

PROJECT IN QUANTUM MECHANICS E2018

PROJECT NO.: 6

TITLE: SPIN AS A RELATIVISTIC CONSEQUENCE

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1 Introduction

Fundamental for quantum mechanics is the concept of particle-wave duality, expressed by the Einstein-de Broglie relations

$$\mathbf{p} = \hbar \mathbf{k} \quad \text{and} \quad E = \hbar \omega, \quad (1.1)$$

where \mathbf{p} and E denotes the momentum and energy of the particle respectively, and \mathbf{k} and ω denotes the wave vector and the frequency of the wave respectively. Implied from these relations is that the particle must be describable by a wave function, which we demand contains the complete information of a particle's state (of motion) at a given time t , hence the wave function must satisfy a differential equation in time, which is the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = \hat{H} \psi(\mathbf{r}, t), \quad (1.2)$$

where \hat{H} is the Hamiltonian. This, however, does not contain all the information we seek from a particle. We are missing a part of the puzzle: The spin of the particle. The complete description of a particle is postulated in [1, chapter 4.4] to be a combination of the spatial wave function, $\psi(\mathbf{r}, t)$, and a spinor, $\chi(\mathbf{s}, t)$,

$$\Psi = \psi(\mathbf{r}, t) \chi(\mathbf{s}, t). \quad (1.3)$$

In the following a more general equation, the Dirac Equation, will be deduced, wherefrom the spin can be found as an integrated part of the particle's state.

2 The Schrödinger equation

Considering a non-relativistic particle with mass m and momentum \mathbf{p} in a potential V , the total energy can be found as

$$E = T + V = \frac{\mathbf{p}^2}{2m} + V. \quad (2.1)$$

Using the operator representations of the energy and momentum,

$$E \rightarrow i\hbar \frac{\partial}{\partial t}, \quad \mathbf{p} \rightarrow \frac{\hbar}{i} \nabla, \quad (2.2)$$

in equation (2.1) and letting it operate on the wave function of a particle, the equation becomes

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = -\frac{\hbar^2}{2m} \nabla^2 \Psi(\mathbf{r}, t) + V \Psi(\mathbf{r}, t), \quad (2.3)$$

which is the Schrödinger equation, hence the Schrödinger equation originate from the non-relativistic equation of momentum, but this changes when in the relativistic realm, hence the energy also changes, and a relativistic Schrödinger-like equation is therefore needed to describe relativistic particles.

Considering now the same particle, but free from any potential, i.e. $V = 0$, the solution is a generalisation to three dimensions of that found in [1, eq. 2.94],

$$\Psi(\mathbf{r}, t) = A \exp \left(i \left[\mathbf{k} \cdot \mathbf{r} - \frac{\hbar \mathbf{k}^2}{2m} t \right] \right) = A \exp \left(\frac{i}{\hbar} [\mathbf{p} \cdot \mathbf{r} - Et] \right), \quad (2.4)$$

using the Einstein-de Broglie relations, equation (1.1), and the total energy of the particle is equal to kinetic energy of it due to the lack of potential.

Wanting to construct a relativistic Schrödinger-like equation one may first consider the structure of the Schrödinger equation itself. The Schrödinger equation a differential equation of first order with respect to time and of second order with respect to position, but in special relativity, equations must be covariant, due to Einstein's principle of relativity - the laws of physics are the same in all frames of

reference - hence time and space are treated equally. It is therefore reasonable to assume a relativistic Schrödinger-like equation to be a differential equation of either first or second order with respect to both time and position.

3 The Klein-Gordon Equation

The approach is to find a Schrödinger-like equation by replacing the non-relativistic energy with that of a relativistic particle, but otherwise do as normal. Considering a free particle with momentum with momentum $p = |\mathbf{p}|$ and invariant mass m_0 , the relativistic energy is [2, eq. 12.34]

$$E = \sqrt{(\mathbf{p}c)^2 + (m_0c^2)^2}. \quad (3.1)$$

A Hamiltonian with the above eigenenergy when applied to a momentum-eigenstate $|\mathbf{p}\rangle$ with eigenvalue \mathbf{p} must be found, [3, chap. 8.1], but the square root turns out to be a problem in the early efforts to derive a relativistic equation, since the way of dealing with the square root is via a Taylor expansion,

$$H = \sqrt{\mathbf{p}^2c^2 + m_0^2c^4} = m_0c^2 \left(1 + \frac{\mathbf{p}^2}{m_0^2c^2}\right)^{\frac{1}{2}} = m_0c^2 + \frac{\mathbf{p}^2}{2m_0} - \frac{\mathbf{p}^4}{8m_0^3} + \frac{\mathbf{p}^6}{16m_0^5} + \dots \quad (3.2)$$

This, though, yields a non-covariant wave equation, since the time derivative from equation (1.2) will be associated with different order spacial derivatives, which is not desirable.

