FYTA12:S2 – Exercises in Quantum Mechanics

The wave nature of particles

1. Electrons are accelerated over a potential difference of 100 V. They are then reflected by a crystal and hit a screen. You will see an interference pattern on the screen.
a) If you repeat the experiment with photons, what energy would the photons have to produce a similar interference pattern?
b) What energy would neutrons have?

2. Use Bohr's quantisation condition (the angular momentum is a multiple of Planck's constant divided by 2π, $\frac{h}{2\pi} = \hbar$) to estimate the energy levels in a harmonic oscillator. The total energy of a harmonic oscillator is given by $p^2/2m + m\omega^2 r^2/2$, i.e. the force is $m\omega^2 r$ (spring force) where r is the distance from the origin. Assume that you have circular orbits.

The wave function

3. A particle moves in a one-dimensional potential

$$V(x) = \begin{cases} \infty, & x < 0 \text{ or } x > a \\ 0, & 0 < x < a \end{cases}$$

and is described at a certain time by the wave-function

$$\Phi(x) = \begin{cases} 0, & x < 0 \text{ or } x > a \\ Ax^2 + Bx + C, & 0 < x < a \end{cases}$$

a) Use the continuity condition and the normalisation condition to determine the constants A, B, and C.
b) Then compute the expectation values of x, x^2, p, and p^2. Try to use possible shortcuts.

4. Use the result from the previous problem and compute Δx and Δp using the definition

$$\Delta A^2 = \left\langle A^2 \right\rangle - \langle A \rangle^2 .$$

Compute $\Delta x \Delta p$ and compare with Heisenberg's uncertainty relation.

5. Use the uncertainty relation to estimate the minimum energy of a proton in a nucleus with radius 5 fm. *Hint:* Assume that the proton is confined in a box with size 5 fm but can move as a free particle inside this box.

The Schrödinger equation

6. The force between two nucleons can be described by a one-dimensional potential energy

$$V(x) = \begin{cases} \frac{a+bx}{x^2}, & x > 0 \\ \infty, & x \leq 0. \end{cases}$$

a) Determine the constants a and b expressed in the range β such that the wave function

$$\Phi(x) = Nx^2 e^{-x/\beta}$$

is a solution the the Schrödinger equation. Compute the binding energy of the system, i.e. the energy required to get the particle free. Draw the potential.
b) Compute the expectation value of the potential energy of the system.

7. Consider a photon trapped in a black hole with radius R. Assume that the wavelength of the photon is of the same size as the radius of the black hole and compute the energy of such a photon. According to the equipartition theorem the energy of the photon will approximately correspond to a temperature given by $k_B T$. Compute this temperature. We can assume that this will be the temperature of the black hole. A blackbody radiator with area A and temperature T radiates a power that is given by Stefan-Boltzmann's law: $P = A\sigma_{SB}T^4$ where σ_{SB} is Stefan-Boltzmann's constant. Compute the power radiated by the black hole. This is the so called Hawking's radiation.

Compute numerically the power radiated by a a black hole with radius l fm. The mass of a black hole is uniquely determined by its radius and given by

$$M = \frac{Rc^2}{2G},$$

where G is the gravitational constant. Compute the mass of the black hole and the relativistic energy equivalent of this mass (by multiplying by c^2). Finally estimate the life-time of the black hole assurning that the radiated energy is provided by a corresponding loss of mass.

8. Assume that the potential in the SE has a negative imaginary part: $\tilde{V}(x) = V(x) - i\alpha$, where $V(x)$ is a real function and α a positive real number. Then show that you have

$$\frac{d}{dt}\int_{-\infty}^{\infty} dx\, |\Psi(x,t)|^2 = -\frac{2\alpha}{\hbar}\int_{-\infty}^{\infty} dx\, |\Psi(x,t)|^2$$

Interpret the result. *Hint:* Modify slightly the steps used in the book for proving the conservation of probability for a real potential.

Piecewise constant potentials

9. A free particle is described at a certain time by the *normalised* wave function (a so called Gaussian wave package):

$$\Phi(x) = \left(\frac{2a}{\pi}\right)^{1/4} e^{ip_0 x/\hbar} e^{-ax^2}$$

Compute Δx and Δp and compare with Heisenberg's uncertainty relation. *Hint:* Use that the normalisation integral is equal to 1. Also use symmetry arguments and that expectation values must be real quantities.

10. A particle with mass m moves in the potential

$$U(x) = \begin{cases} \infty, & x < 0; \\ -4U_0, & O \le x \le a \quad (U_0 > 0); \\ 0, & x > a. \end{cases}$$

The particle is in a stationary state with energy $E = -U_0$. This is possible only for certain values of U_0. Compute the smallest one. *Hint:* Graphical solution.

