Chapter 5

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Dirac equation

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Introduction

The non-relativistic case : the Pauli equation

- Preliminary remark on Pauli matrices :

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

  if $\vec{O}_1$ and $\vec{O}_2$ are operators commuting with the Pauli matrices then

$$\left(\vec{\sigma}.\vec{O}_1\right)\left(\vec{\sigma}.\vec{O}_2\right) = \vec{O}_1.\vec{O}_2 + i\vec{\sigma}.\left(\vec{O}_1 \times \vec{O}_2\right)$$

- Applying the previous relation to $\vec{P}$ leads to :

$$\left(\vec{\sigma}.\vec{P}\right)\left(\vec{\sigma}.\vec{P}\right) = \left(\vec{\sigma}.\vec{P}\right)^2 = \vec{P}^2 \Rightarrow H = \frac{\left(\vec{\sigma}.\vec{P}\right)^2}{2m}$$

Introduction

- Reminder (Pauli matrices properties) :

  - $\{\sigma_i, \sigma_j\} = 2\delta_{ij} \quad [\sigma_i, \sigma_j] = 2i\varepsilon_{ijk}\sigma_k$

  - $\sigma_i\sigma_j = \delta_{ij} + i\varepsilon_{ijk}\sigma_k$

  - $(\vec{\sigma}.\vec{O}_1)(\vec{\sigma}.\vec{O}_2) = \vec{O}_1.\vec{O}_2 + i\vec{\sigma}.(\vec{O}_1 \times \vec{O}_2)$

  - For $\vec{u}$ unit vector $\frac{1}{2}(1 \pm \vec{\sigma}.\vec{u})\chi$ eigenfunction of $\vec{\sigma}.\vec{u}$ with eigenvalue $\pm 1 \ \forall \chi$.

  - $\exp\left(-i\dfrac{\theta}{2}\sigma_k\right) = \cos\left(\dfrac{\theta}{2}\right) - i\sigma_k\sin\left(\dfrac{\theta}{2}\right)$

1- The non-relativistic case

- To describe the particle's motion in an E.M. field the covariant derivative prescription leads to :

$$p^\mu \to p^\mu + eA^\mu \text{ i.e. } \begin{cases} i\hbar\partial_t \to i\hbar\partial_t + eA^0 \\ \vec{p} \to \vec{p} + e\vec{A} \end{cases}$$

- The Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t}(\vec{x},t) = \frac{\vec{P}^2}{2m}\psi(\vec{x},t)$$

can be rewritten as

$$i\hbar\frac{\partial\psi}{\partial t}(\vec{x},t) + eA^0\psi(\vec{x},t) = \frac{\left(\vec{\sigma}.\left(\vec{P}+e\vec{A}\right)\right)^2}{2m}\psi(\vec{x},t)$$

1- The non-relativistic case

- Using the Pauli matrices relation :

$$\left(\vec{\sigma}.\left(\vec{P}+e\vec{A}\right)\right)^2 \psi = \left(\vec{P}+e\vec{A}\right)^2 \psi + i\vec{\sigma}.\left(\left(\vec{P}+e\vec{A}\right)\times\left(\vec{P}+e\vec{A}\right)\right)\psi$$

- The last term reads :

$$\left(\left(\vec{P}+e\vec{A}\right)\times\left(\vec{P}+e\vec{A}\right)\right)_i \psi = e\left(\vec{P}\times\vec{A}+\vec{A}\times\vec{P}\right)_i \psi$$

$$= e\,\varepsilon_{ijk}\left(\vec{P}_j\vec{A}_k + \vec{A}_j\vec{P}_k\right)\psi$$

$$\Rightarrow -e\,i\hbar\varepsilon_{ijk}\left(\vec{\partial}_j\vec{A}_k + \vec{A}_j\vec{\partial}_k\right)\psi$$

