracy" of the level) is the number of ways the three quantum numbers $n_1, n_2, n_3$ can be chosen such that $E(n_1, n_2, n_3) = E_n$ .

b) Compute the degeneracy of the energy levels for an isotropic three-dimensional harmonic oscillator and the number of states with energy $E \leq E_n$ .

c) Find the energy levels of a particle confined in a rectangular box with edges of lengths $a$, $b$, $c$ .

d) Still referring to the particle in the rectangular box (of volume $V = abc$), compute the number of states enclosed in the phase space volume:

$$V \times \Big[(|p_1| \leq p_{n_1}) \times (|p_2| \leq p_{n_2}) \times (|p_3| \leq p_{n_3})\Big]\,; \qquad p_{n_1} = \frac{n_1 h}{2a}\,, \quad \text{etc.}$$

and show that, just as in Problem 2.6, the volume-per-state is $h^3$.

**2.8** A particle of mass $m$ in one dimension is subject to the potential $V(x) = \lambda\,(x/a)^{2k}$ with $\lambda > 0$ and $k$ a positive integer.

a) Show that the energy levels obtained through the Bohr quantization rule are:

$$E_n = n^{2k/(1+k)} \left(\frac{h\,\lambda^{1/2k}}{\sqrt{8m}\;a\,C_k}\right)^{2k/(1+k)}, \qquad C_k = \int_{-1}^{+1} \sqrt{1 - x^{2k}}\;\mathrm{d}x\,.$$

b) Explicitly write the energy levels for $k = 1$ and $k = \infty$. Which well known potential does the case $k = \infty$ correspond to?

**2.9** Consider a nonrelativistic electron in a uniform magnetic field $\vec{B}$, moving in a plane orthogonal to $\vec{B}$.

a) Find the energy levels (*Landau levels*) by means of the Bohr quantization rule $\oint \vec{p}\cdot \mathrm{d}\vec{q} = n\,h$, paying attention to the fact that, in presence of a magnetic field, $\vec{p} \neq m\,\vec{v}$.

b) Calculate the distance between energy levels for $B = 1\,\mathrm{T} = 10^4\,\mathrm{G}$.

**2.10** A particle of mass $m$ in one dimension is constrained in the segment $|x| \leq \frac{1}{2}a$ and is subject to the potential:

$$V(x) = \begin{cases} 0 & |x| > \frac{1}{2}b \\ -V_0 & |x| \leq \frac{1}{2}b \end{cases} \qquad b < a\,, \qquad V_0 > 0\,.$$

a) By use of the Bohr quantization rule determine the energy levels with $E_n < 0$, the condition for the existence of at least one level with negative energy, and the number of levels with negative energy.

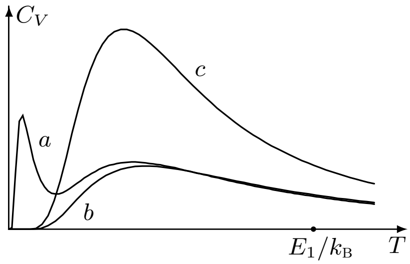
b) Determine the energy levels with $E_n \gg V_0$ (neglecting terms of order $V_0^2/E^2$).

c) Show that the corrections to the 'unperturbed' levels (i.e. those with $V_0 = 0$) found in the previous question, coincide with $-V_0\times$ (probability of finding the particle with $|x| \le \frac{1}{2}b$), where such a probability is the ratio between the time spent in the segment $|x| \le \frac{1}{2}b$ and that spent in the segment $|x| \le \frac{1}{2}a$.

**2.11** Consider a gas of atoms (or molecules) with a ground state $E_0 = 0$, an excited state $E_1$, a third level $E_x$ with $0 \le E_x \le E_1$, as well as other energy levels $E_n \gg E_1$ (a three-level system). Let us consider the contribution to internal energy and heat capacity exclusively due to the three energy levels $E_0$, $E_x$ and $E_1$.

a) Calculate the contribution of the three levels to the internal energy as a function of the temperature $T$ and of $E_x$. For what range of $T$ is it legitimate to ignore the levels with $E_n \gg E_1$?

The three curves ($a$, $b$, $c$) in the figure represent (not necessarily in the same order) $C_V(T)$ for three different values of $E_x$: $E_x = 0$, $E_x = E_1$, $E_x = \frac{1}{10}E_1$.




b) Identify the value of $E_x$ for each curve and explain qualitatively their different features: more precisely, why is the maximum in $c$ higher than in $b$ and why are there two maxima in $a$?

**2.12** Consider a particle of mass $m$ constrained in a segment of size $a$.

a) Show that, for high values of the temperature $T$, the quantum partition function $Z(\beta) = \sum_n \exp\left[-\beta E_n\right]$ $(\beta \equiv 1/k_B T)$ is well approximated by the classical partition function divided by the Planck constant $h$. Explain what 'high values of $T$' means.

**2.13** Consider the gas consisting of the conduction electrons of a conductor with given volume $V$. The conductor being neutral, the ions of the crystal lattice partially screen the charge of the electrons, nearly making their repulsion vanish. In a first approximation the conduction electrons may therefore be considered as a gas of free particles.

a) In Problem 2.7 it has been shown that the phase space volume taken by each quantum state is $h^3$. Calculate the number of (quantum) electron states with energy $\vec{p}^{\,2}/2m_e$ less than $E_F$.