11. A particle with mass m moves in the potential

$$V(x) = \begin{cases} \infty, & x < 0 \text{ or } x > b; \\ -V_0, & 0 \le x \le a \\ 0, & a \le x \le b. \end{cases} \qquad \left(V_0 = \tfrac{2\pi^2\hbar^2}{9ma^2}\right);$$

Determine the ratio between b and a such that the particle can be in a stationary state with total energy equal to zero.

12. A particle with mass m moves in the potential

$$V(x) = \begin{cases} \infty, & |x| \ge a; \\ -V_0, & -a < x \le 0 \quad (V_0 > 0); \\ 0, & 0 < x < a. \end{cases}$$

Determine the smallest value of a such that there is a stationary state with energy $E = V_0/3$.

13. A particle with mass m moves along a line (the x axis) in a potential

$$V(x) = \begin{cases} \infty, & |x| > 2a \\ 0, & a < |x| < 2a \\ -V_0, & |x| < a \qquad (V_0 > 0) \end{cases}$$

For certain values of V_0 there is a stationary state with energy $E = 0$. Show that the smallest of these is given by the equation

$$ka \tan ka = 1, \; k = \sqrt{\frac{2mV_0}{\hbar^2}}$$

Hint: Use the symmetry. Investigate even and odd solutions separately and use graphics.

14. Butadien is a long narrow molecule with length 5.7 Å. We assume that there are four electrons that can move along the molecule. In a first approximation to model the molecule you can assume that the electrons move in a square well potential with infinite walls. The width of the potential is then 5.7 Å. We neglect a possible interaction between the electrons. Give the energy levels in this model expressed in eV. What energy must a photon have to excite the system from its ground state to its first excited state? Note that because of the Pauli principle there can be only two electrons (with different spins) in each energy level.

15. In a simplified model of an atomic nucleus we assume that a specific nucleon moves in the potential

$$V(x) = \begin{cases} 0, & |x| < a \\ V_0, & |x| > a \quad (V_0 > 0) \end{cases}$$

In the model we consider we have

$$V_0 = \frac{30\pi^2\hbar^2}{8ma^2},\ m = \text{nucleon mass}$$

How many bound states are there?

16. A particle with mass m moves in a one-dimensional potential given by

$$V(x) = \begin{cases} \infty, & |x| > a \\ -V_0, & -a \leq x < 0 \quad (V_0 > 0) \\ 0, & 0 < x \leq a \end{cases}$$

The probability of finding the particle in a small region around the origin is zero.
a) What does this tell you about the wavefunction?
This is possible only for certain values of V_0 and a.
b) Show that for all these values the ratio of the probability of finding the particle to the right of the origin and the corresponding probability of finding it to the left of the origin is

$$\frac{P(x > 0)}{P(x < 0)} = \frac{V_0 + E}{E}$$

Operators and linear algebra

17. a) Show that $e^{-a\frac{\partial}{\partial x}} f(x) = f(x - a)$. *Hint:* Taylor expand both sides of the equation.
b) Describe in words the action of the operator $e^{-a\frac{\partial}{\partial x}}$.

18. Show that a Hermitian operator is also linear. *Hint:* Use the definition of a Hermitian operator with $v = av_1 + bv_2$.

19. Show by explicitly doing the integrals that the solutions to the square well potential with infinite walls are orthogonal.

20. A particle can move freely in one dimension between two plates at distance d from each other. The particle is in the ground state. One of the plates is suddenly moved such that the distance between the plates becomes $2d$. We assume that this happens so quickly that the wave function remains the same (sudden approximation). Compute the probability that the particle immediately after this event is in the new ground state. *Hint:* Model the situations with square well potentials with infinite walls. The particle will after the event be in a superposition of eigenfunctions to the new square well potential.

21. A particle moves in a square well potential on $[0, a]$. It is at a certain moment in a state where the wave function (and thus the probability density) is constant for $0 < x < a/2$ and zero everywhere else. Compute the probability that if you measure the total energy of the particle you will get the value $E = \frac{\pi^2\hbar^2}{2ma^2}$

Measurements

22. Show that for the ground state of the one dimensional harmonic oscillator, the expectation values of the kinetic and potential energies are the same.