- Developing the last term :

$$-e\,i\hbar\varepsilon_{ijk}\left(\vec{\partial}_j\vec{A}_k + \vec{A}_j\vec{\partial}_k\right)\psi =$$

$$-e\,i\hbar\varepsilon_{ijk}\left(\vec{\partial}_j\left(\vec{A}_k\psi\right) + \vec{A}_j\left(\vec{\partial}_k\psi\right)\right) =$$

$$-e\,i\hbar\varepsilon_{ijk}\left((\vec{\partial}_j\vec{A}_k)\psi + \underbrace{\vec{A}_k\left(\vec{\partial}_j\psi\right) + \vec{A}_j\left(\vec{\partial}_k\psi\right)}_{=0}\right) =$$

$$-e\,i\hbar\varepsilon_{ijk}(\vec{\partial}_j\vec{A}_k)\psi =$$

$$-e\,i\hbar\left(\vec{\nabla}\times\vec{A}\right)_i\psi =$$

$$e\,i\hbar\vec{B}_i\psi$$

1- The non-relativistic case

- Finally the Pauli equation reads

$$i\hbar \frac{\partial \psi}{\partial t}(\vec{x},t) = \frac{\left(\vec{P}+e\vec{A}\right)^2}{2m}\psi(\vec{x},t) - \frac{e\hbar}{2m}\left(\vec{\sigma}.\vec{B}\right)\psi(\vec{x},t) - eA^0\psi(\vec{x},t)$$

   where the wavefunction is a 2D object.

- The action of the spin operator is explicit.

- N.B. developing $\vec{P}+e\vec{A}$ leads to $\vec{L}.\vec{B}$. One gets the complete equation through the substitution $\vec{L} \rightarrow \vec{L}+2\vec{S}$ with $\vec{S} = \frac{\hbar}{2}\vec{\sigma}$

2- The Dirac equation

- Generalization to the relativistic case : the starting point is always

$$E^2 = \vec{p}^2 c^2 + m^2 c^4$$

which is the only covariant form for the canonical quantization :

$$\left[\left(i\hbar \partial_t \right)^2 - \left(\vec{\sigma}.\vec{P} \right)^2 \right] \psi(\vec{x},t) = m^2 \psi(\vec{x},t)$$

$$\left[i\hbar \partial_t + i\hbar \vec{\sigma}.\vec{\nabla} \right]\left[i\hbar \partial_t - i\hbar \vec{\sigma}.\vec{\nabla} \right] \psi = m^2 \psi$$

- Let's take auxiliary variables :

$$\psi^{(1)} = \psi$$

$$\psi^{(2)} = \frac{1}{m}\left[i\hbar \partial_t - i\hbar \vec{\sigma}.\vec{\nabla} \right] \psi$$

2- The Dirac equation

- The following system

$$\begin{cases} \left[i\hbar\partial_t - i\hbar\vec{\sigma}.\vec{\nabla} \right]\psi^{(1)} = m\psi^{(2)} \\ \left[i\hbar\partial_t + i\hbar\vec{\sigma}.\vec{\nabla} \right]\psi^{(2)} = m\psi^{(1)} \end{cases}$$

is equivalent to

$$\begin{cases} i\hbar\partial_t\varphi + i\hbar\vec{\sigma}.\vec{\nabla}\chi = m\varphi \\ -i\hbar\partial_t\chi - i\hbar\vec{\sigma}.\vec{\nabla}\varphi = m\chi \end{cases} \quad \text{with} \quad \begin{cases} \varphi = \psi^{(2)} + \psi^{(1)} \\ \chi = \psi^{(2)} - \psi^{(1)} \end{cases}$$

- In a matrix form this equation reads :

$$\begin{pmatrix} i\hbar\partial_t & i\hbar\vec{\sigma}.\vec{\nabla} \\ -i\hbar\vec{\sigma}.\vec{\nabla} & -i\hbar\partial_t \end{pmatrix}\begin{pmatrix} \varphi \\ \chi \end{pmatrix} = m\begin{pmatrix} \varphi \\ \chi \end{pmatrix}$$

$$\Leftrightarrow \begin{pmatrix} i\hbar\partial_t & i\hbar\vec{\sigma}.\vec{\nabla} \\ -i\hbar\vec{\sigma}.\vec{\nabla} & -i\hbar\partial_t \end{pmatrix}\psi_{4D} = m\psi_{4D}$$

with $\quad \psi_{4D} \equiv \begin{pmatrix} \varphi \\ \chi \end{pmatrix} = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}$