Due to the *Pauli principle*, at most two electrons are allowed to occupy the same quantum state; furthermore, at temperature $T = 0\,\text{K}$, the gas has, compatibly with the Pauli principle, the lowest possible energy.

b) Let $N$ be the number of conduction electrons in the volume $V$. Calculate the maximum energy $E_{\rm F}$ a conduction electron may have at $T = 0\,\text{K}$. ($E_{\rm F}$ is known as the *Fermi energy* of the system.)

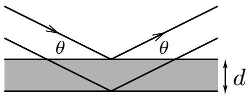
c) Under the same conditions specified above, calculate the value $E$ of the total energy of the gas (approximate sums with integrals) and its pressure $p$. (For $T = 0\,\text{K}$ the pressure is $p = -\partial E/\partial V$). Verify that $pV = \frac{2}{3}E$. (Actually this relation holds also for $T > 0$.)

d) Knowing that for silver the density is $10.5\,\text{g/cm}^3$, the atomic weight is $A = 108$ and that one conduction electron is available for each atom, calculate the value (in atmospheres) of the pressure $p$ at $T = 0\,\text{K}$ and the value of the *Fermi temperature* $T_{\rm F} \equiv E_{\rm F}/k_{\rm B}$ for the electron gas.

**2.14** Neutrons produced in a nuclear reactor and then slowed down ('cold' neutrons) are used in an interferometry experiment. Their de Broglie wavelength is $\lambda = 1.4\,\text{Å}$.

a) Calculate the energy of such neutrons and the energy of photons with the same wavelength (neutron mass $m_{\rm n} \simeq 1.7\times 10^{-24}\,\text{g}$).

The neutrons are fired at a silicon crystal and the smallest angle $\theta$ (see the figure), for which Bragg reflection is observed, is $\theta = 22°$.




b) Calculate the distance $d$ between the lattice plains of the crystal responsible for Bragg reflection.

c) Say for how many angles Bragg reflection can be observed.

**2.15** 'Ultracold' neutrons are free neutrons whose de Broglie wavelength is some hundred Å.

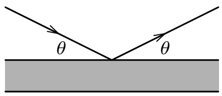
a) Calculate the speed and energy of neutrons with $\lambda = 900\,\text{Å}$ and their 'temperature' ($T \equiv E/k_{\rm B}$).

A way to obtain ultracold neutrons is to inject cold neutrons vertically into a tower of height $D \simeq 35\,\text{m}$.

b) Say what the initial wavelength $\lambda_{\rm i}$ of the cold neutrons must be in order that, at the top of the tower, the final wavelength is $\lambda_{\rm f} = 900\,\text{Å}$.

A nonabsorbing material behaves for neutrons as a region where the potential is about $V_0 \simeq 10^{-7}\,\text{eV}$ (a *repulsive* potential). For aluminium $V_0 = 0.55\times 10^{-7}\,\text{eV}$.

c) Calculate the refractive index of aluminium (i.e. the ratio between the wavelengths in vacuum and in the medium) for the neutrons with $\lambda = 900\,\text{Å}$.




Neutrons with $\lambda = 900\,\text{Å}$ impinge on the surface of a plate of aluminium.

d) Say for what range of angles (see the figure) does total reflection occur.

# Solutions

## 2.1

a) Since for photons $\lambda[\text{Å}] \times E[\text{eV}] = 12400$ eV Å one has:

| 7500 Å | | 6200 | 5900 | | 5390 | | 4860 | 4680 | | 4000 |
|---|---|---|---|---|---|---|---|---|---|---|
| 1.65 eV | | 2 | 2.1 | | 2.3 | | 2.55 | 2.65 | | 3.1 |
| | red | orange | | yellow | | green | blue | | violet | |

## 2.2

a) One has:

$$R_\infty = \frac{m_\mathrm{e} e^4}{4\pi\hbar^3 c} = \frac{e^4}{\hbar^2 c^2} \times \frac{m_\mathrm{e} c}{4\pi\hbar} = \frac{\alpha^2}{2\lambda_c}\,; \qquad E_\mathrm{I} = R_\infty hc = \frac{\alpha^2 hc}{2\lambda_c} = \frac{1}{2}\,\alpha^2 m_\mathrm{e} c^2.$$

b) $\dfrac{\varDelta R_\infty}{R_\infty} = 5.9 \times 10^{-12}; \qquad \dfrac{\varDelta\alpha}{\alpha} = 2.3 \times 10^{-10}; \qquad \dfrac{\varDelta m_\mathrm{e}}{m_\mathrm{e}} = 1.2 \times 10^{-8}.$

c) With $\mu_\mathrm{e}$ the reduced mass of the $(e,\, p)$ system,

$$R_\mathrm{H} = R_\infty \times \frac{\mu_\mathrm{e}}{m_\mathrm{e}} = \frac{R_\infty}{1 + m_\mathrm{e}/m_\mathrm{p}}$$

$$\frac{\varDelta R_\mathrm{H}}{R_\mathrm{H}} = \frac{\varDelta R_\infty}{R_\infty} + \frac{\varDelta(m_\mathrm{e}/m_\mathrm{p})}{1 + m_\mathrm{e}/m_\mathrm{p}} \simeq \frac{\varDelta R_\infty}{R_\infty} + \varDelta(m_\mathrm{e}/m_\mathrm{p})$$

$$= 5.9 \times 10^{-12} + 0.05 \times 10^{-12} = 6 \times 10^{-12}$$

then $R_\mathrm{H}$ has 12 significant digits as $R_\infty$: $R_\mathrm{H} = 109\,677.583\,4063(7)\,\mathrm{cm}^{-1}$.

