Chapter 5 : Klein-Gordon Equation

→ Relativistic quantum mechanics for massive spinless particles

→ We will see that the concept of single-particle wave functions and the concept of conserved norm of a wave function leads to paradoxies.

These problems are related to :
- * particles can be created and annihilated if kinematically allowed (mass is just one form of energy)
- * existence of antiparticles

The rules of non-relativistic quantum mechanics for a fixed number of particles are only a special case of a more general formulation for restricted kinematic situation that are characteristic for non-relativistic problems.

From a general perspective : We are eventually forced to generalize the quantum theory for massive particles to a theory that resembles the quantum theory for photons.

↳ "Relativistic Quantum Field Theory"

5.1. Klein-Gordon Equation

→ Aim: Relativistic "Schrödinger equation" for a free spin-less (scalar) particle with mass m (e.g. Higgs boson, π^0 particle)

↳ Use relativistic on-shell relation and the correspondence principle

$$p^\mu = \begin{pmatrix} E \\ \vec{p} \end{pmatrix} \longleftrightarrow \begin{pmatrix} i\frac{\partial}{\partial t} \\ -i\frac{\partial}{\partial \vec{x}} \end{pmatrix} = i\frac{\partial}{\partial x_\mu} = i\partial^\mu$$

First try: $E = \sqrt{\vec{p}^2 + m^2}$

$$\Rightarrow i\frac{\partial}{\partial t}\psi(t,\vec{x}) = (m^2 - \vec{\nabla}^2)^{1/2}\psi(t,\vec{x}) \iff \left(i\partial_t - \left(m^2 - \frac{\partial^2}{\partial \vec{x}^2}\right)^{1/2}\right)\psi(t,\vec{x}) = 0$$

Problems :
- * $\sqrt{\ }$ -operator mathematically problematic
- * not manifest Lorentz-covariant formulation

$\Big\}\rightarrow$ Failure !

Second try: $E^2 = \vec{p}^2 + m^2$

$$\Rightarrow (i\partial_t)^2\psi(x) = (m^2 - \vec{\nabla}^2)\psi(x)$$

D'Alambert operator : $\Box = \partial_t^2 - \vec{\nabla}^2$

$$\Leftrightarrow \quad \boxed{(\partial_\mu \partial^\mu + m^2)\,\psi(x) = (\Box + m^2)\,\psi(x) = 0}$$

"Klein-Gordon equation"

$\rightsquigarrow$ * obviously Lorentz-covariant

* Obvious physical/mathematical issue:
  KG equation depends on 2nd derivative w.r. to time
  $\hookrightarrow$ To obtain a solution one needs two initial conditions : $\psi(t=x_0)$ and $\dot{\psi}(t=x_0)$

  $\rightsquigarrow$ Signal of a deeper problem related to the existence of particle and antiparticle degrees of freedom.

5.2. Charged Particle and e.m. Interaction

$\longrightarrow$ Let's assume the particle has electric charge q.
We elevate our knowledge from non-relativistic quantum mechanics concerning the coupling of a massive particle to the e.m. field to the relativistic case:

"kovariant derivative"

$$\vec{p} \rightarrow \vec{p} - q\vec{A} \quad \Rightarrow \quad p^\mu \rightarrow p^\mu - q A^\mu \;, \quad \partial^\mu \rightarrow D^\mu \equiv \partial^\mu + iqA^\mu \qquad (p^\mu = i\partial^\mu)$$

$\rightsquigarrow$ KG equation of a scalar particle with mass m and el. charge q in an e.m. field :

$$\boxed{(D^\mu D_\mu + m^2)\,\psi(x) = 0}$$

$$D_\mu D^\mu = (\partial_\mu + iqA_\mu)(\partial^\mu + iqA^\mu) = \partial_\mu\partial^\mu + iq\,\partial_\mu A^\mu + iq\,A_\mu\partial^\mu - q^2 A_\mu A^\mu$$

$\longrightarrow$ Gauge invariance: The KG equation in the presence of an electromagnetic field is gauge invariant under the transformations:

$$\boxed{\begin{aligned} A^\mu(x) &\longrightarrow A^\mu(x) - \partial^\mu\Lambda(x) \\ \psi(x) &\longrightarrow e^{iq\Lambda(x)}\,\psi(x) \end{aligned}}$$

∂^μ acts only on $\Lambda(x)$!