23. A particle with mass m moves in the one dimensional potential $V(x) = \frac{1}{2}m\omega^2x^2$. You know that if you measure the energy of the particle you can only get the values $\frac{1}{2}\hbar\omega$ and $\frac{3}{2}\hbar\omega$). You also know that the probability of finding the particle in a small interval dx around the origin is given by $\frac{1}{9}\sqrt{\frac{a}{\pi}}dx$. Compute the probability of getting the respective energy values when you measure the energy of the particle. The normalised wave functions of the ground state and first excited stated are

$$\Phi_0(x) = \left(\frac{a}{\pi}\right)^{\frac{1}{4}} e^{-ax^2/2},\ \Phi_1(x) = \left(\frac{a}{\pi}\right)^{\frac{1}{4}} \sqrt{2a}\, x\, e^{-ax^2/2},\ a = \frac{m\omega}{\hbar}$$

24. A particle with mass m is in a harmonic oscillator potential. At time $t = 0$ it is described by the wave function

$$\Psi(x,0) = \begin{cases} \frac{1}{\sqrt{d}}, & 0 \le x \le d, \\ 0, & x < 0 \text{ or } x > d, \quad d = \sqrt{\frac{2}{a}} = \sqrt{\frac{2\hbar}{m\omega}} \end{cases}$$

Compute the probability to get the value $\frac{3}{2}\hbar\omega$ when you measure the energy of the particle.

Separation of variables in 3D

25. A particle with mass m moves in a three-dimensional square well

$$V(x,y,z) = \begin{cases} 0, & 0 \le x \le a \text{ and } 0 \le y \le b \text{ and } 0 \le z \le c \\ \infty, & \text{elsewhere} \end{cases}$$

a) Write down the SE for the system and indicate how it can be separated in cartesian coordinates.
b) Write down the eigenfunctions and eigenvalues of the system.
c) Sketch an energy level diagram and give the degeneration of all levels with an energy less than $3E_0$, where E_0 is the ground state energy. You know that $b = c = a/2$.

26. A particle with mass m moves in a plane. It is in a stationary state and is described by the wave function

$$\Phi(x,y) = N\,xy\,e^{-a(x^2+y^2)/2},\ a = \frac{m\omega}{\hbar}$$

You know that for $x = y = 0$ the potential energy is 0. Determine the energy of the state and the kind of potential that it moves in.

27. A particle moves in a two-dimensional potential

$$V(x,y) = \frac{1}{2}m\omega^2(x^2+y^2)$$

It is described by a wave function

$$\Phi(x,y) = N\,xy\,e^{-a(x^2+y^2)/2}$$

a) Determine the constant a and the energy of the system.
b) What is the largest distance from the origin that a classical particle with the same energy can have?

28. Experimentally it can be shown that the bensene molecule is flat. An electron in the molecule then can be described by a two-dimensional wave function

$$\Phi(x,y) = N\,e^{-a(x^2+y^2)/2}$$

What is the most probable distance between the electron and the origin? *Hint:* Introduce polar coordinates and investigate the probability of finding the electron in the region $[r, r+dr]$.

29. Consider a hydrogen atom in its ground state. It can be described by a wave function $\Phi_{n\ell m}$ given by

$$\Phi_{100} = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0},\ a_0 = \frac{4\pi\epsilon_0\hbar^2}{me^2} = \text{the Bohr radius}$$

a) Sketch a graph showing the probability density of finding the electron at distance r from the nucleus, i.e. in a shell between r and $r + dr$. What is the most probable distance?

b) Compute the probability of finding it at a distance from the nucleus that is larger than the Bohr radius.

30. The wave function of a particle in a central field potential is $\Psi(r, \theta, \varphi) = f(r)\, u(\theta, \varphi)$. The wave function is assumed to be normalised such that

$$\int_0^\infty |f(r)|^2\, r^2 dr = 1 \text{ and } \int |u(\theta, \varphi)|^2\, d\Omega = 1.$$

Determine the normalisation constant and compute the probability in a measurement of finding the particle in the first octant, i.e. $x, y, z > 0$, in the case that $u(\theta, \varphi) = N(1 - \cos\theta)\cos\varphi$, where N is the normalisation constant.

31. A spherically symmetric potential is given by

$$V(r) = \begin{cases} 0, & r > a \\ -V_0, & r \le a \quad (V_0 > 0) \end{cases}$$

Compute a if you know that the ground state of the system is bound and has energy $-V_0/2$ and that the system is in an **s** state ($\ell = 0$). The wave function must be finite in the origin.

