Lecture # 13

Relativistic quantum mechanics and Dirac equation.

The problem: in special relativity, the Nature is invariant under Lorentz transformations,

$$x \to x' = \gamma\left(x - \frac{v}{c}(ct)\right); \quad ct \to ct' = \gamma\left(ct - \frac{v}{c}x\right)$$

$$\gamma = \left(1 - v^2/c^2\right)^{-1}$$

The quantum mechanics we considered so far this is not the case,

$$-\frac{\hbar}{i}\frac{\partial\psi}{\partial t} = H\psi$$

1st derivative in time

second derivative in space

How to generalize QM to get it consistent with special (and general) relativity?

Consistent treatment: relativistic quantum field theory (special relativity, see lectures of Prof. Rattazzi). For GR the problem is open.

We will follow here the historical line, to see how heuristic (and not necessarily correct) arguments may lead to discoveries.

<u>1st failed attempt</u>

Energy of the relativistic particle:

$$E = \sqrt{m^2c^4 + p^2c^2} \qquad (*)$$

Let us use the general rules of quantum mechanics and replace

$$p \to \hat{p} = -i\hbar \frac{\partial}{\partial \vec{x}} \Rightarrow$$

Proposal for relativistic Hamiltonian is

$$\hat{H} = \sqrt{m^2c^4 + \hat{p}^2c^2},$$ and for

Schrödinger equation:

$$-\frac{\hbar}{i}\frac{\partial \psi}{\partial t} = \sqrt{m^2c^4 - \hbar^2c^2\vec{\nabla}^2}\,\Psi$$

If we go this way, we get a problem with locality: time evolution of wave function at point x depends on the wave function far away from x:

$$\sqrt{m^2c^4-\hbar^2c^2\bar{\nabla}^2}\,\psi(x)=\int dx'\,F(x,x')\,\psi(x'),$$

with $F(x,x')\sim\int d^3p\, e^{ip(\bar{x}-\bar{x}')}\sqrt{p^2+m^2}$.

This does not look to be consistent with special relativity, as the speed of signal propagation must be finite.

(Will use from now on the system of units with $\hbar=c=1$).

<u>2nd failed attempt</u>

Why not to change Schrödinger equation?

Square of (*): $E^2=m^2+\bar{p}^2$; $\Longrightarrow$

$$\left(-\frac{1}{i}\frac{\partial}{\partial t}\right)^2\psi=(m^2-\nabla^2)\,\psi \qquad (**)$$

This is certainly Lorentz-invariant equation,

$$-\Box\psi = m^2\psi \; ; \quad \Box = \frac{\partial^2}{\partial t^2} - \vec{\nabla}^2$$

However, we are in trouble because of 2 reasons:

1. time evolution of the states with definite momentum:

$$\psi \sim \exp[i\varepsilon t], \quad \varepsilon = \pm\sqrt{p^2+m^2}$$

So, we get particles with negative energy?

2. In QM, probability to have a particle somewhere is conserved,

$$\frac{d}{dt}\int \psi^*\psi \, d^3x = 0, \quad \text{and} \quad \psi^*\psi > 0.$$

This comes from <u>first order</u> character of time evolution:

$$\frac{d}{dt}\int \psi^*\psi \, d^3x = \int (\dot{\psi}^*\psi + \psi^*\dot{\psi})\, d^3x$$

$$= \int d^3x \left[(i\hat{H}\psi)^* \psi - \psi^* (i\hat{H}\psi) \right] = 0,$$

as H is hermitean.

Since (**) is a second order equation,

$$\frac{d}{dt} \int \psi^* \psi \, d^3x \neq 0.$$

Way out: maybe, probability is not $\psi^* \psi$ anymore?

A proposal for conserved quantity:

$$\rho(x) = \frac{i}{2m} \left(\psi^* \frac{\partial}{\partial t} \psi - \psi \frac{\partial}{\partial t} \psi^* \right)$$

This is real, and

$$\frac{d}{dt} \int d^3x \, \rho(x) = 0$$

However, $\rho(x)$ is not positive in general.

Nothing works: second order differential equation in time: negative or not-conserved probabilities, negative energies.

First order derivatives – non-local evolution.

Dirac proposal, 1928

Let us try to construct H which is linear in momenta and keep Schrödinger equation as it is in non-relativistic QM:

$$H = \alpha_i p_i + \beta m \qquad (***)$$

We want to have H linear in p since we want to have space and time to enter on equal footing.

Can we get a relativistic relation between energy and momentum from $(***)$?

