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October 31st, 2024
WS 2024/25

Problem 3.1: Symmetric top

[**Written** | 2 pt(s)]

ID: ex_symmetric_top:aqt2425

> **Learning objective**
>
> The rotational states of molecules can be very well described by employing the model of a quantum mechanical rigid rotor in which the distance of the atoms within the molecules is assumed to be fixed. In this problem, you consider the special case of a symmetric rotor (or symmetric top), which is analytically solvable, where two moments of inertia are equal and the third moment of inertia has a different value.

Consider a symmetric rigid rotor (symmetric top) where two moments of inertia are the same ($I_x = I_y \equiv I_\perp$) and the third moment of inertia has a different value ($I_z \equiv I_\parallel$).

a) Express the Hamiltonian of such a system in terms of the angular momentum operators L^2 and L_z. Provide examples for molecules whose rotation can be well described by this Hamiltonian. **1** pt(s)

b) Determine the eigenvalues and eigenstates of the Hamiltonian. **1** pt(s)

Problem 3.2: Bound states of a spherical potential well

[**Oral** | 3 pt(s)]

ID: ex_bound_states_spherical_potential_well:aqt2425

> **Learning objective**
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> Here we will derive the bound states of a spherically symmetric potential well. To do so, we will exploit the rotation symmetry of the problem and show that the radial solutions are given by *spherical Bessel functions* (see lecture). The idea is to explicitly derive the transcendental equation that determines the eigenenergies for bound states with angular momentum $l = 0$.

Consider the Hamiltonian of a particle in three dimensions

$$H = \frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{r}) \tag{1}$$

with the spherically symmetric and piecewise constant potential

$$V(\boldsymbol{r}) = V(r) = \begin{cases} 0 & r > R \\ V_0 & r \le R \end{cases} \tag{2}$$

with $r = |\boldsymbol{r}|$, $R > 0$ the radius of the potential well and $V_0 < 0$ the potential depth.

Your goal is to find the bound states and eigenenergies of this system and the conditions that are necessary for their existence.

a) Make the separation ansatz $\Psi(\boldsymbol{r}) = R_l(r) \cdot Y_{lm}(\theta, \varphi)$ with spherical harmonics Y_{lm} and show that the eigenvalue problem reduces to **1pt(s)**

$$\left[\rho^2 \partial_\rho^2 + 2\rho\partial_\rho + \rho^2 - l(l+1)\right] \tilde{R}_l(\rho) = 0 \tag{3}$$

with $\rho \equiv K_r r$ and $\tilde{R}_l(\rho) \equiv R_l(r)$ where $K_r \equiv \sqrt{\frac{2m(E-V(r))}{\hbar^2}}$.

b) Write down the general solution of the radial problem in the two regions $r > R$ and $r \leq R$ for a given angular momentum l and formulate the continuity and boundary conditions that the eigenstates must satisfy. **1pt(s)**

Hint: Use that the solutions of the differential equation

$$\left[x^2 \partial_x^2 + 2x\partial_x + x^2 - l(l+1)\right] y(x) = 0 \tag{4}$$

are given by the *spherical Bessel functions*

$$j_l(x) = (-x)^l \left(\frac{1}{x}\partial_x\right)^l \frac{\sin(x)}{x} \quad \text{and} \quad y_l(x) = -(-x)^l \left(\frac{1}{x}\partial_x\right)^l \frac{\cos(x)}{x} \tag{5}$$

for $l \in \mathbb{N}_0$. (The functions y_l are sometimes denoted n_l and referred to as *spherical Neumann functions.*) Write the eigenstates in terms of these functions.

c) Consider the simplest case for $l = 0$. Find explicit expressions for the bound states and derive a transcendental equation to determine their eigenenergies. At which potential depth V_0 appears the first bound state? **1pt(s)**

Hint: Use your knowledge of the one-dimensional potential well to analyze the transcendental equation.