Exercise-sheet 10 (2nd and 3rd of July)

1 In class exercise:

1.1 Potential and perturbation

Consider a potential consisting of two infinite walls at $x = 0$ and $x = a$, and an additional perturbation:

$V_1(x) = \lambda \frac{\hbar^2 \pi^2}{2ma^2} \begin{cases} sin^2(\frac{\pi x}{a}) & , 0 < x < a \\ 0 & , otherwise \end{cases}$

Calculate the eigenfunctions to order λ and the eigenvalues to order λ^2, by using perturbation-theory.

2 Homework - due date 8th of July 2009 (30 points)

This is the last 'regular' homework. For those students which are slightly below our point-criteria of 50 %, there will be a few more exercises.

2.1 Perturbation-theory (10 points)

A system is described by the following Hamilton-matrix:

$$\begin{pmatrix} E_1 & 0 & a \\ 0 & E_1 & b \\ a^* & b^* & E_2 \end{pmatrix} \text{ with } |a|, |b| \ll |E_2 - E_1|$$

The matrix-elements a and b are considered as a perturbation of the same order of magnitute. Calculate the eigenvalues of H with the help of perturbation-theory (till second order). Compare this result with the exact one.

2.2 Hubbard model (10 points)

We consider a model for a hydrogen-molecule: This consists of two sites (each one describing one orbital around one nucleous) and two electrons, which can occupy these sites. The hopping from one site to another one should give an energy of t, while when there are two antiparallel spins occupying the same site, this should cost an energy of U .

2.1. Explain why this system has the following hamiltonian:
$$H = -t \sum_{\sigma=\uparrow,\downarrow} (c^\dagger_{1\sigma} c_{2\sigma} + c^\dagger_{2\sigma} c_{1\sigma}) + U \sum_{i=1}^{2} n_{i\uparrow} n_{i\downarrow},\ n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$$

2.2. Why H commutes with the number-operator $N = \sum_{i,\sigma} n_{i\sigma}$?

2.3. H is diagonal in the particle number because of (2). How many states are there with 0,1,2 particles? Write H as matrix in this basis. Why does H vanish in states with two parallel spins on the two sites ($H|\uparrow,\uparrow\rangle = 0$)?

2.4. For the relevant two-particle states H only the matrix in $\{|\uparrow,\downarrow\rangle,\ |\downarrow,\uparrow\rangle,\ |\uparrow\downarrow,-\rangle,\ |-,\uparrow\downarrow\rangle\}$ is trivial. Calculate the eigenvalues and -states of this matrix.

2.5. Now we assume $U \gg t$. Show that then the eigenvalues from (4) are:
$\{-\frac{4t^2}{U},\ 0,\ U,\ U + \frac{4t^2}{U}\}$
therefore forming two pairs with splitting.

2.6. Show that for the eigenstates the singlett-state - meaning the antiparallel ones, such as: $|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle$ - have always lower energy than the "triplett"-states, which is the symmetric one.

2.3 Perturbation theory Hydrogen-atom (10 points)

The core of the hydrogen-atom is not a 'point-charge'; As a simplification we can consider it as a homogeniously charged ball (radius $R \approx 1fm$) . Explain the Ansatz:
$V(r) = \frac{e^2}{4\pi\epsilon_0 R}(\frac{r^2}{2R^2} - \frac{3}{2}) + \frac{1}{4\pi\epsilon_0}\frac{e^2}{r}$ with $r < R$ otherwise $V(r) = 0$
for the perturbating potential. Which change in energy is there for the $n = 1$ and $n = 2$ states in

first order perturbation theory?
Because $R/a_0 \approx 10^{-5}$ (a_0 : Bohr radius) it is sufficient to evalute the integrals only to leading order in R/a_0.