"Obviously" not

$$(\alpha_i p_i + \beta m)(\alpha_j p_j + \beta m) = \qquad \text{(square)}$$

$$= \alpha_i \alpha_j p_i p_j + m(\beta \alpha_i + \alpha_i \beta) \cdot p_i + \beta^2 m^2$$

It looks like this can never be $m^2 + \vec{p}^{\,2}$.

However, this is only true if α and β are "simple" numbers. Suppose that α_i and β are in fact matrices.

If they satisfy the relations

$$\{\alpha_i, \alpha_j\}_+ = 2\delta_{ij}$$

$$\{\alpha_i, \beta\}_+ = 0$$

$\beta^2 = 1$, then square gives us

what we want:

$$\alpha_i \alpha_j p_i p_j = \frac{1}{2}\{\alpha_i, \alpha_j\}_+ p_i p_j = \bar{p}^2 ;$$

$$\beta\alpha_i + \alpha_i\beta = 0 ;$$

Extra requirement: H must be Hermitean:

$$\alpha_i^+ = \alpha_i ; \quad \beta^+ = \beta$$

What kind of matrices we should have?

Let us find their dimension.

Important properties of α_i and β:

$$Tr\, \alpha_i = Tr\, \beta = 0$$

Indeed,

$$Tr\, \alpha_i = Tr\, \alpha_i \beta^2 = Tr[\beta\alpha_i\beta] = -Tr[\alpha_i\beta^2]$$
$$= -Tr\, \alpha_i ;$$

$$Tr\beta = Tr\beta\alpha_1^2 = Tr[\alpha_1\beta\alpha_1] = -Tr[\beta\alpha_1^2] =$$
$$-Tr\beta$$

Since $\alpha_i^2 = 1$ and $\beta^2 = 1$, the eigenvalues of α and β are ± 1. Since $Tr\,\alpha_i = Tr\,\beta = 0$, it means that we must have $n \times n$ matrices with n even.

2×2: $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ after diagonalisation

4×4: $\begin{pmatrix} 1 & & & \\ & 1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix}$ — " —

Let us take first 2×2 case. There are 4 basis matrices, σ_i (Pauli) and $\mathbb{1}$, with help of which we can construct any 2×2 matrix.

However, it is impossible to satisfy $Tr\,\alpha_i = 0$, $Tr\,\beta = 0$, as we have only 3 trace-less basis matrices, σ_i.

Next step: 4×4. The choice is:

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \; ; \; \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

unit 2×2 matrix

So, Dirac Hamiltonian is 4×4 matrix

$$H_D = \alpha_i p + \beta m \; ; \; -\frac{1}{i}\frac{\partial \psi_D}{\partial t} = H_D \psi_D .$$

Dirac wave function has 4 components, since H_D is 4×4 matrix.

So, it must describe something with 4 internal degrees of freedom. We will argue that $4 = 2+2$: 2: spin, another 2: – antiparticle (So, we have electron with 2 spin states and positron with 2 spin states.)

Other general property: if we define probability as

$\rho(x) = \Psi^{+}\Psi$, then it is positive and conserved. Positive - obvious, conserved - comes from the fact that H is Hermitean

Let us study the eigenvalues and eigenvectors of H:

$$H_D\Psi = \varepsilon\Psi.$$

Take Fourier harmonics: $\Psi \sim e^{ikx/\hbar} \Rightarrow$

$$H_D = mc^2\beta + \alpha_i k_i c =$$

$$= \begin{pmatrix} mc^2 & \vec{\sigma}\vec{k}c \\ \vec{\sigma}\vec{k}c & -mc^2 \end{pmatrix}$$

Take, for simplicity, $k \parallel z \Rightarrow$

$$\mathcal{H}_D = \begin{pmatrix} mc^2 & 0 & kc & 0 \\ 0 & mc^2 & 0 & -kc \\ kc & 0 & -mc^2 & 0 \\ 0 & -kc & 0 & -mc^2 \end{pmatrix}$$

This can be viewed as 2 separated 2×2 matrices:

$$\mathcal{H}_1 = \begin{pmatrix} mc^2 & kc \\ kc & -mc^2 \end{pmatrix} \quad \text{and} \quad \mathcal{H}_2 = \begin{pmatrix} mc^2 & -kc \\ -kc & -mc^2 \end{pmatrix}$$