2- The Dirac equation

- Gamma matrices definition :

$$\gamma^0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \gamma_0 \text{ and } \vec{\gamma}^i = \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix} = -\vec{\gamma}_i$$

- Basic properties :

$$\left\{ \gamma^\mu, \gamma^\nu \right\} = \gamma^\mu \gamma^\nu + \gamma^\nu \gamma^\mu = 2g^{\mu\nu}$$

$$\left(\gamma^0 \right)^2 = 1 \text{ and } \left(\gamma^i \right)^2 = -1$$

$$\gamma^{\mu\dagger} = \gamma^0 \gamma^\mu \gamma^0$$

- "Slash" notation : $\not{a} = a_\mu \gamma^\mu$

2- The Dirac equation

- The previous matrix equation writes :

$$\begin{pmatrix} i\hbar\partial_t & i\hbar\vec{\sigma}.\vec{\nabla} \\ -i\hbar\vec{\sigma}.\vec{\nabla} & -i\hbar\partial_t \end{pmatrix}\begin{pmatrix} \varphi \\ \chi \end{pmatrix} = m\begin{pmatrix} \varphi \\ \chi \end{pmatrix} \Leftrightarrow i\hbar\left(\gamma^0\partial_0 + \gamma^i\partial_i\right)\psi = m\psi$$

$$\left(i\hbar\gamma^\mu\partial_\mu - m\right)\psi = 0 \qquad \textbf{Dirac Equation}$$

- In details :

$$\sum_{\mu=0,1,2,3}\sum_{b=1,2,3,4}\left(i\hbar\left(\gamma^\mu\right)_{ab}\partial_\mu - m\delta_{ab}\right)\psi_b = 0$$

3- Adjoint representation

- Let's start from the "conjugate" equation :

$$\left(i\hbar \gamma^\mu \partial_\mu - m \right)\psi = 0 \Rightarrow \psi^\dagger \left(i\hbar \gamma^{\mu\dagger}\overleftarrow{\partial}_\mu + m \right) = 0$$

- Using the gamma matrices property : $\gamma^{\mu\dagger} = \gamma^0 \gamma^\mu \gamma^0$ one gets

$$\psi^\dagger \left(i\hbar \gamma^0 \gamma^\mu \gamma^0 \overleftarrow{\partial}_\mu + m\gamma^0 \gamma^0 \right) = 0$$

$$\psi^\dagger \gamma^0 \left(i\hbar \gamma^\mu \gamma^0 \overleftarrow{\partial}_\mu + m\gamma^0 \right) = 0 \quad \leftarrow (\times \gamma^0)$$

$$\overline{\psi}\left(i\hbar \gamma^\mu \overleftarrow{\partial}_\mu + m \right) = 0 \text{ where } \boxed{\overline{\psi} = \psi^\dagger \gamma^0}$$

3- Adjoint representation

- One defines the adjoint spinor $\quad \bar{\psi} = \psi^{\dagger}\gamma^0$

- The conjugate equations read therefore :

$$\left(i\hbar\gamma^{\mu}\partial_{\mu} - m\right)\psi = 0$$

and

$$\bar{\psi}\left(i\hbar\gamma^{\mu}\overleftarrow{\partial}_{\mu} + m\right) = 0$$

- Reminder : spinless case (K.G.)

$$\partial^{\mu}\partial_{\mu}\psi + m^2\psi = 0$$

and

$$\partial^{\mu}\partial_{\mu}\psi^{*} + m^2\psi^{*} = 0$$

4- Quadri-current

- Formal derivation possibilities :
    - directly from the fundamental and adjoint representations or
    - from the Lagrangian expression ⊕ gauge invariance (looking for the current coupling to the gauge field)

- Question : is the Born probabilistic interpretation possible in the Dirac case (i.e. is the charge density positive to be interpreted as a probability density?).

