Theory of Quantum Matter

Lecturer: Prof. Otfried Gühne (Mon 14:00, Fri 10:00, Room D120)
Exercises: Chau Nguyen (Fri 14:00, Room B030) **Sheet 1**

Hand in: Mon 22.10.2018 *(questions marked as ∗ are optional)*
Discussion date: Fri 26.10.2018

1. Born-Oppenheimer approximation

Consider a system of two particles with Hamiltonian

$$H = \frac{p_1^2}{2M} + \frac{p_2^2}{2m} + \frac{K}{2}x_1^2 + \frac{k}{2}(x_1 - x_2)^2. \tag{1}$$

We first regard the system as a classical system, where (x_k, p_k) with $k = 1, 2$ are the positions and momenta of the particles.

(a) (15pts) Classical mechanics tells that the solution of this Hamiltonian has two oscillation modes of two frequencies. Find these two frequencies.

Hint: If you need a review of classical mechanics, have a look at Landau's Mechanics or Goldstein's Classical Mechanics.

Now we regard the system as a quantum system, that is, the positions and momenta of the particles are regarded as operators subjected to the commutation relation $[x_k, p_l] = i\hbar\delta_{kl}$.

(b) (10pts) What are the exact eigenvalues of H.

(c) (15pts) Solve the quantum mechanical problem in the Born-Oppenheimer approximation (with $m \ll M$), where we consider

$$T_A = \frac{p_1^2}{2M}, \tag{2}$$

as the "atomic" kinetic energy term, first ignored, and solve the "electronic" problem,

$$\frac{p_2^2}{2m} + \frac{K}{2}x_1^2 + \frac{k}{2}(x_1 - x_2)^2 \tag{3}$$

with fixed parameter x_1 (that is, determining the eigenvalues $\epsilon_{n_1}(x_1)$), then later solve the atomic eigenvalue problem

$$\frac{p_1^2}{2M} + \epsilon_{n_1}(x_1). \tag{4}$$

(d) ∗ Compare the approximate solution in (c) with the exact solution in (b).