QM1 Exercises. Sheet 7.

Corrections June 26-27

1) One-dimensional repulsive δ-potential (5 points)

Consider the one-dimensional stationary Schrödinger equation:

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V_0\delta(x)\right]\Psi(x) = E\Psi(x) \tag{1}$$

with $V_0 > 0$ and $E > 0$.

a) What physical situation is described by the Ansatz:

$$\Psi(x) = \begin{cases} e^{iqx} + Re^{-iqx} & \text{for } \; x < 0 \\ Se^{iqx} & \text{for } \; x > 0 \end{cases} \tag{2}$$

b) What boundary conditions does $\Psi(x)$ has to satisfy at $x = 0$?

c) Using the boundary conditions and Eq. (1), determine q, R, and S. All those quantities should be functions of the energy E.

d) Compute the probability current density $j(x)$ (see Exercise 2 sheet 1) for the state $\Psi(x)$. Show that it is constant.

e) Compute the transmission and reflection probabilities. For which value of V_0 does one have perfect reflection.

2) Angular Momentum (5 points)

The wave function of a particle is given by:

$$\Psi(\boldsymbol{x}) = K(x + y + 2z)e^{-\alpha r} \tag{3}$$

where $r = \sqrt{x^2 + y^2 + z^2}$ and α and K are positive constants.

a) Write the wave function using spherical coordinates: $\boldsymbol{x} = r\left[\sin(\theta)\cos(\varphi), \sin(\theta)\sin(\varphi), \cos(\theta)\right]$, $\varphi \in [0, 2\pi]$ and $\theta \in [0, \pi]$. Then write the angular part in terms of spherical harmonics. Here are the expressions for the first few spherical harmonics $Y_{l,m}(\theta, \varphi)$.

$$Y_{0,0} = \frac{1}{\sqrt{4\pi}}, \quad Y_{1,0} = \sqrt{\frac{3}{4\pi}}\cos\theta, \quad Y_{1,1} = -\sqrt{\frac{3}{8\pi}}\sin\theta e^{i\varphi} \tag{4}$$

b) Compute the expectation value of $\hat{L}_z$ and $\hat{\boldsymbol{L}}^2$.

c) If $\hat{L}_z$ were measured what is the probability of obtaining the result $+\hbar$?.

2) Rigid Quantum Rotor (5 points)

Consider the Hamiltonian:

$$\hat{H} = g\hat{\boldsymbol{L}}^2 + \boldsymbol{B} \cdot \hat{\boldsymbol{L}} \tag{5}$$

where $\hat{\boldsymbol{L}}$ corresponds to the angular momentum operator. Note that this type of Hamiltonian would be appropriate to describe the rotational behavior of a molecule in an external magnetic field.

a) Show that $[\hat{\boldsymbol{L}}^2, \hat{H}] = 0$. Use this property to show that the Hamiltonian can be written as

$$\hat{H} = \sum_{l=0}^{\infty} \sum_{m,m'=-l}^{l} h^{(l)}_{m,m'} |l,m\rangle\langle l,m'| \tag{6}$$

In the above $\sum_{l=0}^{\infty}\sum_{m=-l}^{l} |l,m\rangle\langle l,m| = 1$, $\hat{\boldsymbol{L}}^2|l,m\rangle = \hbar^2 l(l+1)|l,m\rangle$, $\hat{L}_z|l,m\rangle = \hbar m|l,m\rangle$ and $h^{(l)}_{m,m'} = \langle l,m|\hat{H}|l,m'\rangle$. Hence you have shown that $\hat{H}$ is block diagonal in the quantum number l.

b) Show that for $l = 1$,

$$h^{(1)} = 2g\hbar^2 + \boldsymbol{B} \cdot \boldsymbol{K} \tag{7}$$

with

$$K_x = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad K_y = \frac{i\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \quad K_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \tag{8}$$

Which commutation rules do those matrices satisfy?

c) Show that the Heisenberg representation of $\hat{\boldsymbol{L}}$,

$$\hat{\boldsymbol{L}}(t) = e^{i\hat{H}t/\hbar}\hat{\boldsymbol{L}}e^{-i\hat{H}t/\hbar}, \tag{9}$$

satisfies the differential equation:

$$\frac{\mathrm{d}}{dt}\hat{\boldsymbol{L}}(t) = \boldsymbol{B} \times \hat{\boldsymbol{L}}(t) \tag{10}$$

d) For $\boldsymbol{B} = (B, 0, 0)$ and the initial state $|\Psi(t=0)\rangle = |l, m=0\rangle$ compute $\langle\hat{\boldsymbol{L}}\rangle(t)$.