University of Regensburg Summer Term 2010

Quantum Theory of Condensed Matter I

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Sheet 2

1. Hydrogen molecule ion (atomic orbitals)

We now consider the same problem of point 1. starting though from the atomic orbitals.

1. Write the Hamiltonian for a 1D hydrogen atom in"atomic units" and discretize it. Diagonalize numerically.
2. Use the ground state calculated at the previous point and assume that the single particle Hilbert space of the hydrogen molecule is spanned by the ground states of the hydrogen atom centered on the first and second hydrogen. Eventually write the equation

$$\left(-\frac{d^2}{d\xi^2}-\frac{2}{|\xi+D/2|}-\frac{2}{|\xi-D/2|}+\frac{2}{D}\right)\psi_n(\xi)=E_n(D)\psi_n(\xi)$$

   in this atomic orbital basis. Calculate now numerically the matrix elements of the Hamiltonian and the overlap matrix S.
3. Solve the eigenvalue problem stated at the previous point first in the approximation $S_{ij}=\delta_{ij}$. Plot the eigenvalues as a function of the interatomic distance D. Check that in the large D limit the 2 eigenenergies coincide and correspond to the energy of the isolated hydrogen atom. Compare the results also with the ones obtained together in the numerical tutorial.
4. Repeat the previous point releasing the approximation done on the overlap matrix S. Check that in this case the correspondence to the solution obtained using molecular orbitals is closer. Still there are some discrepancies for small D. Can you say why?

Frohes Schaffen!