3.1 Derivation of the Klein-Gordon Equation

To avoid these problems first attempts to find a relativistic wave equation used the square of the Hamiltonian, hence the square of the energy, instead of the Hamiltonian, and the energy, itself,

$$E^2 = (\mathbf{p}c)^2 + (m_0c^2)^2. \quad (3.3)$$

Using the operator representations of E and \mathbf{p} from equation (2.2), and letting it operate on the wave function of a particle equation (3.3) becomes

$$-\hbar^2 \frac{\partial^2}{\partial t^2} \Psi(\mathbf{r}, t) = -\hbar^2 c^2 \nabla^2 \Psi(\mathbf{r}, t) + m_0^2 c^4 \Psi(\mathbf{r}, t), \quad (3.4)$$

which is known as the Klein-Gordon equation.

3.2 Properties of the Klein-Gordon equation

The Klein-Gordon equation satisfies nearly all of the desirable qualities of a relativistic wave equation. Firstly it is covariant which a relativistic equation shall be, as stated in chapter 2.

Solutions that we would expect. Conservation of probability. But then the problems are encountered. Probability not positive definite.

REMEMBER TO WRITE SOMETHING LIKE THIS, BUT NOT JUST THIS SINCE IT'S DIRECTLY FROM SAKURAI: There will be solutions to the wave equation with negative energies; these solutions are necessary to form a complete set of basis states, but they have no obvious physical meaning.

4 The Dirac Equation

Most of the difficulties of the Klein-Gordon equation originate from it being a second order differential equation with respect to time. To avoid these issues Dirac tried to, and in 1928 succeeded in, finding a first order differential equation with respect to both time and space. This equation should satisfy the time-evolution equation of quantum mechanics, equation (1.2), and the Dirac Hamiltonian, \hat{H}_D , since

considering a free particle, would only depend on the fundamental constants c and \hbar , the mass of the particle m and the first order derivative with respect to the particle's coordinates, hence the Dirac equation is

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = \hat{H}_D \Psi(\mathbf{r}, t), \quad \hat{H}_D = c\boldsymbol{\alpha} \cdot \mathbf{p} + m_0 c^2 \beta, \quad (4.1)$$

where $\boldsymbol{\alpha}$ and β must be dimensionless coefficients since $c\mathbf{p}$ (som vektor(?)) and $m_0 c^2$ have the dimensions of energy. Also they must be independent of p_i to ensure a linear dependence of the spacial derivative, the momentum, and they must not depend on the coordinates, since this would introduce a force, which shall not be present for a free particle. These independences implies commutation between the momentum and the coefficients.

To gain further information about the coefficients, solutions to the Dirac equation is required to also satisfy the Klein-Gordon equation to secure correct relation between energy and momentum, hence the Dirac Hamiltonian squared must equal the Klein-Gordon Hamiltonian, since the Klein-Gordon equation yields $E^2 \Psi = \hat{H}_{KG} \Psi$ and the Dirac equation $E \Psi = \hat{H}_D \Psi$.

$$c^2 \mathbf{p}^2 + m_0^2 c^4 = (c\boldsymbol{\alpha} \cdot \mathbf{p} + m_0 c^2 \beta)^2 = c^2 (\boldsymbol{\alpha} \cdot \mathbf{p})^2 + m_0^2 c^4 \beta^2 + m_0 c^3 \{(\boldsymbol{\alpha} \cdot \mathbf{p}), \beta\}, \quad (4.2)$$

where $\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$ is the anticommutator. From equation (4.2) it can be seen that $c^2 (\boldsymbol{\alpha} \cdot \mathbf{p})^2$ must yield $c^2 \mathbf{p}^2$ since it is the only term of second order in momentum and in light speed, $m_0^2 c^4 \beta^2$ must yield $m_0^2 c^4$ since it is the only term of second order in mass and fourth order in light speed, hence $m_0 c^3 \{(\boldsymbol{\alpha} \cdot \mathbf{p}), \beta\} = 0$ since the Klein-Gordon equation does not contain momentum and mass of first order or light speed of third order. Firstly it can be seen, that β^2 must be the identity since $m_0 c^4 = m_0 c^4 \beta^2$. Secondly, writing the zero-term it can be seen that

