Advanced Quantum Mechanics - Problem Set 10

Winter Term 2022/23

Due Date: Hand in solutions to problems marked with * to mailbox 39 with label "Advanced Quantum Mechanics" inside ITP room 105b before the lecture on Friday, 06.01.2023, 09:15. The problem set will be discussed in the tutorials on Monday 09.01.2023 and Wednesday 11.01.2023.

*1. Quantisation of the Radiation Field

2+3+3 Points

In the absence of charges, and in the Coulomb gauge $\nabla \cdot \mathbf{A} = 0$, the electromagnetic field is described by the Lagrangian

$$L(t) = \frac{1}{2} \int_{\Omega} d^3x \left[\epsilon_0 \left(\partial_t \mathbf{A} \right)^2 + \frac{1}{\mu_0} \mathbf{A} \cdot \nabla^2 \mathbf{A} \right].$$

Here ϵ_0 denotes the vacuum dielectric constant, μ_0 is the vacuum permeability, and Ω is a cuboid with extensions L_x , L_y , and L_z . Note that the speed of light is $c = 1/\sqrt{\epsilon_0 \mu_0}$.

- (a) Write down the Lagrange equation for A.
- (b) Find eigenfunctions ${\pmb A}_{\pmb k}$ and eigenvalues $\omega_{\pmb k}^2$ of the equation

$$-\nabla^2 \boldsymbol{A}(\boldsymbol{x}) = \frac{\omega_{\boldsymbol{k}}^2}{c^2} \boldsymbol{A}(\boldsymbol{x}),$$

by using periodic boundary conditions. It may be useful to introduce, for each k, a set of orthonormal vectors $\{\hat{\boldsymbol{\xi}}_{k,1}, \hat{\boldsymbol{\xi}}_{k,2}\}$ which are both perpendicular to k. The time-dependent solution then has a series expansion

$$\mathbf{A}(\mathbf{x},t) = \frac{1}{\sqrt{\Omega}} \sum_{\mathbf{k},j} \alpha_{\mathbf{k},j}(t) e^{i\mathbf{k}\cdot\mathbf{x}} \hat{\boldsymbol{\xi}}_{\mathbf{k},j}.$$

Insert this series expansion in the Lagrangian, and find the momenta

$$\pi_{\mathbf{k},i} = \frac{\partial L}{\partial \dot{\alpha}_{\mathbf{k},i}},$$

canonically conjugate to the coordinates $\alpha_{k,i}$. Use the Legendre transform $H = \sum_{k,i} \pi_{k,i} \dot{\alpha}_{k,i} - L(\pi_{k,i}, \alpha_{k,i})$ to obtain the Hamiltonian.

Hint: The first equation can be obtained from the Euler-Lagrange equation in (a) by using that $\mathbf{A}(\mathbf{x},t) = \mathrm{e}^{-i\omega_{\mathbf{k}}t}\mathbf{A}(\mathbf{x})$. Here, assume that $\mathbf{A}(\mathbf{x})$ is real. Using this it can be shown that $\alpha_{-\mathbf{k},j} = \alpha_{\mathbf{k},j}^{\dagger}$.

(c) The classical Hamiltonian $H(\{\pi_{\mathbf{k},i},\alpha_{\mathbf{k},i}\})$ can be quantised by imposing canonical commutation relations

$$[\alpha_{\mathbf{k},i}, \alpha_{\mathbf{q},j}] = 0, \quad [\pi_{\mathbf{k},i}, \pi_{\mathbf{q},j}] = 0, \quad [\alpha_{\mathbf{k},i}, \pi_{\mathbf{q},j}] = i\hbar \delta_{\mathbf{k},\mathbf{q}} \delta_{i,j},$$

on the coordinates $\alpha_{k,i}$ and their canonically conjugate momenta $\pi_{k,j}$. In analogy to the one-dimensional harmonic oscillator, we define photon creation and annihilation operators

$$a_{\mathbf{k},j}^{\dagger} = \sqrt{\frac{\epsilon_0 \omega_{\mathbf{k}}}{2\hbar}} \left(\alpha_{-\mathbf{k},j} - \frac{i}{\epsilon_0 \omega_{\mathbf{k}}} \pi_{\mathbf{k},j} \right), \quad a_{\mathbf{k},j} = \sqrt{\frac{\epsilon_0 \omega_{\mathbf{k}}}{2\hbar}} \left(\alpha_{\mathbf{k},j} + \frac{i}{\epsilon_0 \omega_{\mathbf{k}}} \pi_{-\mathbf{k},j} \right).$$

Show that $a_{k,j}$ and $a_{k,j}^{\dagger}$ obey the commutation relations of harmonic oscillator ladder operators, and express the Hamiltonian in terms of $a_{k,j}$ and $a_{k,j}^{\dagger}$.

2. Coulomb and Exchange Integrals for Helium 6+3 Points

The energy of excited states in helium can be shown to be, to leading order in perturbation theory, given by

$$E_{nl,\pm} = -\frac{Z^2}{2} \left(1 + \frac{1}{n} \right) + J_{nl} \pm K_{nl},$$

where the Coulomb- and exchange integrals for helium are given by

$$J_{nl} = \frac{e^2}{4\pi\epsilon_0} \langle u_{100}(\mathbf{r_1}) u_{nlm}(\mathbf{r_2}) | \frac{1}{|\mathbf{r_1} - \mathbf{r_2}|} | u_{100}(\mathbf{r_1}) u_{nlm}(\mathbf{r_2}) \rangle,$$

and

$$K_{nl} = \frac{e^2}{4\pi\epsilon_0} \langle u_{100}(\mathbf{r_1}) u_{nlm}(\mathbf{r_2}) | \frac{1}{|\mathbf{r_1} - \mathbf{r_2}|} | u_{nlm}(\mathbf{r_1}) u_{100}(\mathbf{r_2}) \rangle,$$

respectively. Here u_{nlm} is the hydrogen wave-function with Z=2.

(a) Calculate the Coulomb and exchange integrals for n = 2, l = 0, 1.

Hint: Express $1/|\mathbf{r_1} - \mathbf{r_2}|$ as a sum over spherical harmonics and use orthogonality of these to perform the angular integrals.

(b) Make a sketch of the energy levels $E_{nl,\pm}$ of the terms ¹S, ³S, ¹P, and ³P.

Hint: Recall that the superscript denotes the spin and is given by 2S + 1 whilst the letter denotes the total orbital angular momentum $L = L_1 + L_2$ (L = 0 for S, L = 1 for P).