$$h = \frac{\alpha^2 m_\mathrm{e} c}{2R_\infty} \quad \Rightarrow \quad \frac{\varDelta h}{h} = \cancel{2\frac{\varDelta\alpha}{\alpha}} + \frac{\varDelta m_\mathrm{e}}{m_\mathrm{e}} + \cancel{\frac{\varDelta R_\infty}{R_\infty}} = 1.2 \times 10^{-8}$$

$(\varDelta R_\infty/R_\infty,\ \varDelta\alpha/\alpha \ll \varDelta m_\mathrm{e}/m_\mathrm{e})$, then $h = 6.626\,070\,040(80) \times 10^{-27}$ erg s.

**2.3**

a) $\nu_{\mathrm{H}} = R_{\mathrm{H}}\, c\Big(\dfrac{1}{4} - \dfrac{1}{n^2}\Big) \quad \Rightarrow \quad \dfrac{1}{n^2} = \dfrac{1}{4} - \dfrac{\nu_{\mathrm{H}}}{R_{\mathrm{H}}\, c}\,.$

If $n^2 \lesssim 10^4$ it is sufficient to make calculations with 6 significant digits ($R_{\mathrm{H}}$ is given in the solution of Problem 2.2):

$$\frac{1}{n^2} \simeq \frac{1}{4} - \frac{0.799192 \times 10^{15}}{109677 \cdot 299792 \times 10^5} = 0.007 \quad \Rightarrow \quad n^2 \simeq 143 \;\Rightarrow\; n = 12\,.$$

b) As the frequencies are proportional to the reduced masses, one has:

$$\frac{\nu_{\mathrm{H}}}{\nu_{\mathrm{D}}} = \frac{1 + m_{\mathrm{e}}/m_{\mathrm{d}}}{1 + m_{\mathrm{e}}/m_{\mathrm{p}}} \quad \Rightarrow \quad \frac{m_{\mathrm{e}}}{m_{\mathrm{d}}} = \frac{\nu_{\mathrm{H}}}{\nu_{\mathrm{D}}}\big(1 + m_{\mathrm{e}}/m_{\mathrm{p}}\big) - 1$$

and, with $m_{\mathrm{e}}/m_{\mathrm{p}}$ given in the text of Problem 2.2,

$$\frac{m_{\mathrm{e}}}{m_{\mathrm{d}}} = \frac{799\,192}{799\,409} \times 1.000544 - 1 \simeq 2.724 \times 10^{-4} \quad \Rightarrow \quad \frac{m_{\mathrm{d}}}{m_{\mathrm{e}}} \simeq 3670\,.$$

**2.4**

a) Positronium differs from the hydrogen atom only for the value of the reduced mass, which is a half of the mass common to electron and positron. Then:

$$E_{\mathrm{B}} = \frac{e^2}{4a_{\mathrm{B}}} = \frac{1}{2}\,13.6\,\mathrm{eV} = 6.8\,\mathrm{eV}\,.$$

b) In the center-of-mass reference frame the two photons have the same energy $m_{\mathrm{e}}c^2$ (binding energy neglected):

$$E_\gamma = m_{\mathrm{e}}c^2 = 0.51\,\mathrm{MeV}\,, \qquad \lambda = \frac{hc}{E_\gamma} = \frac{12400}{0.51 \times 10^6} = 0.024\,\text{Å}$$

which is the Compton electron wavelength $\lambda_c = h/m_{\mathrm{e}}c$.

c) The maximum release of energy from the photon to an electron takes place when the photon is scattered backwards $(\theta = 180°)$. In this case the wavelength of the scattered photon is

$$\lambda(\pi) = \lambda(0) + 2\lambda_c = 3\lambda_c \quad \Rightarrow \quad E_\gamma^{\mathrm{f}} = \frac{1}{3}E_\gamma^{\mathrm{i}}$$

and as a consequence the energy released to the electron is

$$E_{\mathrm{e}} = \frac{2}{3}E_\gamma^{\mathrm{i}} = \frac{2}{3}m_{\mathrm{e}}c^2 = 0.34\,\mathrm{MeV}\,.$$

d) The momentum of the electron is

$$p = \frac{E_\gamma^{\mathrm{i}}}{c} - \frac{-E_\gamma^{\mathrm{f}}}{c} = \frac{4}{3}m_{\mathrm{e}}c$$

so the radius of curvature of the electron trajectory is

$$\rho = \frac{p\,c}{eB} = \frac{4}{3}\,\frac{m_{\mathrm{e}}c^2}{eB} = \frac{4}{3}\,\frac{hc}{4\pi\,\mu_{\mathrm{B}}B} = 2.3\,\mathrm{cm}$$

where $\mu_{\mathrm{B}} \equiv e\,\hbar/2m_{\mathrm{e}}c = 5.8 \times 10^{-9}\,\mathrm{eV/G}$ is the Bohr magneton.