$$0 = \{(\boldsymbol{\alpha} \cdot \mathbf{p}), \beta\} = \left\{ \sum_{i=1}^3 \alpha_i p_i, \beta \right\} = \sum_{i=1}^3 \alpha_i p_i \beta + \beta \alpha_i p_i = \sum_{i=1}^3 (\alpha_i \beta + \beta \alpha_i) p_i, \quad (4.3)$$

hence $\{\alpha_i, \beta\} = 0$ since equation (4.3) must be valid for an arbitrary p_i . Lastly

$$\mathbf{p}^2 = (\boldsymbol{\alpha} \cdot \mathbf{p})^2 = \sum_{i=1}^3 \alpha_i p_i \sum_{j=1}^3 \alpha_j p_j = \sum_{i=1}^3 \sum_{j=1}^3 p_i p_j \alpha_i \alpha_j = \begin{cases} \sum_{i=1}^3 \sum_{j=i}^3 p_i^2 \alpha_i^2 \\ \sum_{i=1}^3 \sum_{j \neq i}^3 p_i p_j \{\alpha_i \alpha_j\} \end{cases}, \quad (4.4)$$

so $\alpha_i^2 = 1$, and for every choice of i and j where $j \neq i$, there will be two terms, with equal p_i and p_j combination, because there is a sum over both indices, and since \mathbf{p}^2 only consist of quadratic terms of p_i , then

$$0 = p_i p_j \alpha_i \alpha_j + p_j p_i \alpha_j \alpha_i = p_i p_j \{\alpha_i \alpha_j\}, \quad (4.5)$$

hence $\{\alpha_i, \alpha_j\} = 2\delta_{ij}$. For Ψ to satisfy both the Dirac equation and the Klein-Gordon equation we find that $\boldsymbol{\alpha}$ and β must satisfy

$$\{\alpha_i, \alpha_j\} = 2\delta_{ij}, \quad \{\alpha_i, \beta\} = 0, \quad \text{and} \quad \beta^2 = 1, \quad (4.6)$$

which defines the Clifford algebra. (SOMETHING MORE HERE(?))

Another demand of the Dirac equation is that the Dirac Hamiltonian shall be hermitian since the energy is an observable. If \hat{H}_D is hermitian

$$\begin{aligned} c(\boldsymbol{\alpha} \cdot \mathbf{p}) + \beta m_0 c^2 &= \hat{H}_D = \hat{H}_D^\dagger = c(\boldsymbol{\alpha} \cdot \mathbf{p})^\dagger + m_0 c^2 \beta^\dagger \\ \Rightarrow c(\boldsymbol{\alpha} - \boldsymbol{\alpha}^\dagger) \cdot \mathbf{p} &= m_0 c^2 (\beta^\dagger - \beta), \end{aligned} \quad (4.7)$$

since \mathbf{p} is an observable, $\mathbf{p} = \mathbf{p}^\dagger$. By the principle of relativity choosing the frame of reference for the particle, where $\mathbf{p} = \mathbf{0}$, to calculate β is valid (OMFORMULERING???)

$$0 = m_0 c^2 (\beta^\dagger - \beta) \Rightarrow \beta = \beta^\dagger, \quad (4.8)$$

and using this to calculate α for an arbitrary \mathbf{p} yields

$$0 = c(\alpha - \alpha^\dagger) \cdot \mathbf{p} \Rightarrow \alpha = \alpha^\dagger, \quad (4.9)$$

hence both α and β shall be hermitian for \hat{H}_D to be hermitian.

It turns out also to be important for the coefficients to be traceless, [4], with trace being the sum of the diagonal elements of a matrix, and these requirements along with linearly independence narrows the possible options to a few, that in the Dirac-Pauli representation are:

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \quad \text{and} \quad \beta = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}, \quad (4.10)$$

with I_2 being the identity matrix and σ_i being the hermitian Pauli spin matrices [3, eq. 3.2.32]

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \text{and} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (4.11)$$

Per identities from [3, p. 169] it can be realised, that α and β satisfy the above stated requirements.