Their eigenvalues are found from

$$(mc^2 - \varepsilon_1)(-mc^2 - \varepsilon) - (kc)^2 = 0$$

$$(mc^2 - \varepsilon_2)(-mc^2 - \varepsilon) - (kc)^2 = 0$$

and equal to

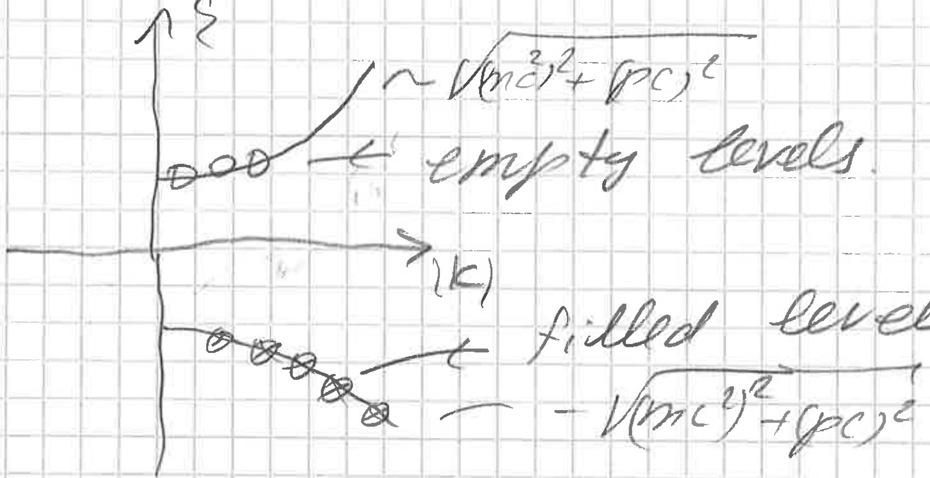
$$-(mc^2)^2 + \varepsilon_{1,2}^2 - (kc)^2 = 0 \Rightarrow$$

$$\varepsilon_{1,2} = \pm \sqrt{(kc)^2 + (mc^2)^2}$$

The problem of negative energy states is still there!

Dirac solution of this problem:

- suppose that the particles which D. equation describes are fermions. (electron at this time)
- The system „wants" to have smallest energy, and thus „wants" to have particles on all negative energy levels:



- So, ground state of the system is the state where all negative energy levels are occupied. It is stable due to Pauli exclusion principle.
- Then we have two types of excitations:
  - occupied positive energy level
  - unoccupied negative energy level will have <u>positive energy</u> and opposite electric charge in comparison with occupied state:

energy of a hole corresponding to some $\vec{k}$:

$$\underbrace{\left(-\varepsilon_{k_1}-\varepsilon_{k_2}-\ldots-\varepsilon_{k_N}\right)}_{\substack{\text{no } \varepsilon_k, \\ \text{state with a "hole"}}} - \underbrace{\left(-\varepsilon_1-\varepsilon_2-\ldots-\varepsilon_k-\varepsilon_{k_N}\right)}_{\substack{\text{state - vacuum,} \\ \text{without a hole}}} =$$

$$= +\varepsilon_k$$

Electric charge, the same story.

Prediction: there must be antiparticle with positive energy, but opposite electric charge. Prediction has been confirmed - Nobel to Dirac in 1933.

(In fact, there are some flows in the arguments: one can construct a relativistic equation for fermions just with 2 components - "Majorana" fermions. Also, "negative" energies appear in bosonic case as well, and this can not be cured in Pauli-Dirac way.

Let us now show that Dirac equation goes to Pauli equation in non-relativistic limit.

– Step # I – inclusion of electromagnetic field: – as usual, replace

$$p^\mu \to p^\mu - \frac{e}{c} A^\mu, \text{ where } A^\mu \text{ is}$$

the vector – potential.

in more detail: A_0 is the scalar potential, $A_0 \equiv \Phi$

$$-\frac{\hbar}{i}\frac{\partial}{\partial t} \to -\frac{\hbar}{i}\frac{\partial}{\partial t} - e\Phi$$

$$-i\hbar\frac{\partial}{\partial x} \to -i\hbar\frac{\partial}{\partial x} - \frac{e}{c}\vec{A} \quad \text{, leading to}$$

$$-\frac{\hbar}{i}\frac{\partial \Psi}{\partial t} = \left[\left(c\vec{\alpha}\,\overbrace{\left(\vec{p} - \frac{e}{c}\vec{A}\right)}^{\vec{\pi}}\right) + \beta mc^2 + e\Phi\right]\Psi \quad (*)$$

For hydrogen atom: $\varepsilon_{min} = \sqrt{1-(\alpha Z)^2}\,m - m$ $\left[\alpha = \frac{e^2}{\hbar c}\right.$

Remark: this equation can be used to determine energy levels of electron in Coulomb field accounting for relativistic corrections

: put $\vec{A} = 0$, $\Phi = 1/r$

Let us try to solve (*), assuming that $mc^2 \gg (pc)$ (non-relativistic approximation and weak fields:

$e\varphi \ll mc^2$; $|e\vec{A}| \ll mc^2$

write $\psi = \begin{pmatrix} \tilde{\varphi} \\ \tilde{\chi} \end{pmatrix}$ } 2-component „spinors"