$\leftarrow$ Obvious: ψ is a complex field !

act on everything on the right

$$D^\mu\psi(x) \longrightarrow (\partial^\mu + iqA^\mu - iq\partial^\mu\Lambda)\,e^{iq\Lambda}\,\psi(x) = e^{iq\Lambda}\,(\partial^\mu + \cancel{iq\partial^\mu\Lambda} + iqA^\mu - \cancel{iq\partial^\mu\Lambda})\,\psi(x) = e^{iq\Lambda}\,D^\mu\psi(x)$$

$$D_\mu D^\mu\psi(x) \longrightarrow e^{iq\Lambda}\,D_\mu D^\mu\psi(x)$$

$$\longrightarrow \quad 0 = (D_\mu D^\mu + m^2)\,\psi(x) \longrightarrow e^{iq\Lambda}\,(D_\mu D^\mu + m^2)\,\psi(x) = 0 \quad \checkmark$$

$\longrightarrow$ Conserved current: The gauge invariance represents a continuous symmetry.
According to the Noether theorem there is a conserved charge and thus a conserved current. $\rightsquigarrow$ This is just the electric charge/current.

$$(D_\mu D^\mu + m^2)\psi(x) = 0 \quad \Longrightarrow \quad \psi^*(x)(D_\mu D^\mu + m^2)\psi(x) = 0$$

↓ compl. conj. Subtract

$$(D_\mu^* D^{\mu *} + m^2)\psi^*(x) = 0 \quad \Longrightarrow \quad \psi(x)(D_\mu^* D^{\mu *} + m^2)\psi^*(x) = 0$$

$$\Rightarrow \quad 0 = \psi^* D_\mu D^\mu \psi - \psi D_\mu^* D^{\mu *}\psi^* = \psi^*\left(\vec{D}_\mu \vec{D}^\mu - \overleftarrow{D}_\mu^* \overleftarrow{D}^{\mu *}\right)\psi$$

$$= \psi^*\left[(\vec{\partial}_\mu + iqA_\mu)(\vec{\partial}^\mu + iqA^\mu) - (\overleftarrow{\partial}_\mu - iqA_\mu)(\overleftarrow{\partial}^\mu - iqA^\mu)\right]\psi \qquad \leftarrow \partial \text{ act outside parentheses}$$

$$= \psi^*\left[\vec{\partial}_\mu \vec{\partial}^\mu - \overleftarrow{\partial}_\mu \overleftarrow{\partial}^\mu + iq\left(\vec{\partial}_\mu A^\mu + A_\mu \vec{\partial}^\mu + A_\mu \overleftarrow{\partial}^\mu + \overleftarrow{\partial}_\mu A^\mu\right)\right]\psi \qquad \leftarrow \partial \text{ act outside parentheses}$$

$$= \psi^*\left[\vec{\partial}_\mu \vec{\partial}^\mu - \overleftarrow{\partial}_\mu \overleftarrow{\partial}^\mu + 2iq\left(\overleftarrow{\partial}_\mu A^\mu + A_\mu \vec{\partial}^\mu + (\partial_\mu A^\mu)\right)\right]\psi$$

$$= -i\,\partial_\mu\left[\psi^* i\left(\vec{\partial}^\mu - \overleftarrow{\partial}^\mu + 2iqA^\mu\right)\psi\right] = -i\,\partial_\mu\left[-i\left((D^\mu\psi)^*\psi - \psi^*(D^\mu\psi)\right)\right]$$

$\Rightarrow$ Conserved current: $j^\mu(x) = (\rho(x), \vec{j}(x))$

$$\boxed{j^\mu(x) = -i\left((D^\mu\psi(x))^*\psi(x) - \psi^*(x)(D^\mu\psi(x))\right), \quad \partial_\mu j^\mu(x) = 0}$$

→ <u>Conserved (total) charge:</u> $\partial_\mu j^\mu(x) = \partial_t \rho(x) + \vec{\nabla}\vec{j}(x) = 0$

$$\Rightarrow \quad 0 = \int_{\text{all space}} d^3\vec{x}\, \partial_\mu j^\mu(x) = \partial_t \int d^3\vec{x}\, \rho(x) + \underbrace{\cancel{\int d^3\vec{x}\, \vec{\nabla}\vec{j}(x)}}_{\text{current cannot leave space!}}{}^{=0}$$

$\Longrightarrow$ The total electric charge is conserved.

