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Höhere Quantenmechanik

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Exercise sheet 11

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Exercise 1: Dirac equation in two spatial dimensions (graphene) *(6 Points)*

When one is in two spatial dimensions, it is possible to write down a Dirac equation with two-dimensional spinors. This is not possible in three space dimensions. A possible representation is given by

$$i\hbar\partial_t\psi = \left[c\left(p_x\sigma_x + p_y\sigma_y\right) + mc^2\sigma_z\right]\psi, \tag{1}$$

where $\psi = \psi(x, y, t)$ is the two-component wave function and σ_i are the Pauli matrices. Find the energy eigenfunctions and eigenvalues for massless particles obeying Eq. (1), by using the Ansatz of plane waves. Sketch the energy as a function of k_x, k_y. Comment the difference between the energy dispersion of massless ($m = 0$) and massive ($m \neq 0$) particles.

Physical context: Graphene is an allotrope of carbon consisting of a single layer of atoms arranged in a two-dimensional honeycomb lattice. Around certain reciprocal lattice vectors within its electronic band structure, the electron dispersion can effectively be described by the 2D Dirac equation (1) with $m = 0$ and $c = v \approx 10^6$m/s. The two components of the wave function are then not related to electron spin (which is to be described separately) but originate from the two atoms per unit cell in graphene. A finite effective mass $m > 0$ can arise, for example, when two graphene sheets are laid on top of each other.

Exercise 2: pionic atom (Klein-Gordon hydrogen atom) *(14 Points)*

We consider the Klein-Gordon equation in presence of a hydrogen-like central potential of the form $V(r) = -\frac{Ze^2}{r}$. This can describe a *pionic atom*, i.e. a negatively charged pion (π^-, charge: $-e$) in presence of the electrostatic potential of a nucleus with Z protons (total charge: Ze). The use of the Klein-Gordon equation is justified by the fact that pions are spinless. For simplicity, let us set $\hbar = 1$ and $c = 1$ throughout the exercise.

(i) Assume that $\psi(\vec{r}, t) = \varphi(\vec{r})e^{iEt}$. Show that the stationary equation for the problem (in spherical coordinates) is

$$\frac{1}{r}\partial_r^2(r\varphi(\vec{r})) + \left(-\frac{\vec{L}^2 - Z^2e^4}{r^2} + E^2 + 2E\frac{Ze^2}{r} - m^2\right)\varphi(\vec{r}) = 0$$

where $\vec{L}$ is the angular momentum operator. *(3 Points)*

(ii) Assume that $\varphi(\vec{r}) = \frac{R_{n,l}(r)}{r}Y_{l,m}(\theta, \phi)$, where $Y_{l,m}(\theta, \phi)$ are spherical harmonics. Find the equation for the radial part of the wave function and highlight the differences with respect to the case of the standard Schrödinger equation for the hydrogen atom. *(4 Points)*

Hint: you can map the radial Schrödinger equation to the radial Klein-Gordon equation by replacing $l(l+1)$, E and e^2 by certain suitable quantities. Find them out. It is helpful for the remainder of the exercise.

(iii) To find the energies of the bound states, we can exploit the analogy to the standard Schrödinger equation for the hydrogen atom, whose eigenvalues can be written as

$$E = E(n_r, l) = -\frac{m(Ze^2)^2}{2(n_r + l + 1)^2}$$

where $n_r = n - l - 1 \geq 0$ is the *radial quantum number* which counts the number of nodes in the radial part of the wave function[1]. Using the information gathered in the previous point (i.e., how to replace $l(l+1)$, E and e^2), modify the expression for $E(n_r, l)$ to obtain the energies of the Klein-Gordon equation for the hydrogen atom. *(4 Points)*

Hint: take the solution $E > 0$, such that $Z \to 0$ gives $E = m$ (particle at rest).

(iv) In the non-relativistic case, bound states are characterized by $E < V(\infty) = 0$ (for the Coulomb potential, which vanishes at infinite distance). What is the condition for the energy of a bound state in the relativistic case? *(1 Point)*

(v) Show that in the limit $Ze^2 \ll 1$ you recover the expected energies at the lowest orders (expand to second order in Ze^2). *(2 Points)*

[1] For this exercise, using n_r is more convenient than using n, because only the former is integer-valued in the Klein-Gordon case.