Advanced Quantum Mechanic – Winter Term 2017/18

Problem Sheet 01 – due on October 11th

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Problem 1.1

For the discussion of quantum mechanics of a charged particle in an electromagnetic field we will need the following results from electrodynamics.

The equation of motion of a charged particle (charge q, mass m) in an electromagnetic field is given by:

$$m\,\ddot{\vec{x}}(t) \;=\; q\,\vec{E}(\vec{x}(t),t) \;+\; \frac{q}{c}\,\dot{\vec{x}}(t)\;\times\;\vec{B}(\vec{x}(t),t)\;. \tag{1}$$

The $\vec{E}$- and $\vec{B}$-fields can be represented by a vector potential $\vec{A}(\vec{x},t)$ and a scalar potential $\phi(\vec{x},t)$:

$$\vec{E}(\vec{x},t) \;=\; -\frac{1}{c}\frac{\partial}{\partial t}\,\vec{A}(\vec{x},t) \;-\; \nabla\,\phi(\vec{x},t) \quad , \quad \vec{B}(\vec{x},t) \;=\; \nabla\;\times\;\vec{A}(\vec{x},t)\;. \tag{2}$$

Insert this in (1) and show that the equations of motion assume the form

$$\begin{aligned} m\,\ddot{x}_j(t) \;&=\; -\frac{q}{c}\,\dot{A}_j(\vec{x}(t),t) - q\,\frac{\partial\,\phi}{\partial x_j}(\vec{x}(t),t) \\ &\quad + \frac{q}{c}\sum_k \dot{x}_k(t)\left(\frac{\partial\,A_k}{\partial x_j}(\vec{x}(t),t) - \frac{\partial\,A_j}{\partial x_k}(\vec{x}(t),t)\right). \end{aligned} \tag{3}$$

Show that this equation of motion corresponds to the Lagrange function

$$L \;=\; \frac{m}{2}\,\dot{\vec{x}}(t)^{\,2} \;+\; q\,\left(\frac{1}{c}\dot{\vec{x}}(t)\cdot\vec{A}(\vec{x}(t),t) \;-\; \phi(\vec{x}(t),t)\right)\;, \tag{4}$$

by evaluating the Euler-Lagrange equations

$$\frac{d}{dt}\frac{\partial}{\partial \dot{x}_j}\,L \;-\; \frac{\partial}{\partial x_j}\,L \;=\; 0\;. \tag{5}$$

Finally perform the Legendre transformation to the Hamilton function,

$$H \;=\; \vec{p}\cdot\dot{\vec{x}} \;-\; L\;, \tag{6}$$

where the components of the generalized momentum are given by $p_j = \partial L/\partial \dot{x}_j$. Show that

$$H \;=\; \frac{1}{2m}\left(\vec{p}(t) \;-\; \frac{q}{c}\,\vec{A}(\vec{x}(t),t)\right)^2 \;+\; q\,\phi(\vec{x}(t),t)\;. \tag{7}$$

Problem 1.2

A short repetition of calculating with the Pauli matrices and some application to spin.

Remember/show the following identities of the Pauli matrices:

$$\mathrm{Tr}\,\sigma_j = 0 \ , \qquad \sigma_j^2 = \mathbb{1} \ , \qquad \sigma_j \cdot \sigma_k \ = \ i\,\epsilon_{jkl}\,\sigma_l \ \ (k \neq j) \ . \tag{8}$$

Denote by $\vec{\sigma}$ the vector of the three Pauli matrices, such that $\vec{a}\cdot\vec{\sigma}$ is the matrix $\sum_j a_j \sigma_j$. Using these identities show that

$$(\,\vec{a}\cdot\vec{\sigma}\,)^2 \ = \ \vec{a}^{\,2}\,\mathbb{1} \quad , \qquad (\,\vec{a}\cdot\vec{\sigma}\,)(\,\vec{b}\cdot\vec{\sigma}\,) \ = \ \vec{a}\cdot\vec{b}\,\mathbb{1} \ + \ i\,\vec{\sigma}\cdot(\vec{a}\times\vec{b}) \ . \tag{9}$$

Finally, let $\vec{n}$ be an arbitrary vector of length 1 and $\beta \in [0,\pi]$ and show

$$U(\beta,\vec{n}) \ \equiv \ e^{i\beta\,\vec{n}\cdot\vec{\sigma}} \ = \ \cos(\beta)\mathbb{1} + i\sin(\beta)\,\vec{n}\cdot\vec{\sigma} \ . \tag{10}$$

The identity can be obtained by expanding the exponential in a power series. Demonstrate that $U(\beta,\vec{n})$ is a unitary matrix with determinant 1, i.e., $U(\beta,\vec{n})$ is in the group SU(2) (special unitary 2×2 matrices).