- Reminder : not the case in the spinless case where negative energy solutions and negative charge density should have been re-interpretated.

$$\psi(x) = N e^{i(\vec{p}.\vec{x} - Et)/\hbar} \Rightarrow \rho = 2|N|^2 \times \underbrace{E}_{>0 \text{ or } 0<}$$

4- Quadri-current

Direct derivation :

$$\left. \begin{array}{l} \left(i\hbar\gamma^{\mu}\partial_{\mu} - m\right)\psi = 0 \\[2mm] \overline{\psi}\left(i\hbar\gamma^{\mu}\overleftarrow{\partial}_{\mu} + m\right) = 0 \end{array} \right\} \oplus$$

$$\overline{\psi}\gamma^{\mu}\left(\overleftarrow{\partial}_{\mu} + \partial_{\mu}\right)\psi = 0 \Leftrightarrow \partial_{\mu}\left(\overline{\psi}\gamma^{\mu}\psi\right) = 0$$

- Conserved current : $\boxed{J^{\mu} \equiv c\left(\overline{\psi}\gamma^{\mu}\psi\right)}$

- Conserved charge density : $\rho \equiv J^{0}\big/c = \overline{\psi}\gamma^{0}\psi = \psi^{\dagger}\underbrace{\gamma^{0}\gamma^{0}}_{=1}\psi$

$$\Rightarrow \rho = \psi^{\dagger}\psi = \sum_{a=1,2,3,4}\psi_{a}^{*}\psi_{a} > 0$$

4- Quadri-current

Derivation from gauge invariance :

- Lagrangian of free particles : $\boxed{\mathcal{L}_{free} = \bar{\psi}\left(i\gamma^{\mu}\partial_{\mu} - m\right)\psi}$

- *U(1)* invariance ➔ use of covariant derivatives :

$$\mathcal{L}_{int.} = \bar{\psi}\left(i\gamma^{\mu}D_{\mu} - m\right)\psi$$

$$= \bar{\psi}\left(i\gamma^{\mu}\left(\partial_{\mu} + ieA_{\mu}\right) - m\right)\psi$$

$$= \bar{\psi}\left(i\gamma^{\mu}\partial_{\mu} - m\right)\psi - e\underbrace{\bar{\psi}\gamma^{\mu}\psi}_{\propto J^{\mu}}A_{\mu}$$

where the interaction term appears on the form $\boxed{-J_{\mu}A^{\mu}}$ as for spinless particles.

5- Dirac spinors

Free particle solutions.

- By analogy with the non-relativistic case we may write a general spin-½ wavefunction in terms of factorized solutions :

$$\psi = u \times \left(\text{plane wave}\right)$$

$$= u \times \exp(-ip^{\mu}x_{\mu}) = u \times \exp(-ipx)$$

$$= u(p)e^{\left[i(\vec{p}.\vec{x}-Et)\right]}$$

where u is a 4-components spinor.

- The explicit expression of the spinor is more easily deduced from the Hamiltonian formalism of the Dirac equation...

5- Dirac spinors

- The solution to the Dirac equation may be written as :

$$u = N_p \begin{pmatrix} u_A \\ \dfrac{\vec{\sigma}.\vec{p}}{E+m} u_A \end{pmatrix}$$

where u_A is a 2D spinors $\quad u_A = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ or $u_A = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

- The E - p relation reads :

$$\left(\vec{\sigma}.\vec{p}\right)\left(\vec{\sigma}.\vec{p}\right)u_A = \vec{p}^{\,2}u_A = (E-m)(E+m)u_A \Rightarrow \boxed{E = \pm E_p}$$

5- Dirac spinors

Summary.