→ <u>Norm and scalar product:</u> For $A^\mu = 0$ the current $j^\mu(x) = (\rho(x), \vec{j}(x))$ is also conserved!

$$\left.\begin{aligned} \rho(x) &= -i\left((\partial_t\psi^*(x))\psi(x) - \psi^*(x)(\partial_t\psi(x))\right) \\ \vec{j}(x) &= i\left((\vec{\nabla}\psi^*(x))\psi(x) - \psi^*(x)(\vec{\nabla}\psi(x))\right) \end{aligned}\right\} \rightarrow \frac{d}{dt}\int d^3\vec{x}\, \rho(x) = 0$$

We can use $\rho(x)$ to define a <u>time-independent norm</u> and a <u>time-independent scalar product</u>

$\Rightarrow$

<u>Scalar product:</u> $\psi(x) = \langle \vec{x} | \psi(t) \rangle$, $\phi(x) = \langle \vec{x} | \phi(t) \rangle$

$$\langle \psi | \phi \rangle = \int d^3\vec{x}\, \psi^*(x)\, i\overleftrightarrow{\partial_t}\, \phi(x), \quad \overleftrightarrow{\partial_t} \equiv \vec{\partial}_t - \overleftarrow{\partial}_t$$

<u>But:</u> The norm and the scalar product are <u>not invariant under Lorentz transformations</u>! They are only meaningful to be used in a particular inertial frame.

5.3. Solutions of the Free KG Equation

We start with the ansatz: $\phi(x) = N e^{-ip.x} = N e^{-iEt} e^{i\vec{k}\vec{x}}$ $\qquad p^\mu = (E, \vec{k})$

↳ $(\partial_\mu \partial^\mu + m^2)\phi(x) = (-E^2 + \vec{k}^2 + m^2)\phi(x) = (-p^2 + m^2)\phi(x) = 0$

⟹ (1) $p^2 = m^2$: on-shell condition for particle with rest mass m

(2) We have 2 solutions for the energy : $E = \pm\sqrt{\vec{k}^2 + m^2}$ ⟵ What does this mean?

↳ Conserved current : $\rho(x) = -i(2iE)|N|^2 = 2E|N|^2$

$\vec{j}(x) = i(-2i\vec{k})|N|^2 = 2\vec{k}|N|^2$

$\Big\} \; j^\mu(x) = 2p^\mu |N|^2$

Problems :
* Solutions with negative energy have negative norm.
* Due to completeness one cannot throw away the solutions with negative energy.

} What is going on?

History : For some time the KG equation was not considered to be a valid relativistic wave equation for a scalar particle due to the appearance of ∂_t^2.
This lead to the development of the Dirac equation in 1927 which only contains a single time derivative. The Dirac equation, however, also has negative energy solutions

Today accepted paradigm:

Feynman - Stückelberg Interpretation

Solution with positive energy $\xrightarrow{\text{describes}}$ Particle that propagates forward in time

Solution with negative energy ⟶ Particle that propagates backward in time

} Appear in Lorentz-covariant theory

↓ is physically interpreted as
↑ is mathematically described by

Does not appear in the manifest Lorentz-covariant theory { Antiparticle with positive energy that propagates forward in time

Convention: particle A ⟶ antiparticle $\bar{A}$ (with a few exceptions)

Properties of particles and the associated antiparticles:

* The rest masses of particles and the associated antiparticles are exactly equal. (CPT symmetry)
  ⊕ lifetimes

* All additive quantum numbers (e.g. electr. charge) for particles and associated antiparticles have opposite signs. → Way out of the negative norm issue: $\rho(t,\vec{x})$ is related to particle / antiparticle number $\rho(t,\vec{x}) \longrightarrow q\,\rho(t,\vec{x})$ (q = particle charge)

* For a neutral particle (i.e. all additive quantum numbers = 0) it is possible that the particle is its own antiparticle (i.e. particle = antiparticle).

* What one calls particle and antiparticle is pure convention mathematically.

* Particles and associated antiparticles can annihilate each other and turn completely into photons.

