Exercise sheet 8
Theoretical Physics 3: QM WS2023/2024

20.12.2023

Exercise 0.

How much time did you take to complete this homework sheet?

Exercise 1. Hydrogen atom (30 points + 10 bonus)

The normalized hydrogen wave functions are:

$$\psi_{nlm}(r,\theta,\phi) = \frac{2}{n^2}\sqrt{\frac{(n-l-1)!}{[a(n+l)!]^3}}\, e^{-\frac{r}{na}} \left(\frac{2r}{na}\right)^l L^{2l+1}_{n-l-1}(\tfrac{2r}{na})\, Y_l^m(\theta,\phi)$$

Where $L^p_{q-p}(x)$ are the associated Laguerre polynomials and $Y_l^m(\theta,\phi)$ are the spherical harmonics.

a) *(10 p.)* Consider the electron is in the state $\psi_{nlm}(r,\theta,\phi)$. What is the probability $P_{nl}(r)$ to find it somewhere?

b) *(20 p.)* Check explicitly that $P_{nl}(r)$ is correctly normalized to unity for $n=3$.
Hint: use $\int_0^\infty \mathrm{d}x\, e^{-x}x^n = n!$.

c) *(10 p.) (Bonus)* Show that $\int_0^\infty \mathrm{d}x\, e^{-x}x^n = n!$. *Hint*: Use the mathematical induction method.

Exercise 2. (45 points)

To solve the radial equation for an infinite spherical well, we introduce spherical Bessel functions $j_l(x)$ of order l defined as:

$$j_l(x) \equiv (-x)^l \left(\frac{1}{x}\frac{\mathrm{d}}{\mathrm{d}x}\right)^l \frac{\sin x}{x}\,.$$

A spherical Bessel functions is a particular case of a Bessel function $J_\alpha(x)$ defined as:

$$J_\alpha = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!\Gamma(n+\alpha+1)} \left(\frac{x}{2}\right)^{2n+\alpha}\,,$$

for α half integer, so $J_{n+1/2} = \sqrt{\frac{2x}{\pi}}\, j_n(x)$.

a) *(25 p.)* Using the definition of the Bessel function, compute $J_{1/2}$ and $J_{3/2}$ and check that, indeed, the relation between $J_{l+1/2}$ and j_l is correct.

The spherical Bessel functions have well defined $x \ll 1$ and $x \gg 1$ limits:

$$j_l(x) \to \frac{2^l l!}{(2l+1)!}x^l \qquad \text{for } x \ll 1$$
$$j_l(x) \to \frac{1}{x}\cos\left(x - \frac{(l+1)\pi}{2}\right) \qquad \text{for } x \gg 1$$

b) *(10 p.)* Compute both limits for j_0, j_1 and j_2 using the definition given at the beginning and confirm with the asymptotic behaviour listed above.
Hint: Calculate the formulas for $j_0,\ j_1$ and j_2 first. For the lower limit use the first few terms of the Taylor expansions of the trigonometric functions and keep only the lowest non-zero one in the final result.

c) *(10 p.)* Compute j_3 using the definition given at the beginning.

Math hints:

$$\sin(x) = \sum_{m=0}^{\infty} (-1)^m \frac{x^{2m+1}}{(2m+1)!}$$
$$\Gamma(m+1/2) = \frac{1 \cdot 3 \cdot 5 \cdot (2m-1)}{2^m}\sqrt{\pi}$$
$$\int_0^{\pi} \sin^n(x)\mathrm{d}x = \frac{\Gamma(1/2+n/2)}{\Gamma(1+n/2)}\sqrt{\pi}$$

Exercise 3. (25 points + 20 bonus)

Consider a particle confined in a three-dimensional square box with side length "a" and *periodic* boundary conditions:

$$\begin{cases} \Psi(r_i = a,\, t) = \Psi(r_i = 0,\, t), \\ \frac{\partial}{\partial r_i}\Psi(r_i = a,\, t) = \frac{\partial}{\partial r_i}\Psi(r_i = 0,\, t). \end{cases}$$

a) *(25 p.)* Solve the Schrödinger equation in Cartesian coordinates.
Hint: Separate variables as

$$\psi(x, y, z) = X(x)Y(y)Z(z)$$

to reduce the problem to one-dimensional and solve it.

b) *(10 p.) (bonus)* Write down the energy spectrum.
What are the degrees of degeneracy of the four lowest energy states?

c) *(10 p.) (bonus)* Consider (fictitious) generalisation of the problem to *four* spatial dimensions.
How would the spectrum be compared to the spectrum of the isotropic harmonic oscillator?
Hint: There is the Lagrange's four-square theorem, which states that every natural number can be represented as the sum of four integer squares:

$$\forall n \in \mathbb{N}:\ \exists\, i, j, k, l \in \mathbb{Z}:\ n = i^2 + j^2 + k^2 + l^2.$$