PH 204: Quantum Mechanics II
Take Home examination
Exam starts on 29.03.2019 at 9AM. To be submitted by 30.03.2019 at 11AM in the Physics Auditorium. Total Marks: 140

(*If the answer sheets of any two persons appear to us to be similar, both persons will be penalized equally. The judgement for any two papers to be equal/equivalent is entirely the examiner's call, and no argument will be entertained on this.*)

1. Consider a system of N particles (either fermions or bosons) that obey:

$$\left[\left(-\frac{\hbar^2}{2m}\nabla_i^2-\frac{Ze^2}{r_i}\right)+\frac{e^2}{r_{ij}}\right]\psi(r_1,r_2,\cdots,r_N)=E\psi(r_1,r_2,\cdots,r_N)$$

The singlet particle eigenstates satisfy the eigenvalue equation:

$$\left[-\frac{\hbar^2}{2m}\nabla_i^2-\frac{Ze^2}{r_i}\right]\phi_i(r)=\varepsilon_i\phi_i(r).$$

The Hartree and Exchange terms are:

$$V_{H_{ij}}=\int drdr'\phi_i^*(r)\phi_j^*(r')\frac{1}{|r-r'|}\phi_i(r)\phi_j(r')$$

$$V_{E_{ij}}=-\int drdr'\phi_i^*(r)\phi_j^*(r')\frac{1}{|r-r'|}\phi_i(r')\phi_j(r)$$

Given a three level system with $\varepsilon_1<\varepsilon_2<\varepsilon_3$.

(a) (10 points) If two bosons are given at temperature $T=0$, express the total ground state energy in terms of ε_i, $V_{H_{ij}}$ and $V_{E_{ij}}$.

(b) (30 points) If we instead have two fermions, then find the two possible lowest energy states.

[Hint: You need to express the final resut in terms of $\varepsilon_{1,2,3}$, $V_{H_{11}}$, $V_{H_{12}}$, $V_{E_{11}}$, $V_{E_{12}}$ etc. as appropriate. If some terms do not arise or vanishes to zero, you need to explain the corresponding reasons.]

2. (50 points) Hund's rule:
Consider the following three possible states of two electrons placed in the $l=1$ states in some radial quantum number n of some atom.
(i) both electrons are in the $l=1,\ l_z=1$ state, with their spins forming a singlet,
(ii) one electron is in the $l=1,\ l_z=0$ and the other in the $l=1,\ l_z=1$ state in a symmetric combination, with their spins forming a singlet,
(iii) one electron is in the $l=1,\ l_z=0$ and the other in the $l=1,\ l_z=1$ state in an antisymmetric combination, with their spins forming a triplet.
These three states are degenerate if the Coulomb interaction between the electrons is ignored.

Assuming that the Coulomb interaction between the two electrons is described by the 'simplified' Hamiltonian $H_{int}=U\,\delta^3(\vec{r}_1-\vec{r}_2)$, compute the expectation value of H_{int} in terms of U in the three states described above. Which state has the lowest energy if $U>0$? (We do not need to know the explicit forms of the spatial wave functions to answer this question).

3. (30 points) Given a Hamiltonan of a two level system as

$$H=\begin{bmatrix}\beta_1 t & V\\ V & \beta_2 t\end{bmatrix},$$

where V, $\beta_{1,2}$ are constant in time (t). Show that the transition probabilities between the two levels (also known as hopping probability) is:

$$P=e^{-2\pi V^2/\hbar|\beta_1-\beta_2|}.$$

[A useful hint: The solution of the 2nd order ODE $\ddot{y}(t)+iA(t)\dot{y}(t)+By(t)=0$ is $|y(t\to\infty)|^2=1-e^{2\pi B/\dot{A}}$with the boundary condition $y(t\to-\infty)=0$.]

4. (20 points) Consider any operator A_s in the Schrödinger picture that transforms in the interaction picture as

$$A_I(t) = U_0^\dagger(t, t_0) A_S U_0(t, t_0),$$

where

$$U_0(t, t_0) = \exp[-\frac{i}{\hbar} H_0 (t - t_0)],$$

with

$$H = H_0 + V(t).$$

(H_0 being the time independent Hamiltonian.)

Find the two possible equations of motion for $A_I(t)$.