University of Regensburg Summer Term 2010

Quantum Theory of Condensed Matter I

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Sheet 1

1. Rules of the game

Nothing else than "hands-on" approach helps to fix ideas, we will give than a lot of importance to the written exercises proposed on a weekly basis. In particular:

1. An exercise sheet is posted on line every Wednesday at the address `http://homepages-nw.uni-regensburg.de/~doa17296/fisica/Teaching/SS10_QTKM1/SS10_QTKM1.html`. **Clearly written** solutions of the exercise sheets should be handed in by Tuesday of the following week at 12:00 in the post box of the course located in "*Treppenhaus 1. Etage* (*Bibliothek Physik*)". The exercise solutions will be then discussed during Wednesday exercise class.
2. One tutorial (depending on time also one lecture) in April will be dedicated to the computational laboratory. The corresponding exercise sheet will consist of a task to be solved with a computer simulation. You will be asked to develop a simple code that allows you to calculate and visualize some of the results obtained in the course. Linux CIP pool will be available for coding and running the MATLAB® simulations. Group sizes of 2-3 people are encouraged. The solution of easy numerical tasks will be also required during the entire course.

2. Hydrogen molecule (discretize the Schrödinger equation)

Let us consider a 1D model of a hydrogen molecule. In particular we study only one electron in the system thus restricting ourselves to the hydrogen molecule ion.

1. Write the Hamiltonian for the system in Born-Oppenheimer approximation. Prove that, if all lengths are written in units of the Bohr radius a_0, and all energies in units of the modulus of the eigenenergy $|E_1|$ of the $1s$ orbital of hydrogen, the Schrödinger equation reads:

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

   where D is the (renormalized) distance between the protons and $V_0(\xi)=\frac{2}{|\xi|}$ is the Coulomb interaction.

   Hint: The Bohr radius a_0 and the hydrogen eigenenergy E_1 in terms of fundamental constants read, respectively:

$$a_0=\frac{4\pi\varepsilon_0\hbar^2}{me^2}\approx 0.053\,\mathrm{nm}$$
$$E_1=\frac{me^4}{2(4\pi\varepsilon_0)^2\hbar^2}\approx -13.6\,e\mathrm{V}$$

   where e and m are the charge and the rest mass of the electron and ε_0 the vacuum dielectric constant.

Now you will discretize the equation stated at point 1 and thus transform the eigenvalue problem to make it suitable for a numerical calculation.

2. Replace the continuous space variable ξ with the discrete set of numbers ξ_i with $i=1,\ldots,N$. The wave-function is thus replaced by a vector: which one?
3. Work out the discrete version of the derivative. Eventually represent it as a matrix acting on the discrete wave function calculated in the previous point.

4. Also the second derivative is an operator which acts on the wave function. Find out which is its matrix representation in the discrete space introduced in the previous points.

5. Complete the discretization process and write the full eigenvalue problem as an algebraic equation:

$$\mathbf{H}\mathbf{\Psi}_n = E_n\mathbf{\Psi}_n$$

(Hint: Remember that the potential operator acts locally $(V\psi)(\xi) = V(\xi)\psi(\xi)$.)

Frohes Schaffen!