1. Ammonia molecule

The stable configuration of the ammonia molecule NH_3 forms a pyramid with

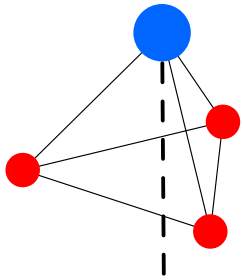

Abbildung 1: *Ammonia molecule*

three hydrogen atoms forming a triangular base and the nitrogen atom at the apex. The molecule as a whole can perform rotations and/or translations. We will focus on the internal dynamics, namely the vibrations. Due to its heavy mass the nitrogen atom can be considered as fixed and rigid and the entire hydrogen base (which is essentially rigid) moves up and down along the dashed line.
The problem, thus, reduces to a one-dimensional one. We denote by x the distance of the nitrogen atom from the hydrogen plane. Obviously, the corresponding potential $V(x)$ is symmetric in x and has a double-well shape. For the sake of simplicity, we will simplify the Potential even further

$$V(x) = \begin{cases} \infty & \text{region I} \quad x < -a, \\ 0 & \text{region II} \quad -a \leq x \leq -b \\ V_0 & \text{region III} \quad -b < x < b \\ 0 & \text{region IV} \quad b \leq x \leq a \\ \infty & \text{region V} \quad x > a \end{cases} .$$

1. Determine the general solutions of the Schrödinger equation in the 5 regions separately.

2. Simplify the coefficients by exploiting the fact that the solutions have definite parity.

3. Enforce the appropriate boundary conditions, yielding conditions for the coefficients and for the allowed energy levels.
   Introduce natural, dimensionless units.

4. Solve the equations for the eigenenergies numerically.

5. Discuss the physical meaning of the result.

6. Simulate and discuss the time evolution of the wavefunction which starts with $\psi(x, t = 0) = \Phi_1(x) + \Phi_2(x)$, with $\Phi_\alpha(x), \quad \alpha = 1, 2$ being the two lowest eigenvectors of the Hamiltonian.