**2.5**

a) The energy levels of muonium differ from those of the hydrogen atom only because of the different value of the reduced mass. The highest energy of the emitted photons is equal to the ionization energy of muonium and is $2.5 \times 10^3/13.6 = 184$ times that of the hydrogen atom, therefore the reduced mass $\mu$ of the system $(\mu^- p)$ is 184 times the electron mass:
$$m_\mu = \frac{m_\mathrm{p}\,\mu}{m_\mathrm{p} - \mu} = \frac{1840\,m_\mathrm{e} \times 184\,m_\mathrm{e}}{1840\,m_\mathrm{e} - 184\,m_\mathrm{e}} = 204\,m_\mathrm{e}\;.$$

b) Also the dimensions of the orbits of the $\mu^-$ meson are reduced by a factor 184 with respect to those of the electron. As a consequence the size of muonium in its ground state is $a_\mathrm{B}/184 = 0.53\,\text{Å}/184 = 2.9 \times 10^{-3}\,\text{Å}$.

c) The reduced mass of the system $(\mu^- d)$ is $193\,m_\mathrm{e}$, whence:
$$\frac{\Delta\nu}{\nu} = \frac{\Delta\mu}{\mu} = \frac{193 - 184}{184} \simeq 5\%\;.$$

**2.6**

a) The curve described by the equation $p^2 + m^2\omega^2 q^2 = 2mE_n$ is an ellipse whose semiaxes are $\sqrt{2mE_n}$ and $\sqrt{2E_n/m\omega^2}$, so the enclosed area is
$$A_n = \frac{2\pi E_n}{\omega} = n\,h \quad\Rightarrow\quad A_n - A_{n-1} = h\;.$$

b) In the case of a particle in a segment, the Bohr quantization rule gives $p_n = \pm n\,h/2a$, so the volume of the phase space where $E \le E_n$ is the area of the rectangle whose base and height respectively are $a$ and $2|p_n|$, therefore:
$$A_n = 2|p_n|a = n\,h \quad\Rightarrow\quad A_n - A_{n-1} = h\;.$$
Equivalently:
$$A_n = \int\limits_{E\le E_n} \mathrm{d}q\,\mathrm{d}p = a\int\limits_{-\sqrt{2mE_n}}^{+\sqrt{2mE_n}} \mathrm{d}p = 2a\,n\sqrt{\frac{h^2}{4a^2}} = n\,h\;.$$

c) The volume of the phase space where $E \le E_n$ is
$$A_n = \left|\int_{E\le E_n} \mathrm{d}q\,\mathrm{d}p\right|$$
and by Stokes theorem (the surfaces are oriented):
$$\int_{E\le E_n} \mathrm{d}q\,\mathrm{d}p = -\oint_{E=E_n} p\,\mathrm{d}q$$
(indeed, the flux of the curl of the two-dimensional vector $\vec{B}$ with components $B_q = -p,\ B_p = 0,\ \mathrm{curl}\,\vec{B} = \partial B_p/\partial q - \partial B_q/\partial p = 1$, equals the circulation of the vector $\vec{B}$) therefore, owing to Bohr quantization rule, $A_n = n\,h$.

d) One has:

$$\oint \sum_i p_i \,\mathrm{d}q_i = \sum_i \int_{\text{period}} p_i \,\dot{q}_i \,\mathrm{d}t = 2\,\frac{2\pi}{\omega}\,\overline{E_c} = \frac{2\pi}{\omega}\,E_n = n\,h \;\Rightarrow\; E_n = n\,\hbar\,\omega\;.$$

Making the change of variables $p_i = \sqrt{m\omega}\,p_i'$, $q_i = q_i'/\sqrt{m\omega}$ (the Jacobian is 1), the surface of energy $E_n$ becomes the surface of the sphere of radius $\sqrt{2E_n/\omega}$ . The volume of the sphere of radius $R$ in $d$ dimensions is

$$V_d = \frac{\pi^{d/2} R^d}{\Gamma\big(d/2+1\big)} \qquad \Rightarrow \qquad V_{E\le E_n} = \frac{n^3}{6} h^3$$

where use has been made of the fact that $d = 6$ and that, for integer $k$, the Euler $\Gamma$ function has the value $\Gamma(k) = (k-1)!$ .

The meaning of the obtained result is that the number of states of the oscillator with energy $E \le E_n$ is of the order of $n^3/6$ (approximately one state for each cell of the phase space with volume $h^3$).