- Positive-energy solutions :

$$\psi^{(+)(s=1,2)}(x) \equiv u^{(s=1,2)}(p)\, e^{[-ipx]} \qquad u^{(s)}(p) \propto \begin{pmatrix} \varphi^{(s)} \\ \dfrac{\vec{\sigma}.\vec{p}}{E+m}\varphi^{(s)} \end{pmatrix}$$

- Negative-energy solutions :

$$\psi^{(-)(s=1,2)}(x) \equiv v^{(s=1,2)}(p)\, e^{[+ipx]} \qquad v^{(s)}(p) \propto \begin{pmatrix} \dfrac{\vec{\sigma}.\vec{p}}{E+m}\chi^{(s)} \\ \chi^{(s)} \end{pmatrix}$$

with the spin-up/down 2D spinors $\varphi, \chi^{(s=1)} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\varphi, \chi^{(s=2)} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

- Warning on spin direction : negative-energy solution with spin-$\uparrow$ = positive-energy solution with spin-$\downarrow$

5- Dirac spinors

- Dirac equation in p-space :

$$\left(\gamma^\mu p_\mu - m\right)u(p) = 0$$

$$\left(\gamma^\mu p_\mu + m\right)v(p) = 0$$

- Adjoint spinors (same procedure as in x-space) :

$$\overline{u}(p)\left(\gamma^\mu p_\mu - m\right) = 0$$

$$\overline{v}(p)\left(\gamma^\mu p_\mu + m\right) = 0$$

- Ortho-normalization relations :

$$\overline{u}^{(s)}(p)u^{(s')}(p) = \delta_{ss'} \qquad \overline{v}^{(s)}(p)v^{(s')}(p) = -\delta_{ss'}$$

$$\overline{u}^{(s)}(p)v^{(s')}(p) = 0 \qquad \overline{v}^{(s)}(p)u^{(s')}(p) = 0$$

5- Dirac spinors

Some useful relations :

$$\sum_{s=1,2} u^{(s)}(p)\overline{u}^{(s)}(p) = \left(\not{p} + m \right)$$

$$\sum_{s=1,2} v^{(s)}(p)\overline{v}^{(s)}(p) = \left(\not{p} - m \right)$$

- 'Energy' projectors :

$$\Lambda_+ = \frac{\left(\not{p} + m \right)}{2m} \text{ such as } \Lambda_+ u = u \text{ and } \Lambda_+ v = 0$$

$$\Lambda_- = \frac{\left(-\not{p} + m \right)}{2m} \text{ such as } \Lambda_- v = v \text{ and } \Lambda_- u = 0$$

$$\Lambda_\pm^2 = \Lambda_\pm \text{ and } \Lambda_+ + \Lambda_- = 1$$

6- Feynman's prescription

Summary.

- Klein-Gordon equation ➔ {
  negative probabilities

  negative energies
}

- Dirac equation ➔ {
  positive (only) probabilities

  negative energies
}

- Dirac's historical interpretation : the 'vacuum' state consists of all negative-energy states filled with electrons. The Pauli principle forbids any positive-energy electron from falling into these lower energy states.