Spherical symmetric potentials; Spherical harmonics

32. For the hydrogen atom the non-relativistic approximation of the electron is often sufficiently good as a first approximation. This is no longer the case for heavier hydrogen-like ions. Compute the smallest value of Z (the charge of the nucleus is Ze) such that the electron in the ground state must be treated as relativistic if you as a condition for this choose $\langle p^2 \rangle < m^2c^2/3$ where m is the mass of the electron and c the speed of light. The wave function for the ground state of a hydrogen-like ion is given by

$$\Phi(r) = \sqrt{\frac{Z^3}{\pi a_0^3}} e^{-Zr/a_0},\ a_0 = \frac{\hbar}{mc}\frac{1}{\alpha},\ \alpha = \frac{1}{137} = \text{fine structure constant}$$

33. A body with moment of inertia I is rotating around its centre of mass.
a) Give the classical expression for the kinetic energy of the body expressed by I and the angular momentum L of the system.
b) A freely rotating body has no potential energy. Translating to quantum mechanics, we change to operators in the total energy to get the Hamiltonian. What is the Schrödinger equation for the rotating body?
c) What is the energy spectrum (energy eigenvalues)? Estimate numerically the energies of a hydrogen molecule rotating around an axis perpendicular to the connection line between the two atoms. Estimate the typical minimum temperature to excite higher rotational states. Can we see this experimentally, and if so how? What is the result for an oxygen molecule? The distance between the nuclei in a hydrogen atom is $0.75 \cdot 10^{-10}$ m and in an oxygen molecule $1.2 \cdot 10^{-10}$ m.

34. For spherical harmonics with $\ell = l$ you have

$$Y_1^{\pm 1}(\theta, \varphi) = \mp\sqrt{\frac{3}{8\pi}} \sin\theta e^{\pm i\varphi},\ Y_1^0(\theta, \varphi) = \sqrt{\frac{3}{4\pi}} \cos\theta.$$

a) Show that the Cartesian coordinates can be written

$$x = r\sqrt{\frac{2\pi}{3}} \left(-Y_1^1 + Y_1^{-1}\right),\ y = ir\sqrt{\frac{2\pi}{3}} \left(Y_1^1 + Y_1^{-1}\right),\ z = r\sqrt{\frac{4\pi}{3}} Y_1^0.$$

b) A quantum-mechanical particle is described by the wave function

$$\Psi = N\frac{x}{r} e^{-ar^2/2}\sqrt{r}.$$

Use your results above to normalise the wave function.
Hint: $\int Y_\ell^{m*} Y_{\ell'}^{m'}\, d\Omega = \delta_{\ell\ell'}\delta_{mm'}$.
c) Which values of the total angular momentum and its z-component are possible to get if you measure them, and what are the respective probabilities to get these values?

Perturbation theory and scattering

35. A particle moves in a one-dimensional square well potential on $[0, a]$ with infinite walls. How is the ground state energy changed if you introduce a perturbation potential

$$v(x) = -\lambda \sin\frac{\pi x}{a}?$$

36. A particle moves in the usual one-dimensional harmonic oscillator potential. The ground state wave function then is

$$\Phi(x) = \left(\frac{a}{\pi}\right)^{1/4} e^{-ax^2/2},\ a = \frac{m\omega}{\hbar}$$

and the energy eigenvalue is $E = \frac{1}{2}\hbar\omega$.
a) Within which interval can a corresponding classical particle move?
b) We add an extra potential that in the classical region is given by $v(x) = -q|x|$ and is zero outside this region. Compute the change in the ground state energy.

37. A particle moves in a potential

$$V(x) = \begin{cases} \frac{V_0}{\sin\frac{\pi x}{a}}, & 0 < x < a \quad (V_0 > 0) \\ \infty, & \text{otherwise} \end{cases}$$

a) Sketch the potential and compute an approximate value of the ground state energy by considering this potential as a perturbation of a suitable known potential.
b) Why would first order perturbation theory not be a good idea for highly excited states?

38. Compute the differential cross section of the scattering potential

$$V(x) = V_0 e^{-r/a}$$

in the Born approximation.

39. When we derive energy levels and eigenfunctions of a hydrogen-like atom we assume that the electron moves in a central field of a point charge.
a) Use first order perturbation theory to estimate the change of the ground state energy induced by the finite size of the nucleus. The nucleus can be taken to be a homogeneously charged sphere vith radius $R \approx (\text{Bohr radius}) \cdot l0^{-5}$. The potential energy of the electron is in this case

$$V(x) = \begin{cases} -\frac{Z\alpha}{2}\left(\frac{3}{R} - \frac{r^2}{R^3}\right), & r < R \\ \\ -\frac{Z\alpha}{r}, & r > R \end{cases} \qquad \left(\alpha = \frac{e^2}{4\pi\epsilon_0}\right)$$

Hint: You can make life easier by using the fact that the ratio $R/(\text{Bohr radius})$ is extremely small. Also try to write the potential energy for $r < R$ as a known potential plus a perturbation.
(This has actually been used to estimate the radius of the nucleus but with a muonic atom instead of an electronic atom. The muon has a mass which is 207 times the electron mass. Why would a muonic atom be better for this purpose than an electronic atom?)
$*$b) Try to prove the expression for the potential! *Hint:* Gauss' theorem!