**2.7**

a) As the Hamiltonian $H$ is a separate variables one: $H = H_1 + H_2 + H_3$, its energy levels are:

$$E(n_1,n_2,n_3) = n_1\hbar\,\omega_1 + n_2\hbar\,\omega_2 + n_3\hbar\,\omega_3\;.$$

b) In the case of an isotropic oscillator $\omega_1 = \omega_2 = \omega_3 \equiv \omega$ and

$$E(n_1,n_2,n_3) = (n_1+n_2+n_3)\,\hbar\,\omega \equiv n\,\hbar\,\omega\,, \qquad\qquad n = n_1+n_2+n_3\;.$$

Choosing $n_1 = n-k$, $\;(k = 0,\,\cdots\, n)$, $n_2$ and $n_3$ may be chosen in $k+1$ ways: $n_2 = k,\; n_3 = 0;\; n_2 = k-1,\; n_3 = 1;\; \cdots\; n_2 = 0,\; n_3 = k$. So the degeneracy of the level $E_n$ is

$$g_n = \sum_0^n (k+1) = \frac{(n+1)(n+2)}{2}$$

and the number of states with energy $E \le E_n$ is

$$\sum_0^n g_k = \frac{1}{2}\sum_0^n (k^2+3k+2) =$$

$$= \frac{1}{2}\Big(\frac{n(n+1)(2n+1)}{6} + 3\frac{n(n+1)}{2} + 2(n+1)\Big) = \frac{(n+1)(n+2)(n+3)}{6}\;.$$

Compare this result – that will be confirmed by quantum mechanics – with what has been found in question d) of Problem 2.6.

c) Also in the case of a particle in a box the Hamiltonian is a separate variables one: $H = p_1^2/2m + p_2^2/2m + p_3^2/2m$, therefore:

$$E(n_1,n_2,n_3) = \frac{n_1^2\,h^2}{8ma^2} + \frac{n_2^2\,h^2}{8mb^2} + \frac{n_3^2\,h^2}{8mc^2} = \frac{h^2}{8m}\Big(\frac{n_1^2}{a^2} + \frac{n_2^2}{b^2} + \frac{n_3^2}{c^2}\Big)\;.$$

d) Due to $p_{n_1} = n_1 h/2a$, $p_{n_2} = n_2 h/2b$, etc. the required volume is given by $V \times 2^3\, p_{n_1} p_{n_2} p_{n_3} = n_1 n_2 n_3\, h^3$ and, since the number of states with quantum numbers less or equal to $n_1$, $n_2$, $n_3$ is $n_1 n_2 n_3$, the result follows.

**2.8**

a) $$\oint p\, \mathrm{d}x = \oint \sqrt{2m\big(E - V(x)\big)}\, \mathrm{d}x = \sqrt{2mE} \oint \Big(1 - \frac{\lambda}{E}\frac{x^{2k}}{a^{2k}}\Big)^{1/2} \mathrm{d}x\,.$$

Putting $y = (\lambda/E)^{1/2k}\, x/a$,

$$\oint p\, \mathrm{d}x = 2\sqrt{2m\,E}\; a\Big(\frac{E}{\lambda}\Big)^{1/2k} \int_{-1}^{+1} \sqrt{1 - y^{2k}}\, \mathrm{d}y = n\,h \quad \Rightarrow$$

$$E_n^{(1+k)/2k} = n\, \frac{h\,\lambda^{1/2k}}{\sqrt{8m}\; a\, C_k} \quad \Rightarrow \quad E_n = n^{2k/(1+k)} \left(\frac{h\,\lambda^{1/2k}}{\sqrt{8m}\; a\, C_k}\right)^{2k/(1+k)}.$$

b) For $k = 1$ $C_1 = \pi/2$ and $E_n = n\,\hbar\,\sqrt{2\lambda/ma^2}$: these are the energy levels of a harmonic oscillator with $\frac{1}{2}m\omega^2 = \lambda/a^2$.
For $k = \infty$ the potential is that of an infinite potential well of width $2a$ ($x^{2k} \to 0$ for $|x| < 1$, $x^{2k} \to \infty$ for $|x| > 1$), $C_\infty = 2$ and the energy levels are $E_n = n^2 h^2/8m(2a)^2$.

Only in the two cases $k = 1$ and $k = \infty$ (up to the additive constant $\frac{1}{2}\hbar\,\omega$ in the case of the oscillator) the energy levels found by means of the Bohr quantization rule will turn out to be identical to those predicted by quantum mechanics: in general, the energy levels calculated using the Bohr–Sommerfeld quantization rule agree with those predicted by quantum mechanics only for large values of the quantum number $n$.

**2.9**

a) The electron follows a circular trajectory with cyclotron angular frequency $\omega_{\mathrm{c}} = eB/m_{\mathrm{e}}c$ (twice the Larmor frequency) and velocity $v = \omega_{\mathrm{c}} r = eB\,r/m_{\mathrm{e}}c$. One has:

$$\vec{p} = m_{\mathrm{e}}\,\vec{v} - \frac{e}{c}\vec{A}\,; \qquad \oint \vec{p}\cdot \mathrm{d}\vec{q} = \frac{2\pi}{\omega_{\mathrm{c}}}\, m_{\mathrm{e}}\, v^2 - \frac{e}{c}\oint \vec{A}\cdot \mathrm{d}\vec{q}$$