The Dirac equation is a relativistic equation, hence it must obey the principle of relativity. This mean(s)(?) that it must be covariant for it to preserve the invariant space-time interval. SHOW COVARIANCE(?) SHOW POSITIVE PROBABILITY DENSITY(?)

4.1 Existence of the spin

For the Dirac equation to also be a Schrödinger-like equation, it must have the same properties as the Schrödinger equation, one of them being the conservation of angular momentum $\hat{\mathbf{L}}$. This can be shown using Ehrenfests theorem, stating that the time-dependence of an operator \hat{Q} can be found as

$$\frac{d}{dt}\langle Q \rangle = \langle [\hat{H}, \hat{Q}] \rangle + \left\langle \frac{\partial \hat{Q}}{\partial t} \right\rangle. \quad (4.12)$$

Since time is explicit present in neither the Schrödinger Hamiltonian nor the Dirac Hamiltonian, the angular momentum is conserved if $\hat{\mathbf{L}}$ and \hat{H} commutes. For the Dirac Hamiltonian the commutator is calculated componentwise using the property of linearity alongside $[\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}$, the canonical commutator and the commutation of α and β with both \mathbf{r} and \mathbf{p} . This becomes

$$\begin{aligned} [\hat{L}_j, \hat{H}_D] &= \left[(\mathbf{r} \times \mathbf{p})_j, c\alpha \cdot \mathbf{p} + \beta m_0 c^2 \right] = i\hbar (\alpha_k p_l - \alpha_l p_k) = i\hbar (\alpha \times \mathbf{p})_j \\ \Rightarrow [\hat{\mathbf{L}}, \hat{H}_D] &= i\hbar \alpha \times \mathbf{p} = i\hbar \epsilon_{jkl} \mathbf{j} \alpha_k p_l, \end{aligned} \quad (4.13)$$

where \mathbf{j} denotes the direction vector, and ϵ_{jkl} is the Levi-Civita symbol, which is 1 if the indices are a cyclic permutation, xyz , yzx or zxy , -1 if they are an anticyclic permutation, i.e. zyx , yxz or xzy , and zero if two or more indices are equal. Equation (4.13) is not zero, hence the Dirac equation do not conserve the angular momentum. To compensate the spin operator and spin matrix

$$\hat{\mathbf{S}} = \frac{\hbar}{2} \boldsymbol{\sigma}', \quad \boldsymbol{\sigma}' = \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix}, \quad (4.14)$$

is introduced, where $\boldsymbol{\sigma} = \sum_{j=1}^3 \sigma_j \mathbf{j}$, with \mathbf{j} as the direction vector, denotes the pauli vector. Computing the commutator of $\hat{\mathbf{S}}$ and \hat{H}_D as for $\hat{\mathbf{L}}$ yields

$$!!! \text{LIGNINGER HER} !!! \quad (4.15)$$

....

Considering now the sum of the angular momentum and the spin operator $\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}}$, and calculating the commutator between this $\hat{\mathbf{J}}$ and the Dirac Hamiltonian

$$[\hat{\mathbf{J}}, \hat{H}_D] = [\hat{\mathbf{L}} + \hat{\mathbf{S}}, \hat{H}_D] = [\hat{\mathbf{L}}, \hat{H}_D] + [\hat{\mathbf{S}}, \hat{H}_D] = 0, \quad (4.16)$$

hence the angular momentum $\hat{\mathbf{L}}$ along with the spin operator describe the particle's state. For $\hat{\mathbf{J}}$ to be the total angular momentum $\hat{\mathbf{S}}$ must be verified as an angular momentum by obey [1, eq. 4.99, 4.118].

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Thus $\hat{\mathbf{S}}$ is an angular momentum, more precisely the intrinsic or rotational angular momentum, more commonly known as spin, while $\hat{\mathbf{L}}$ is the orbital angular momentum, thus a non-moving particle can still an angular momentum, the spin.