Comment: Physically matter and antimatter can be distinguished due to a small imbalance in their CP properties. → particle physics lecture

Examples: * electron e^-, $Q(e^-) = -e$ $\qquad m_{e^-} = m_{e^+} = 0.5$ MeV
positron e^+, $Q(e^+) = +e$ $\qquad e^+ + e^- \longrightarrow n\gamma$ (dominant channel: $n=2$)

* proton p ⟷ antiproton $\bar{p}$

* positively charged pion (π^+) ⟷ negat. charged pion (π^-)

Conventions for the solutions: From now on we will always use the following notations.

* Energy: $E > 0$. Negative energies always have an explicit minus sign.

* Particle with electric charge q and 4-momentum $p^\mu = (E, \vec{k})$, $E = \sqrt{\vec{k}^2 + m^2}$:

→ wave function: $\boxed{\psi_{\vec{k}}^{(+)}(x) = N e^{-ip.x} = N e^{-i(Et - \vec{k}\vec{x})}}$

electric current: $j^\mu_{el} = q\, j^\mu_{\psi,\psi} = 2q|N|^2 (E, \vec{k}) = 2q|N|^2 p^\mu$

* Antiparticle with electric charge $-q$ and 4-momentum $p^\mu = (E, \vec{k})$, $E = \sqrt{\vec{k}^2 + m^2}$:

↳ Is described in theory by a particle with el. charge $+q$ and 4-momentum $\bar{p}^\mu = (-E, -\vec{k})$ (and that propagates backward in time).

→ wave function: $\boxed{\psi_{\vec{k}}^{(-)}(x) = N e^{+ip.x} = N e^{+i(Et - \vec{k}\vec{x})}}$

electric current: $j^\mu_{el} = q\, j^\mu_{\psi,\psi} = -2q|N|^2 (E, \vec{k}) = -2q|N|^2 p^\mu = 2q|N|\bar{p}^\mu$

Comment on gauge transformations:

The notations are designed such that $\varphi^{(+)}$ and $\varphi^{(-)}$ are both particle wave functions.
Therefore the charge-dependent gauge transformations act on both types exactly the same way:

Q: el. charge operator $\qquad \varphi^{(\pm)} \longrightarrow e^{iQ\Lambda}\varphi^{(\pm)} = e^{iq\Lambda}\varphi^{(\pm)}$

This notation is mandatory for a manifest Lorentz-covariant formulation of the theory and, thus, also the basis of being able to carry out calculations that are manifest Lorentz-covariant.

Scalar product:

$\longrightarrow$ We see that the scalar product has consistent features. $\qquad p^\mu = (E_k, \vec{k}),\ p'^\mu = (E_{k'}, \vec{k}')$

$$\langle \varphi_k^{(\pm)} | \varphi_{k'}^{(\pm)} \rangle = \int d^3\vec{x}\ \varphi_k^{(\pm)*}(x)\ i\overleftrightarrow{\partial_t}\ \varphi_{k'}^{(\pm)}(x) = \pm |N|^2 \int d^3\vec{x}\ e^{\pm ip\cdot x}(E_k + E_{k'})\, e^{\mp ip'\cdot x}$$

$$= \pm |N|^2 (2\pi)^3 (E_k + E_{k'})\, e^{\pm i(E-E')t}\, \delta^{(3)}(\vec{k}-\vec{k}')$$

$$= \pm 2 E_k (2\pi)^3 |N|^2 \delta^{(3)}(\vec{k}-\vec{k}') \stackrel{!}{=} \pm \delta^{(3)}(\vec{k}-\vec{k}') \implies \boxed{N = \frac{1}{\sqrt{2E_k}}\frac{1}{(2\pi)^{3/2}}}$$

$$\langle \varphi_k^{(\pm)} | \varphi_{k'}^{(\mp)} \rangle = \int d^3\vec{x}\ \varphi_k^{(\pm)*}(x)\ i\overleftrightarrow{\partial_t}\ \varphi_{k'}^{(\mp)}(x) = \pm |N|^2 \int d^3\vec{x}\ e^{\pm ip\cdot x}(E_k - E_{k'})\, e^{\pm ip'\cdot x}$$

$$= \pm |N|^2 (2\pi)^3 (E_k - E_{k'})\, e^{\pm i(E+E')t}\, \delta^{(3)}(\vec{k}-\vec{k}') = 0 \qquad \text{o.k.} \checkmark$$

$$\leadsto \boxed{\begin{aligned} \varphi_k^{(+)}(x) &= \frac{1}{\sqrt{2E_k}}\frac{1}{(2\pi)^{3/2}}\, e^{-ip\cdot x} \\ \varphi_k^{(-)}(x) &= \frac{1}{\sqrt{2E_k}}\frac{1}{(2\pi)^{3/2}}\, e^{+ip\cdot x} \end{aligned}}$$