The unperturbed ground state wave function is

$$\Phi(r) = \sqrt{\frac{Z^3}{ma^3}} e^{-Zr/a},\ a = \text{Bohr radius} = \frac{4\pi\epsilon_0\hbar^2}{me^2} = 52.82\text{pm}.$$

Answers

1. a) 10 keV (X-rays) b) 0.05 eV (thermal neutrons)

2. $E = n\hbar\omega$

3. a) $A = \sqrt{\frac{30}{a^5}}$, $B = -aA$, $C = 0$,
b) $\langle x \rangle = a/2$, $\langle x^2 \rangle = 2a^2/7$, $\langle p \rangle = 0$, $\langle p^2 \rangle = 10\hbar^2/a^2$

4. $\Delta x \Delta p = \sqrt{\frac{10}{28}}\hbar \approx 0.6\hbar$

5. Of the order of MeV

6. $a = \frac{\hbar^2}{m}$, $b = -\frac{2\hbar^2}{m\beta}$, $E = -\frac{\hbar^2}{2m\beta^2}$, $\langle V \rangle = -\frac{4}{3}\frac{\hbar^2}{2m\beta^2}$

7. The power is of the order of 10^{16} W. The mass of the black hole is of the order of 10^{12} kg. The life-time is of the order of 10^{12} s, or 10^5 years.

9. $\Delta x = \frac{1}{2\sqrt{a}}$, $\Delta p = \hbar\sqrt{a}$, $\Delta x \Delta p = \hbar/2$

10. $U_0 = \frac{2\pi^2\hbar^2}{27ma^2}$

11. $b/a = 1 + \sqrt{27}/2\pi$

12. $a = \sqrt{\frac{3\hbar^2}{2mV_0}} \arctan\sqrt{2}$

14. $E_n \approx n^2 \cdot 1$ eV, $E_{\text{photon}} \approx 5$ eV

15. 6

20. $P = \frac{32}{9\pi^2} \approx 0.36$

21. $4/\pi^2 \approx 0.4$

23. 1/9, 8/9

24. $\sqrt{\frac{2}{\pi}}\left(1 - e^{-1}\right)^2 \approx 0.319$

25. $\Phi(x,y,z) = \sqrt{\frac{8}{abc}} \sin\frac{n_x\pi x}{a} \sin\frac{n_y\pi y}{b} \sin\frac{n_z\pi z}{c}$, $E = \frac{\hbar^2\pi^2}{2m}\left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right)$

26. $E = 3\hbar\omega$, $V(x,y) = \frac{1}{2}m\omega^2\left(x^2 + y^2\right)$

27. $E = 3\hbar\omega$, $a = \frac{m\omega}{\hbar}$, $r_{\max} = \sqrt{\frac{6}{a}}$

28. $r = 1/\sqrt{2a}$

29. $r = a_0$, $P(r > a_0) = \frac{5}{e^2} \approx 0.68$

30. a) $N = \sqrt{\frac{3}{8\pi}}$, b) $P = \frac{1}{32}$

31. $a = \frac{3\pi\hbar}{4\sqrt{mV_0}}$

32. $Z < 79$

33. c) $\frac{\hbar^2 \ell(\ell+1)}{2I}$

34. b) $N = a\sqrt{\frac{3}{2\pi}}$, c) $P(\ell = 1, m = 1) = P(\ell = 1, m = -1) = 1/2$

35. $\Delta E = -\frac{8\lambda}{3\pi}$

36. a) $|x| < x_0 = \frac{1}{\sqrt{a}}$, b) $\Delta E = -\frac{qx_0(1-e^{-1})}{\sqrt{\pi}}$

37. $E = \frac{4V_0}{\pi} + \frac{\pi^2\hbar^2}{2ma^2}$

38. $\frac{d\sigma}{d\Omega} = \frac{16m^2V_0^2}{\hbar^4 a^2(1/a^2+K^2)^4}$

39. $\Delta E = \left(\frac{Z^2R}{a}\right)^2 \frac{2\alpha}{5a} \approx Z^4 \cdot 10^{-9}$ eV