4.2 Solutions to the Dirac equation for a free particle

Assuming the structure of the solution to the free particle for the Dirac equation to resemble that of the Schrödinger equation, equation (2.4), we make the following ansatz for the solutions of the Dirac equation:

$$\Psi(\mathbf{r}, t) = u(\mathbf{p}) \exp\left(\frac{i}{\hbar} [\mathbf{p} \cdot \mathbf{r} - Et]\right), \quad (4.17)$$

where $u(\mathbf{p})$ is a four column vector, since Ψ is required to be a four-component spinor since the Dirac Hamiltonian is represented as a quadratic matrix of dimension four, and the exponential function represent the expected plane wave. Inserting the ansatz in the Dirac equation, 4.1, yields the eigenvalue equation

$$Eu(\mathbf{p}) = (c\boldsymbol{\alpha} \cdot \mathbf{p} + m_0 c^2 \beta) u(\mathbf{p}) = \begin{pmatrix} mc^2 I_2 & c\boldsymbol{\sigma} \cdot \mathbf{p} \\ c\boldsymbol{\sigma} \cdot \mathbf{p} & -mc^2 I_2 \end{pmatrix} u(\mathbf{p}) = Mu(\mathbf{p}), \quad (4.18)$$

for which the eigenvalue can be found as

$$\begin{aligned} 0 = \det(M - EI_4) &= \det \begin{pmatrix} mc^2 I_2 - EI_2 & c\boldsymbol{\sigma} \cdot \mathbf{p} \\ c\boldsymbol{\sigma} \cdot \mathbf{p} & -mc^2 I_2 - EI_2 \end{pmatrix} = -m^2 c^4 I_2^2 + E^2 I_2 - c^2 \mathbf{p}^2 I_2 \\ &\Rightarrow E^2 = c^2 \mathbf{p}^2 + m^2 c^4 \quad \Rightarrow \quad E^2 = \pm \sqrt{(c\mathbf{p})^2 + (mc^2)^2}, \end{aligned} \quad (4.19)$$

since

$$\boldsymbol{\sigma} \cdot \mathbf{p} = \begin{pmatrix} p_z & p_x - ip_y \\ p_x + ip_y & -p_z \end{pmatrix} \Rightarrow (\boldsymbol{\sigma} \cdot \mathbf{p})^2 = \mathbf{p}^2 I_2. \quad (4.20)$$

Equation (4.19) yields exactly the relativistic connection between the energy and the momentum from equation (3.1), but here there are two possible signs, both positive and negative. Examining the solutions for the different energies (SKRIV EN BRO HER(?))

5 Prediction of antimatter

5.1 The Dirac Sea

A first attempt to explain the negative energy quantum states found predicted in the Dirac equation was the Dirac sea postulated by Dirac in 1930. The model makes use of the Pauli exclusion principle - that two ore more identical fermions can not occupy the same quantum state - to interpret the vacuum as an infinite sea of negatively charged particles, so that all negative-energy states are filled, but none of the positive-energy states.[5] Introducing an electron the only available state for it to be placed is a positive-energy state, and should this electron emit photons and thereby lose energy, it is forbidden to drop to negative energy, hence ... (!!!something with that it then is how we would expect it to be!!!(?)).

Occasionally a negative-energy particle could be supplied(?) with a sufficient amount of energy to be lifted out of the Dirac sea and become a particle of positive energy. This electron would leave behind a hole in the sea, that would act exactly like the positive-energy electron but with opposite charge. The process is known as pair production, where an subatomic particle and its antiparticle, here the electron and the hole, is created form a neutral boson, here a photon. These holes were by Dirac wrongly identified as protons, [6, p. 363], and predicted the annihilation of these particles when the positive-energy electron drops into the hole and fills it up.

Dirac's wrongly interpretation increased confusion about the negative-energy interpretation of the Dirac equation and caused some difficulties(?). One of these problems, the annihilation, was addressed in 1930 by Oppenheimer, who showed that Dirac's proton and the electron would annihilate within 10^{-10} s, which implied the life time of a hydrogen atom to be 10^{-10} s, (but this was not consistent with earlier experimental results(?)). The other problem, the difference in mass of the proton and the electron, was addressed by Herman Weyl using the symmetry of charges in the Maxwell and Dirac equations, which showed the mass of Dirac's proton, the hole in the Dirac sea, to be equal to the mass of the electron.[7, sec. 8] This lead Dirac to (??? reform / rethink ???) his theory and in his paper [8, p. 61] Dirac acknowledges the hole as being an anti-electron, which is now known as a positron.

SOMETHING ABOUT THE EXPERIMENTAL DISCOVERY???(?)[9]

5.2 Modern interpretation of the Dirac equation

Litteratur

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