An Introduction to Quantum Mechanics

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Calculus

Differentiation

Q1: Show, from first principles, that

$$\frac{d\sin x}{dx} = \cos x$$

Q2: Find and identify the nature of the turning points of

$$y = \frac{1}{3}x^3 - 3x^2 + 8x + 4$$

What is the minimum of the function?

Q3: Show how Newton's gravitation force law follows from the gravitational potential

$$\phi_g = \frac{-GMm}{r}$$

Similarly show that Coulomb's law follows from

$$\phi_e = -\frac{Qq}{4\pi\epsilon_0 r}$$

Taylor Expansion

Q4: Find the Taylor expansion for $\sin x$, $\cos x$ and e^x . Find the first three non-zero terms and the *n*th term in the series in each case.

Check that your expansions are consistent with $\frac{d\sin x}{dx} = \cos x$; $\frac{d\cos x}{dx} = -\sin x$; $\frac{de^x}{dx} = e^x$;

Q5: Use your expansions from Q4 to prove Euler's formula

$$e^{ix} = \cos x + i \sin x$$

where $i^2 = -1$.

Integration

Q6: There is another way to formulate mechanics that is equivalent to Newton's laws. One gives a particular number to any trajectory that a particle might travel by (here we really allow any motion to begin with - speed is not connected to position!) - the path with the smallest value of that number is the path taken. The way to define the number that works is through the Action

$$S = \int (T - V)dt$$

T = kinetic energy, V = potential energy

let's do a very simple one dimensional example where

$$T = \frac{1}{2}m\dot{x}^2. \qquad V = V(x)$$

Write out the Action. Imagine that you expand the paths around the true minimum

$$x = x_m + \delta x$$
 $\dot{x} = \dot{x}_m + \delta \dot{x}$

Write out the leading order change in the action ΔS .

Now use Integration by Parts to make the $\delta \dot{x}$ piece look like just δx . You will get a term evaluated at the ends of the path. We will assume that these ends points are held fixed.

If we were at the minimum then the leading order $\Delta S = 0$. Show that this condition is equivalent to Newton's second law.

Classical Physics

Q7: Show that the classical energy of an electron in a circular orbit in a hydrogen atom is given by

$$E = -\frac{Q^2}{8\pi\epsilon_0 r}$$

The Semi-classical Period

Q8: The photoelectric effect is described by the key equation for the energy of the electron

$$\frac{1}{2}m_e v_e^2 + W_f = h\nu$$

where the first term is the kinetic energy of the emerging electron, W_f is the work function - the energy needed to liberate an electron from the material - ν is the frequency of the incident light and $h = 6.6 \times 10^{-34}$ Js is Planck's constant.

The table below shows four different metals and their corresponding work functions.

Metal	Work function ($\times 10^{-19}$ J)
Gold	7.8
Zinc	6.9
Calcium	4.3
Potassium	3.2

a) Calculate the threshold frequencies for each of the four metals listed above.

b) When radiation of frequency 8×10^{14} Hz is applied to Calcium, calculate the speed of the photoelectrons leaving the Calcium.

Q9: Neutrons may be used to study the atomic structure of matter. Diffraction effects are noticeable when the de Broglie wavelength of the neutrons is comparable to the spacing between the atoms. This spacing is typically 2.6 $\times 10^{-10}$ m.

i) Suggest why using neutrons may be preferable to using electrons when investigating matter.

ii) Calculate the speed v of a neutron having a de Broglie wavelength of 2.6 $\times 10^{-10}$ m. The mass of a neutron is 1.7×10^{-27} kg.

Q10: Find the real and imaginary parts of the complex wave function (here A is a complex number)

$$\psi = A e^{i\frac{2\pi}{\lambda}(x-vt)}$$

Exponentials are easier to differentiate than sine waves so people use the trick of writing the solution like this and then take either just the real or imaginary part.

Show that in quantum mechanics

$$E\psi = i\frac{h}{2\pi}\frac{d\psi}{dt}$$

$$p\psi=-i\frac{h}{2\pi}\frac{d\psi}{dx}$$

The Schroedinger equation

Q11: Derive the solutions for an infinite quantum square well. Start from the Schroedinger equation

$$\frac{1}{2m}\left(-\frac{h^2}{(2\pi)^2}\right)\frac{d^2}{dx^2}\psi + V\psi = i\frac{h}{2\pi}\frac{d}{dt}\psi$$

The well has zero potential between x = 0 and L - elsewhere V is infinite.

In time independent solutions you can always find a solution of the form

$$\psi = u(x)e^{-i2\pi E/h}$$

Find an equation for u(x) and then try a solution of the form

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

Make sure your solution vanishes at x = 0, L. Now substitute your guess into your differential equation for u(x).

To fix the overall normalization make sure the probability that the particle is somewhere in the box is one. That is require

$$\int_0^L \psi^* \psi dx = 1$$

Hydrogen Atom Solutions

Q12: In three dimensions and with spherical symmetry the Schroedinger equation takes the form

$$\frac{1}{2m} \left(-\frac{h^2}{(2\pi)^2} \right) \frac{1}{r^2} \left(\frac{d}{dr} r^2 \frac{d}{dr} \right) \psi + V \psi = i \frac{h}{2\pi} \frac{d}{dt} \psi$$

Show, by substitution, that there is a solution of the form

$$u_1 = A e^{-r/a_0} e^{-i2\pi E_1/h}$$

where A is a constant and $a_0 = \frac{\epsilon_0 h^2}{m_e e^2 \pi}$. This is the ground state solution.

There are then excited, spherically symmetric states

$$u_2 = Ae^{-r/2a_0} \left(1 - \frac{r}{2a_0}\right) e^{-i2\pi E_2/h}$$

$$u_3 = Ae^{-r/2a_0} \left(1 - \frac{2r}{3a_0} + \frac{2r^2}{27a_0^2} \right) e^{-i2\pi E_3/h}$$

and so on. They have energy

$$E_n = \frac{E_0}{n^2} \qquad E_0 = \frac{(2\pi)^2 m_e e^4}{32\pi^2 \epsilon_0^2 h^2}$$

What colour is the emission line corresponding to the transition from the n = 3 to n = 2 state?