and, thanks to Stokes' theorem,

$$\frac{e}{c}\oint \vec{A}\cdot \mathrm{d}\vec{q} = \frac{e}{c}\,\pi\, r^2 B = \frac{2\pi}{\omega_{\mathrm{c}}} \times \frac{1}{2} m_{\mathrm{e}}\, \frac{e^2 B^2 r^2}{m_{\mathrm{e}}^2 c^2} = \frac{2\pi}{\omega_{\mathrm{c}}} \times \frac{1}{2} m_{\mathrm{e}}\, v^2$$

then (the energy is only kinetic):

$$\oint \vec{p}\cdot \mathrm{d}\vec{q} = \frac{2\pi}{\omega_{\mathrm{c}}} \times E_n = n\,h \quad \Rightarrow \quad E_n = n\,\hbar\,\omega_{\mathrm{c}} = n\,\hbar\,\frac{eB}{m_{\mathrm{e}}c}\,\cdot$$

b) The Bohr magneton is defined by (see also Problem 2.4):

$$\mu_{\mathrm{B}} \equiv \frac{e\,\hbar}{2m_{\mathrm{e}}c} = 0.93 \times 10^{-20}\,\mathrm{erg/G} = 5.8 \times 10^{-9}\mathrm{eV/G}$$

so the distance between Landau levels is

$$\Delta E_n = 2\mu_{\mathrm{B}} B = 1.16 \times 10^{-4}\,\mathrm{eV}\,.$$

**2.10**

a) For negative energies the particle is confined in the region $|x| \le \frac{1}{2}b$, whence:

$$p_n = \sqrt{2m(E_n + V_0)} = \frac{n\,h}{2b} \quad \Rightarrow \quad E_n = \frac{n^2 h^2}{8mb^2} - V_0$$

$$E_1 < 0 \quad \Rightarrow \quad V_0 > \frac{h^2}{8mb^2}\,; \qquad E_n < 0 \quad \Rightarrow \quad n < \frac{2b\,\sqrt{2mV_0}}{h}$$

and the number of levels is given by the integer part of $2b\,\sqrt{2mV_0}/h$.

b) For $E \ge 0$ the Bohr condition reads:

$$\Big[(a-b)\sqrt{2mE_n} + b\,\sqrt{2m(E_n+V_0)}\Big] = \frac{n\,h}{2}$$

that, for $E_n \gg V_0$ and up to the first order in $V_0/E_n$, takes the form:

$$\sqrt{2mE_n}\,\Big[(a-b) + b\Big(1 + \frac{1}{2}\frac{V_0}{E_n}\Big)\Big] = a\,\sqrt{2mE_n} + \frac{mb\,V_0}{\sqrt{2mE_n}} = \frac{n\,h}{2}$$

that gives, upon solving and neglecting the terms of order $V_0^2/E_n^2$,

$$E_n = \frac{n^2h^2}{8ma^2} - \frac{b}{a}\,V_0\,, \qquad n \gg \frac{2a\,\sqrt{2mV_0}}{h}\,.$$

c) In one period, the time spent by the particle in a given segment, is twice the ratio between the length of the segment and the velocity of the particle: in order to find the result to the first order in $E/V_0$ we must take the velocity of the unperturbed motion (that with $V_0 = 0$), then:

$$t_b = 2\,\frac{b}{v}\,; \quad t_a = 2\,\frac{a}{v} \quad \Rightarrow \quad -V_0\,\frac{t_b}{t_a} = -\frac{b}{a}\,V_0\,.$$

**2.11**

a) Putting $E_0 = 0$ one has:

$$\mathcal{U} = \frac{E_x \mathrm{e}^{-\beta E_x} + E_1 \mathrm{e}^{-\beta E_1}}{1 + \mathrm{e}^{-\beta E_x} + \mathrm{e}^{-\beta E_1}}\,.$$

It is legitimate to neglect the levels with $E_n \gg E_1$ when their population is negligible with respect to that of the level $E_1$, namely when $\mathrm{e}^{-\beta(E_n - E_1)} \ll 1$, i.e when $T \ll (E_n - E_1)/k_{\mathrm{B}}$.

b) Note that, when $E_x = 0 = E_0$, the degeneracy of the level $E_0$ is 2, when $E_x = E_1$ the degeneracy of $E_1$ is 2, while for $E_x = \frac{1}{10}E_1$ the lowest energy level is “quasi degenerate” with $E_x$. So, for high temperatures ($k_{\mathrm{B}}T \gg E_1$), i.e. in the limit of equi-population, if $E_x = E_1$, the internal energy tends to a value that is twice that of the case $E_x = E_0$ ($2E_1/3$ in

the first case, $E_1/3$ in the second) and almost twice (2/1.1) that of the case $E_x = \frac{1}{10}E_1$, and then grows more than in the other cases. For this reason the specific heat of the case $E_x = E_1$ (the curve labeled by $c$) is greater than in the other cases.
If $E_x = \frac{1}{10}E_1$, the level $E_x$ becomes immediately populated (i.e. for temperatures $T \simeq E_x/k_\mathrm{B}$) and the heat capacity grows accordingly; then, as long as $k_\mathrm{B}T \ll E_1$, the system behaves as a two-level system, therefore $C_V$ decreases towards zero to start a new growth when the level $E_1$ starts populating: in conclusion the curve labeled by $a$ corresponds to the case when the lowest energy level is quasi degenerate: $E_x = \frac{1}{10}E_1$.