The quantum mechanical spin operator is given by $\hat{\vec{S}} \ = \ \frac{\hbar}{2}\,\vec{\sigma}$. Consider a spinor given by

$$\psi(t) \ = \ \begin{pmatrix} A_+\,e^{-i\omega t} \\ A_-\,e^{+i\omega t} \end{pmatrix} \ \text{ with } \ A_+^2 \ + \ A_-^2 \ = \ 1 \ . \tag{11}$$

The quantum mechanical expectation value of an operator $\hat{O}$ is given by $\langle\hat{O}\rangle = \psi(t)^\dagger \hat{O}\,\psi(t)$. Compute

$$\langle\hat{\vec{S}}\,\rangle \ = \ \begin{pmatrix} \langle\hat{S}_x\rangle \\ \langle\hat{S}_y\rangle \\ \langle\hat{S}_z\rangle \end{pmatrix} \ . \tag{12}$$

Show that $\langle\hat{\vec{S}}\,\rangle^2 = \langle\hat{S}_x\rangle^2 + \langle\hat{S}_y\rangle^2 + \langle\hat{S}_z\rangle^2 \ = \ \hbar^2/4$ and compare this to $\langle(\hat{\vec{S}}\,)^2\rangle$.

Problem 1.3

Later in the course we will discuss Fock spaces, a useful type of Hilbert spaces for many particle problems. The Fock space construction makes use of creation and annihilation operators as you know them from the algebraic treatment of the harmonic oscillator. We here repeat some basic properties of the formalism.

The eigenstates $|n\rangle, n = 0, 1, 2\ldots$, are given by

$$|n\rangle \;=\; \frac{1}{\sqrt{n!}}\,(a^\dagger)^n\,|0\rangle \quad , \quad n \;=\; 0, 1, 2\ldots\,, \tag{13}$$

where $a^\dagger$ is the creation operator and $|0\rangle$ denotes the ground state (vacuum state) which is normalized, i.e., $\langle 0|0\rangle = 1$. Together with its adjoint operator a, the annihilation operator obeys the commutation operators

$$[\,a\,,\,a\,] \;=\; 0\,, \quad [\,a^\dagger\,,\,a^\dagger\,] \;=\; 0\,, \quad [\,a\,,\,a^\dagger\,] \;=\; 1\,. \tag{14}$$

The annihilation operator a annihilates the vacuum state, i.e., $a|0\rangle = 0$. Use these properties of a and $a^\dagger$ to show that the states $|n\rangle$ are orthonormal,

$$\langle n|m\rangle \;=\; \langle 0|\,\frac{1}{\sqrt{n!}}\,a^n\,\frac{1}{\sqrt{m!}}\,(a^\dagger)^m\,|0\rangle \;=\; \delta_{nm}\,. \tag{15}$$

The number operator $\hat{n}$ is defined as $\hat{n} = a^\dagger a$. Show that it obeys

$$\hat{n}\,|n\rangle \;=\; n\,|n\rangle\,, \tag{16}$$

which implies that the Hamilton operator $\hat{H} \;=\; \hbar\omega\left(\hat{n} + \frac{1}{2}\right)$ has the eigenstates $|n\rangle$:

$$\hat{H}\,|n\rangle \;=\; E_n\,|n\rangle \quad \text{with} \quad E_n = \hbar\omega\left(n + \frac{1}{2}\right)\,. \tag{17}$$

Problem 1.4

Use Rayleigh-Schrödinger perturbation theory (details see below) to compute the first and second order corrections to the energy for an infinitely deep potential well with a perturbation. The Hamilton operator $\widehat{H} = \widehat{H}^{(0)} + \lambda\widehat{H}^{(1)}$ for this 1-d problem is given by

$$\widehat{H}^{(0)} \;=\; -\frac{\hbar^2}{2m}\,\frac{d^2}{dx^2} \,+\, V^{(0)}(x) \quad , \quad \widehat{H}^{(1)} \;=\; V^{(1)}(x)\,, \tag{18}$$

where

$$V^{(0)}(x) = \begin{cases} 0 & \text{for } x \in (0, L) \\ \infty & \text{otherwise} \end{cases}, \; V^{(1)}(x) = \begin{cases} \sin(\pi x/L) & \text{for } x \in (0, L) \\ 0 & \text{otherwise} \end{cases}. \tag{19}$$

Equations for first and second order corrections to the energy (you should already know them):

$$E_n \;=\; E_n^{(0)} \,+\, \lambda\,E_n^{(1)} \,+\, \lambda^2\,E_n^{(2)} \,+\, \mathcal{O}(\lambda^3)\,, \tag{20}$$

$$E_n^{(1)} \;=\; \langle n^{(0)}|\widehat{H}^{(1)}|n^{(0)}\rangle \quad , \quad E_n^{(2)} \;=\; \sum_{m\neq n} \frac{|\langle m^{(0)}|\widehat{H}^{(1)}|n^{(0)}\rangle|^2}{E_n^{(0)} - E_m^{(0)}}\,, \tag{21}$$

$$\psi_n^{(0)}(x) \;=\; \sqrt{\frac{2}{L}}\,\sin(n\pi x/L) \quad , \quad E_n^{(0)} \;=\; \frac{\hbar^2\,\pi^2}{2m\,L^2}\,n^2\,, \tag{22}$$

Two useful integrals:

$$\int_0^\pi dy\, \sin(y)\, \sin(ny)^2 \;=\; \frac{4n^2}{4n^2-1}\,, \tag{23}$$

$$\int_0^\pi dy\, \sin(y)\, \sin(ny)\, \sin(my) \;=\; \frac{-2mn\,(1+(-1)^{m-n})}{1-2(m^2+n^2)+(m^2-n^2)^2}\,. \tag{24}$$