6- Feynman's prescription

- The 'vacuum' (so-called Dirac sea)
  has now infinite negative charge
  and energy but all observations repre-
  sent finite fluctuations w.r.t. the
  vacuum.
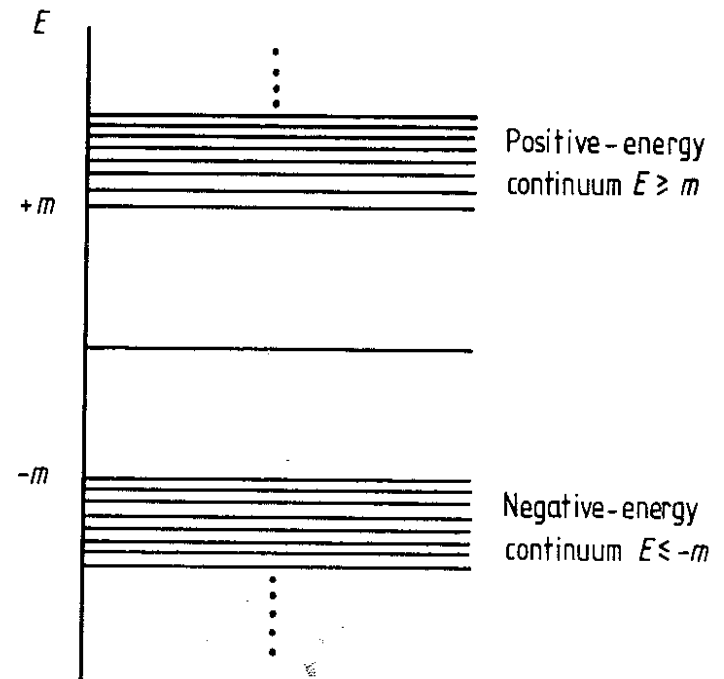
- A 'hole' in the Dirac sea, i.e. the absence of a negative-energy
  electron is equivalent to the presence of a positive-energy
  positively charged version of the electron, namely a positron.

$$\text{energy of 'hole'} = -\left(E_{neg}\right) \rightarrow \text{positive energy}$$

$$\text{charge of 'hole'} = -\left(q_e\right) \rightarrow \text{positive charge}$$

6- Feynman's prescription

- What about solutions to the Klein-Gordon equation (bosons not affected by Pauli principle)?

- Interpretation through Feynman's prescription (1962) :