**2.12**

a) The classical partition function is

$$Z_\mathrm{cl} = \int \exp\Big[-\beta\, p^2/2m\Big]\,\mathrm{d}q\,\mathrm{d}p = 2a\int_0^\infty \exp\Big[-\beta\, p^2/2m\Big]\,\mathrm{d}p$$
$$\simeq 2a\sum\nolimits_n \exp\Big[-\beta\, p_n^2/2m\Big]\times \varDelta p_n$$

and, if we take $p_n = n\,h/2a,\ \varDelta p_n = h/2a$, the thesis follows. Let us now examine the conditions under which approximating the integral by the series is legitimate. One has:

$$Z_\mathrm{cl}/h = \frac{2a}{h}\int_0^\infty \exp\Big[-\beta\, p^2/2m\Big]\,\mathrm{d}p = \frac{2a}{h}\sum_{n=0}^\infty\int_{p_n}^{p_{n+1}} \exp\Big[-\beta\, p^2/2m\Big]\,\mathrm{d}p$$
$$= \frac{2a}{h}\sum_{n=0}^\infty \exp\Big[-\beta\,\overline{p}_n^2/2m\Big]\times\varDelta p_n = \sum_{n=0}^\infty \exp\Big[-\beta\,\overline{p}_n^2/2m\Big]$$

where $p_n < \overline{p}_n < p_{n+1}$. The maximum of the difference with respect to the sum with $p_n$ instead of $\overline{p}_n$ is obtained if one replaces $\overline{p}_n$ with $p_{n+1}$: in this case the two sums differ by the first term that equals 1. The quantum partition function and $Z_\mathrm{cl}/h$ differ by a function of $\beta$ (the $\overline{p}_n$ do depend on $\beta$) bounded by 0 and 1; since $\int \mathrm{e}^{-ax^2}\,\mathrm{d}x = \sqrt{\pi/a}$, one has:

$$Z_\mathrm{cl}/h = \frac{a}{h}\sqrt{\frac{2\pi m}{\beta}}$$

and in conclusion, if $Z_\mathrm{cl}/h \gg 1$ namely for $\beta \ll ma^2/h^2$ ($k_\mathrm{B}T \gg h^2/ma^2$), the difference is negligible.

**2.13**

a) Since the energy of the electrons is $\vec{p}^{\,2}/2m_\mathrm{e}$, putting $p_\mathrm{F} = \sqrt{2m_\mathrm{e}E_\mathrm{F}}$ one has:

$$\int\limits_{E\le E_\mathrm{F}} \mathrm{d}^3q\,\mathrm{d}^3p = V\times 4\pi\int\limits_{p\le p_\mathrm{F}} p^2\mathrm{d}p = \frac{4\pi}{3}V\big(2m_\mathrm{e}E_\mathrm{F}\big)^{3/2}\,.$$

The number of states is $n = \dfrac{4\pi V}{3h^3}\left(2m_{\mathrm{e}}E_{\mathrm{F}}\right)^{3/2}$.

b) The energy is a minimum if all the states with energy less than $E_{\mathrm{F}}$ are occupied and there are two electrons per state, so:

$$N = 2\,n = 2 \times \frac{4\pi V}{3h^3}\left(2m_{\mathrm{e}}E_{\mathrm{F}}\right)^{3/2} \quad \Rightarrow \quad E_{\mathrm{F}} = \frac{h^2}{8m_{\mathrm{e}}}\left(\frac{3N}{\pi V}\right)^{2/3}.$$

c) The total energy is

$$E = 2 \times \sum_{n_1,n_2,n_3} E_{n_1,n_2,n_3} = 2 \times \sum_{n_1,n_2,n_3} \frac{1}{2m_{\mathrm{e}}}\left(p_{n_1}^2 + p_{n_2}^2 + p_{n_3}^2\right)$$

where $p_{n_1} = n_1 h/2a$, etc. and the sum is performed on all the quantum numbers such that $E_{n_1,n_2,n_3} \le E_{\mathrm{F}}$. The points $\vec{p} = (p_{n_1}, p_{n_2}, p_{n_3})$ in the octant $p_i > 0$ $(i = 1,\,2,\,3)$ of momentum space give rise to a lattice with unit steps $h/2a,\ h/2b,\ h/2c$. So, replacing the sum with the integral:

$$E = 2 \times \frac{1}{8}\frac{8V}{h^3}\,4\pi \int_0^{p_{\mathrm{F}}} \frac{p^2}{2m_{\mathrm{e}}}\,p^2\,\mathrm{d}p = \frac{4\pi V}{5m_{\mathrm{e}}h^3}\,p_{\mathrm{F}}^5 = \frac{3\,h^2 N}{40\,m_{\mathrm{e}}}\left(\frac{3N}{\pi V}\right)^{2/3}$$

and since $E$ is a homogeneous function of $V$ of order $-2/3$:

$$p\,V = -V\,\frac{\partial E}{\partial V} = \frac{2}{3}E \quad \Rightarrow \quad p = \frac{2}{3}\,\frac{E}{V} = \frac{\pi h^2}{60\,m_{\mathrm{e}}}\left(\frac{3N}{\pi V}\right)^{5/3}.$$

d) A mole of atoms of silver occupies the volume $108/10.5 \simeq 10\,\mathrm{cm}^3$, so:

$N/V \simeq 6 \times 10^{22}\,\mathrm{cm}^{-3} \quad \Rightarrow \quad p \simeq 2 \times 10^{11}\,\mathrm{dyn/cm}^2 = 2 \times 10^5\,\mathrm{atm}$.