Dirac eq:

$$-\frac{\hbar}{i}\frac{\partial}{\partial t}\begin{pmatrix} \tilde{\varphi} \\ \tilde{\chi} \end{pmatrix} = c\vec{\sigma}\vec{\pi}\begin{pmatrix} \tilde{\chi} \\ \tilde{\varphi} \end{pmatrix} + e\Phi\begin{pmatrix} \tilde{\varphi} \\ \tilde{\chi} \end{pmatrix} + mc^2\begin{pmatrix} \tilde{\varphi} \\ -\tilde{\chi} \end{pmatrix}$$

Search solution in the form:

$$\begin{pmatrix} \tilde{\varphi} \\ \tilde{\chi} \end{pmatrix} = \exp\left[-\frac{imc^2}{\hbar}t\right]\begin{pmatrix} \varphi \\ \chi \end{pmatrix},$$ to

remove the biggest part $\sim mc^2$:

$$(***) \quad -\frac{\hbar}{i}\frac{\partial}{\partial t}\begin{pmatrix} \varphi \\ \chi \end{pmatrix} = c\vec{\sigma}\vec{\pi}\begin{pmatrix} \chi \\ \varphi \end{pmatrix} + e\Phi\begin{pmatrix} \varphi \\ \chi \end{pmatrix} - 2mc^2\begin{pmatrix} 0 \\ \chi \end{pmatrix}$$

In components:

$$-\frac{\hbar}{i}\frac{\partial\varphi}{\partial t} = c\vec{\sigma}\vec{\pi}\chi + e\Phi\cdot\varphi$$

$$-\frac{\hbar}{i}\frac{\partial\chi}{\partial t} = c\vec{\sigma}\vec{\pi}\varphi + e\Phi\cdot\chi - 2mc^2\chi$$

Let us analyse second equation.

Since $e\Phi << 2mc^2$ [weak fields – valid in the atom: potential energy of electron in the atom ~ binding energy ~ 13 eV << $mc^2 = 5\cdot 10^5$ eV] we can drop the term $e\Phi\chi$.

Rewrite second equation as

$$\chi = \frac{c\vec{\sigma}\vec{\pi}\cdot\varphi}{2mc^2} + \frac{\hbar}{i}\frac{1}{2mc^2}\frac{\partial\chi}{\partial t}$$

and solve it by itterations, assuming that term with $\dot{\chi}$ is small:

$$\chi_0 \approx \frac{c\vec{\sigma}\vec{\pi}}{2mc^2}\varphi \qquad \text{(zero approximation)}$$

$$\chi_1 \approx \frac{c\vec{\sigma}\vec{\pi}\varphi}{2mc^2} + \underbrace{\frac{\hbar}{i}\frac{1}{2mc^2}\frac{\partial}{\partial t}\left[\frac{c\vec{\sigma}\vec{\pi}}{2mc^2}\cdot\varphi\right]}_{}$$

suppressed in comparison with the firs term by extra mc^2!

So, we will keep the first term only.

χ_0 is << than φ. χ is called „small" component, and φ is called „large" component.

insert this solution to equation for the first line in (**):

$$-\frac{\hbar}{i}\frac{\partial}{\partial t}\varphi = c\vec{\sigma}\vec{\pi}\cdot\underbrace{\chi}_{\frac{\vec{\sigma}\vec{\pi}\varphi}{2mc}} + e\phi\cdot\varphi =$$

$$= \left(\frac{\vec{\sigma}\vec{\pi}\;\vec{\sigma}\cdot\vec{\pi}}{2m} + e\phi\right)\varphi$$

Transform the first part:

$$(\vec{\sigma}\cdot\vec{a})(\vec{\sigma}\cdot\vec{b}) = \vec{a}\cdot\vec{b} + i\vec{\sigma}\,\vec{a}\wedge\vec{b}$$

for our case:

$$(\vec{\sigma}\vec{\pi})(\vec{\sigma}\vec{\pi}) = \vec{\pi}^2 + i\sigma\,\underbrace{\vec{\pi}\wedge\vec{\pi}} = \vec{\pi}^2 - \frac{e\hbar}{c}\vec{\sigma}\cdot\vec{B}$$

not zero, as $\vec{p}$ does not commute with $\vec{A}$

At last,

$$-\frac{\hbar}{i}\frac{\partial\varphi}{\partial t} = \left[\frac{(\vec{p}-\frac{e}{c}\vec{A})^2}{2m} - \frac{e\hbar}{2mc}\vec{\sigma}\vec{B} + e\phi\right]\varphi -$$

exactly Pauli equation.