  negative-energy particle solutions propagating backward in time =

  positive-energy antiparticle solutions propagating forward in time

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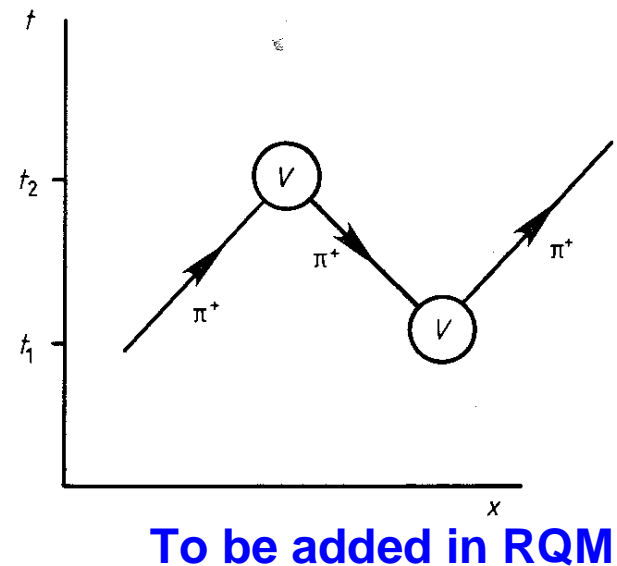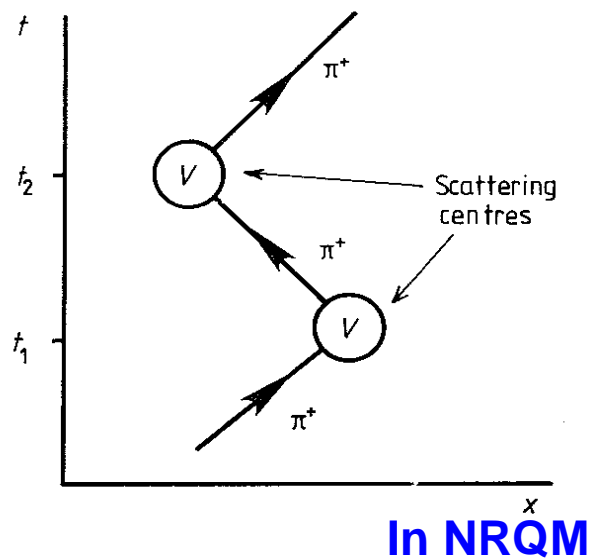
- Consequence of the Feynman prescription :
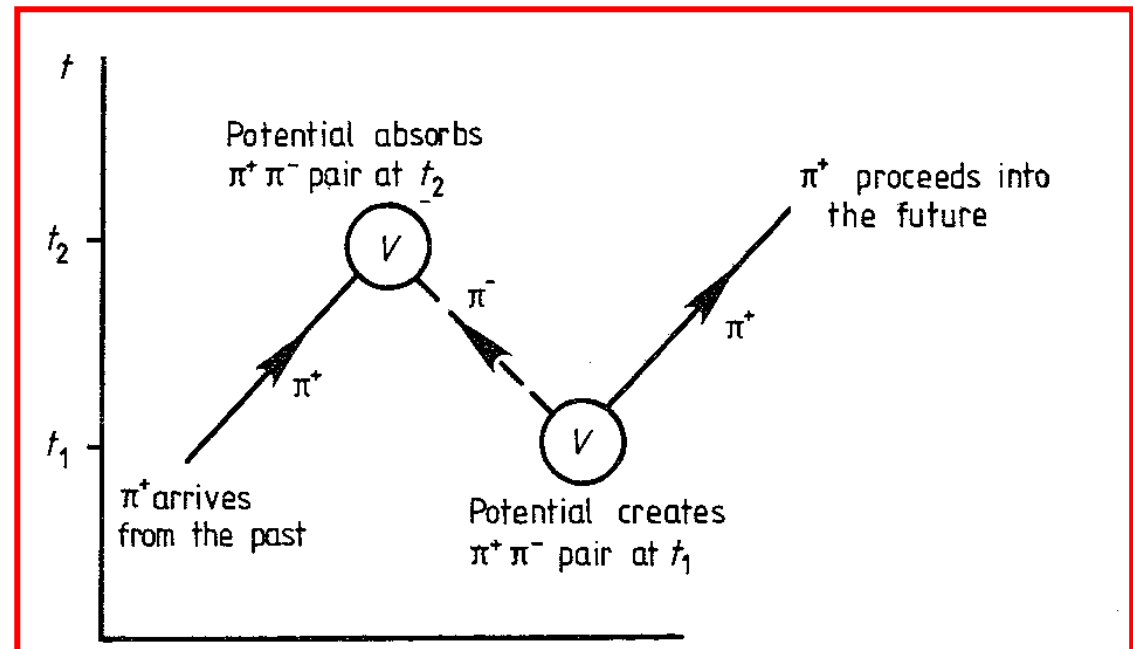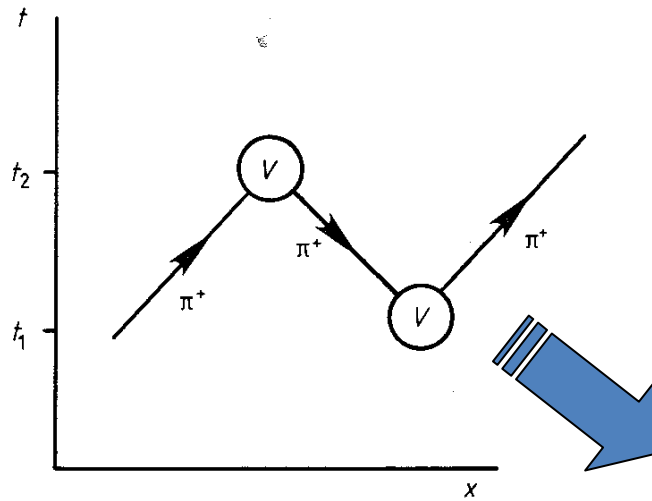
Summary

- Relativistic propagation equations derived from energy definition law => Klein-Gordon (bosons) and Dirac (fermions)

- Gauge invariance imposed to the theory => existence of conserved currents coupled to gauge fields (e.g. photons for EM)

- From classical to quantum field theory : fields => operators

- Lagrangian formalism widely used.