Exercise sheet 13, Theoretical Physics III (Quantum Mechanics)

Solutions to be handed in and class exercise discussed
in the tutorials of Week 14 (01/02/08)

Class exercise P11: Born approximation (2 points for contributions)

a) Calculate the scattering amplitude $f(\theta, \phi)$ to first order in the Born series for scattering off the potential

$$V(r, \theta, \phi) = -V_0 e^{-r/r_0}, \qquad \text{where } V_0 > 0.$$

Hint:

$$\int_0^\infty dx\, x\, e^{-x} \sin qx = \frac{2q}{(1+q^2)^2}. \qquad ☺$$

b) If there is still time, prove the equation ☺.

Ex. H28: Stark effect (7 points)

A hydrogen atom in the first excited state, thus $n = 2$, is exposed to a constant electric field $\mathbf{E} = (0, 0, E)$.

a) Give the potential.

b) For the hydrogen atom with $n = 2$ there is one state with $l = 0$ (2s state) and three with $l = 1$ (2p states). In the absence of external electric field these states would have the same energie, thus the $n = 2$ level would be four-fold degenerate. Consider the external electric effect as a perturbation, and determine the matrix elements of the perturbation in this space of degenerate states.

c) Diagonalize the matrix of perturbations in order to obtain the splitting of the energy levels.

Instructions: Show first that the equation $[L_3, W] = 0$ holds for the perturbing potential W. Deduce that the only matrix elements of the form $\langle \psi_{nlm} | W | \psi_{n'l'm'} \rangle$ that can be non-vanishing are those with $m = m'$. Then write the perturbation in spherical coordinates and use the known wavefunctions ψ_{2lm} to calculate these matrix elements as well.

Ex. H29: Rayleigh-Ritz variational principle and the helium atom (7 points)

This is a method of approximation that can be applied even if a system cannot be represented as a small perturbation of an exactly solvable problem. It is particularly practical for the estimation of ground state energies. The idea is to approximate the ground state wavefunction by a test function that depends on one or more parameters and to minimise the energy with respect to the parameter(s).

a) Consider a Hamiltonian H with eigenvalues E_n, where E_0 denotes the ground state energy. Let $\left|\phi^{(z)}\right\rangle$ be a family of normalized states, not necessarily eigenstates of H which depend on one parameter z. Show that

$$E_0 \leq \left\langle\phi^{(z)}\right| H \left|\phi^{(z)}\right\rangle .$$

Now consider an application to the Hamiltonian of the helium atom (neglecting the spins):

$$H = \frac{\mathbf{P}_1^2}{2m} + \frac{\mathbf{P}_2^2}{2m} - \frac{2e^2}{|\mathbf{X}_1|} - \frac{2e^2}{|\mathbf{X}_2|} + \frac{e^2}{|\mathbf{X}_1 - \mathbf{X}_2|}$$

The last term arises due to the Coulomb interaction between the two interactions. Make the ansatz

$$\left|\phi^{(z)}\right\rangle = \left|\phi_1^{(z)}\right\rangle \left|\phi_2^{(z)}\right\rangle$$

with two one-particle wavefunctions

$$\phi_i^{(z)}(\mathbf{x}_i) = A(z)\, e^{-z|\mathbf{x}_i|/a} \qquad (i = 1, 2).$$

Here $a = \hbar^2/me^2$ is the Bohr radius.

b) Determine the normalization constant $A(z)$.

c) Minimize the matrix element $\left\langle\phi^{(z)}\right| H \left|\phi^{(z)}\right\rangle$ with respect to z to obtain an estimate of the ground state energy.
(Result: $E_0 = -\frac{729}{256}\frac{me^4}{\hbar^2} = -77.5$ eV.)

Remark: The experimental value is $E_0 = -79.0$ eV. To first order in perturbation theory (considering the mutual interaction of the electrons as a perturbation) one obtains only $E_0 = -74.8$ eV.