

# QUANTENMECHANIK

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Sheet 11 Due: 25.06 um 12 Uhr

## 1 Separation of variables (10 P)

The Hamiltonian of a hydrogen atom is given by

$$H = \frac{1}{2m_p} P_p^2 + \frac{1}{2m_e} P_e^2 - \frac{k}{|R_p - R_e|},$$

where  $P_p, R_p$  are the momentum and position operators of the proton, and  $P_e, R_e$  the momentum and position operators of the electron. To simplify the problem, we can define new position and momentum operators, that separate this Hamiltonian into two independent Hamiltonians, one for the centre-of-mass degree of freedom, and another for the relative movement degree of freedom.

Analogous to the classical problem, the position and momentum operators for centre-of-mass and relative movement are given by

$$R_{SP} = \frac{1}{m_p + m_e} (m_p R_p + m_e R_e), \quad R_r = R_p - R_e$$

$$P_{SP} = P_p + P_e \quad P_r = \frac{1}{m_p + m_e} (m_e P_p - m_p P_e)$$

- a) (0,5 P) Show that the new operators are proper position and momentum operators, in that they respect the following commutation relations for an arbitrary component (e.g.  $x$ ):

$$[R_{SP}^x, P_{SP}^x] = i\hbar \quad \text{and} \quad [R_r^x, P_r^x] = i\hbar$$

- b) (1 P) Show that the new degrees of freedom are independent, in that they respect the following commutation relations for an arbitrary component (e.g.  $x$ ):

$$[R_r^x, P_{SP}^x] = 0 \quad \text{and} \quad [R_{SP}^x, P_r^x] = 0$$

- c) (1,5 P) Show that the Hamiltonian with the new operators is given by

$$H = \frac{1}{2M} P_{SP}^2 + \frac{1}{2\mu} P_r^2 - \frac{k}{|R_r|},$$

where

$$M = m_p + m_e \quad \text{and} \quad \mu = \frac{m_p m_e}{m_p + m_e}$$

are the total and reduced masses.

- d) (1 P) A more-or-less realist model for the complete wavefunction of a hydrogen atom is a product between a Gaussian wavepacket for the centre-of-mass degree of freedom and a so-called "1s orbital" for the relative movement degree of freedom. Here we show a one-dimensional cut through the three-dimensional solution. It is given by

$$\psi(x_{SP}, x_r) = \frac{1}{\sqrt[4]{\pi\sigma^2}} \exp\left(-\frac{x_{SP}^2}{2\sigma^2}\right) \frac{1}{\sqrt{a_0}} \exp\left(-\frac{|x_r|}{a_0}\right),$$

and when written in terms of the coordinates for the proton and electron, by

$$\psi(x_p, x_e) = \frac{1}{\sqrt[4]{\pi\sigma^2}} \exp\left(-\frac{(\mu_p x_p + \mu_e x_e)^2}{2\sigma^2}\right) \frac{1}{\sqrt{a_0}} \exp\left(-\frac{|x_p - x_e|}{a_0}\right),$$

where  $\mu_e = m_e/M$  and  $\mu_p = m_p/M$ . This wavefunction is an *entangled* quantum state, that is, it is not a product between a wavefunction  $\varphi_p(x_p)$  for the proton and a wavefunction  $\varphi_e(x_e)$  for the electron. Show that if the wavefunction were a product, the probability density  $|\psi(x_p, x_e)|^2$  would also factorise:

$$|\psi(x_p, x_e)|^2 = \text{Pr}_p(x_p)\text{Pr}_e(x_e),$$

where

$$\text{Pr}_p(x_p) = \int_{-\infty}^{\infty} dx_e |\psi(x_p, x_e)|^2 \quad \text{and} \quad \text{Pr}_e(x_e) = \int_{-\infty}^{\infty} dx_p |\psi(x_p, x_e)|^2.$$

e) (3 P) Show that

$$\text{Pr}_p(x_p) = \frac{1}{2a_0\mu_e} e^{\frac{\sigma^2}{a_0^2\mu_e^2}} \left( \exp\left(\frac{2x_p}{a_0\mu_e}\right) \text{erfc}\left(\frac{\sigma}{a_0\mu_e} + \frac{x_p}{\sigma}\right) + \exp\left(-\frac{2x_p}{a_0\mu_e}\right) \text{erfc}\left(\frac{\sigma}{a_0\mu_e} - \frac{x_p}{\sigma}\right) \right),$$

where

$$\text{erfc}(x) = 1 - \text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_x^{\infty} e^{-t^2} dt$$

is the complementary error function. For the electron the analogous calculation shows that

$$\text{Pr}_e(x_e) = \frac{1}{2a_0\mu_p} e^{\frac{\sigma^2}{a_0^2\mu_p^2}} \left( \exp\left(\frac{2x_e}{a_0\mu_p}\right) \text{erfc}\left(\frac{\sigma}{a_0\mu_p} + \frac{x_e}{\sigma}\right) + \exp\left(-\frac{2x_e}{a_0\mu_p}\right) \text{erfc}\left(\frac{\sigma}{a_0\mu_p} - \frac{x_e}{\sigma}\right) \right),$$

but you don't need to show that.

**Hint:** A useful property of the absolute value function is that  $|x_p - x_e| = x_p - x_e$  for  $x_p \geq x_e$  and  $|x_p - x_e| = -x_p + x_e$  for  $x_p \leq x_e$ .

f) (1 P) Show that

$$|\psi(x_p, x_e)|^2 \neq \text{Pr}_p(x_p)\text{Pr}_e(x_e)$$

to conclude that  $\psi(x_p, x_e)$  is entangled.

**Hint:** It is enough to find a single value of  $(x_p, x_e)$  for which the equality does not hold.

g) (1 P) Plot with a computer  $\text{Pr}_p(x_p)$  together with

$$\text{Pr}_{SP}(x_{SP}) = \int_{-\infty}^{\infty} dx_r |\psi(x_{SP}, x_r)|^2 = \frac{1}{\sigma\sqrt{\pi}} \exp\left(-\frac{x_{SP}^2}{\sigma^2}\right)$$

to show that  $x_{SP}$  is a good approximation for  $x_p$ .

h) (1 P) Plot with a computer  $\text{Pr}_e(x_e)$  together with

$$\text{Pr}_r(x_r) = \int_{-\infty}^{\infty} dx_{SP} |\psi(x_{SP}, x_r)|^2 = \frac{1}{a_0} \exp\left(-\frac{2|x_r|}{a_0}\right)$$

to show that  $x_r$  is *not* a good approximation for  $x_e$ .