# 4 Ammonia molecule

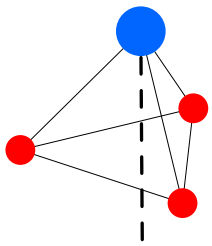

Abbildung 1: *Ammonia molecule*

The stable configuration of the ammonia molecule $NH_3$ forms a pyramid with the 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 the entire hydrogen base moves up and down along the dashed line. Effectively, this can likewise be viewed as if the hydrogen atoms are at rest and the nitrogen moves along the dashed line.

Bottom line is, we have a 1-d potential problem. We denote the distance of the nitrogen atom from the hydrogen plane by $x$. Obviously, the respective 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 parts of the eigenfunctions in the 5 regions separately.

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

3. Evaluate the boundary conditions, yielding conditions for the coefficients and the energy quantization.
   Introduce natural, dimensionless units.

4. Solve the equations for the eigen-energies 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 $\Phi_\alpha(x)$ being the two lowest eigenvectors of the Hamiltonian.