$E_{\mathrm{F}} = 9 \times 10^{-12}\,\mathrm{erg} = 5.6\,\mathrm{eV} \quad \Rightarrow \quad T_{\mathrm{F}} = 6.5 \times 10^4\,\mathrm{K}$.

**2.14**

a) While for a photon:

$$E_\gamma = h\,\nu = \frac{h\,c}{\lambda} \simeq \frac{12400\ \mathrm{eV\,\mathring{A}}}{1.4\,\mathrm{\mathring{A}}} = 8.9 \times 10^3\,\mathrm{eV}\,,$$

for a particle of mass $m \neq 0$, if $m_{\mathrm{e}}$ stands for the electron mass:

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}} \quad \Rightarrow \quad \lambda\sqrt{E} = \frac{h\,c}{\sqrt{2m_{\mathrm{e}}c^2}}\sqrt{\frac{m_{\mathrm{e}}}{m}} = 12.4\sqrt{\frac{m_{\mathrm{e}}}{m}}\ \mathrm{\mathring{A}}\,(\mathrm{eV})^{1/2}$$

and, as a consequence, for neutrons of mass $m_{\mathrm{n}} \simeq 1.7 \times 10^{-24}\,\mathrm{g} = 1840\,m_{\mathrm{e}}$ one has:

$$E_{\mathrm{n}} = \left(\frac{12.4}{1.4}\right)^2 \times \frac{1}{1840} \simeq 4.3 \times 10^{-2}\,\mathrm{eV}\,.$$

b) From the Bragg relation $2\,d\,\sin\theta = n\,\lambda$ with $n = 1$ one obtains:

$$d = \frac{\lambda}{2\sin\theta} \simeq 1.9\,\mathrm{\mathring{A}}\,.$$

c) The number of angles for which there occurs Bragg reflection is the integer part of $2d/\lambda$, namely $2$.

**2.15**

a) $v = \dfrac{p}{m_\mathrm{n}} = \dfrac{h}{m_\mathrm{n}\lambda} = 4.3\,\mathrm{m/s}\,;\ E_\mathrm{f} = \dfrac{h^2}{2m_\mathrm{n}\lambda^2} = 10^{-7}\,\mathrm{eV}\,;\ T = 1.1\times 10^{-3}\,\mathrm{K}\,.$

b) The difference between the initial and final kinetic energy is $3.7\times 10^{-6}\,\mathrm{eV}$, that practically is the same as the initial energy; so, if the energy is expressed in eV and the wavelength in Å (see Problem 2.14), one has:

$$\lambda_\mathrm{i} = \frac{12.4}{\sqrt{E_\mathrm{i}}}\sqrt{\frac{m_\mathrm{e}}{m_\mathrm{n}}} \simeq 150\,\text{Å}$$

or, since $\lambda$ is inversely proportional to the square root of the energy,

$$\lambda_\mathrm{i} = \lambda_\mathrm{f}\sqrt{E_\mathrm{f}/E_\mathrm{i}} = 900\sqrt{10^{-7}/3.8\times 10^{-6}} \simeq 150\,\text{Å}\,.$$

c) In vacuum $\lambda_0 = h/p_0 = h/\sqrt{2m_\mathrm{n}E}$; in the medium $\lambda = h/p = h/\sqrt{2m_\mathrm{n}(E-V_0)}$, therefore $n \equiv \lambda_0/\lambda = \sqrt{1-V_0/E} = 0.67$ (note that $n<1$).

d) Note that, contrary to the convention used in optics, here the incidence angle is measured from the reflection plane. So total reflection occurs for angles $\theta < \theta_r$ where $\cos\theta_r = n$, namely $\theta < 48°$. Equivalently, if $\vec{p}_0$ is the momentum of the neutron in vacuum and $\vec{p}$ is the momentum in the medium, taking the $y$ axis normal to the surface and the $x$ axis in the plane containing the incident beam, one has:

$$E = \frac{p_{0x}^2}{2m_\mathrm{n}} + \frac{p_{0y}^2}{2m_\mathrm{n}} = \frac{p_x^2}{2m_\mathrm{n}} + \frac{p_y^2}{2m_\mathrm{n}} + V_0\,.$$

Since $p_x = p_{0x}$ and $p_{0y} = p_0\sin\theta$, there occur both reflection and refraction when $p_y^2 > 0$, i.e. $E\sin^2\theta > V_0$, therefore $\sin^2\theta_r = V_0/E$, namely $\cos\theta_r = \sqrt{1-V_0/E}$.

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