$\longrightarrow$ propagates forward in time

$\longrightarrow$ propagates backwards in time

Form of a general free particle/antiparticle state

$$\leadsto \varphi(x) = \int d^3\vec{k}\ \left[a_+(\vec{k})\, \varphi_k^{(+)}(x) + a_-^*(\vec{k})\, \varphi_k^{(-)}(x) \right] \qquad a_-^* \leftarrow \text{convention}$$

$$\rightarrow \text{particle number} = \int d^3\vec{x}\ \varphi^*(x)\, i\overleftrightarrow{\partial_t}\, \varphi(x) = \int d^3\vec{k}\ \left(|a_+(\vec{k})|^2 - |a_-(\vec{k})|^2\right)$$

contribution of particle > 0 $\qquad$ contribution of antiparticle < 0

Completeness relation:

We can define a completeness relation : $x^\mu = (t, \vec{x})$, $x'^\mu = (t, \vec{x}')$

$\hookrightarrow$ $$K(x,x') = K(t, \vec{x}, \vec{x}') = \int d^3\tilde{q} \left[\varphi^{(+)}_{\vec{q}}(t,\vec{x})\, \varphi^{(+)*}_{\vec{q}}(t,\vec{x}') - \varphi^{(-)}_{\vec{q}}(t,\vec{x})\, \varphi^{(-)*}_{\vec{q}}(t,\vec{x}') \right]$$

$$= \int \frac{d^3\vec{q}}{(2\pi)^3} \frac{1}{2E_{\vec{q}}} \left[e^{-iE_q t} e^{i\vec{q}\vec{x}} \left(e^{-iE_{\vec{q}} t} e^{i\vec{q}\vec{x}'} \right)^* - e^{+iE_q t} e^{-i\vec{q}\vec{x}} \left(e^{-iE_{\vec{q}} t} e^{-i\vec{q}\vec{x}'} \right)^* \right]$$

$$= \int \frac{d^3\vec{q}}{(2\pi)^3} \frac{1}{2E_{\vec{q}}} \left[e^{-iE_q t} e^{i\vec{q}\vec{x}} \left(e^{-iE_{\vec{q}} t} e^{i\vec{q}\vec{x}'} \right)^* - e^{+iE_q t} e^{i\vec{q}\vec{x}} \left(e^{-iE_{\vec{q}} t} e^{i\vec{q}\vec{x}'} \right)^* \right]$$

$$\delta(q^2 - m^2) = \delta\left((q_0 + \sqrt{\vec{q}^2 + m^2})(q_0 - \sqrt{\vec{q}^2 + m^2}) \right) = \delta\left((q_0 + E_{\vec{q}})(q_0 - E_{\vec{q}}) \right)$$

$$= \frac{1}{2E_{\vec{q}}} \left(\delta(q_0 - E_{\vec{q}}) + \delta(q_0 + E_{\vec{q}}) \right)$$

$$= \int \frac{d^4 q}{(2\pi)^3} \delta(q^2 - m^2) \left[\theta(q_0) - \theta(-q_0) \right] e^{-iq\cdot x} \left(e^{-iqx'} \right)^*$$

This is a completeness relation with respect to the scalar product $\langle \psi | \varphi \rangle = \int d^3\vec{x}\, \psi^*(x)\, i \overleftrightarrow{\partial_t}\, \varphi(x)$!

We have:

$$\int d^3\vec{x}'\, K(x,x')\, i\overleftrightarrow{\partial_t}\, \underset{\substack{\uparrow \\ \text{defined above}}}{\varphi(x)} = \int d^3\tilde{k} \left[a_+(\vec{k})\, \varphi^{(+)}_{\vec{k}}(x) + a^*_-(\vec{k})\, \varphi^{(-)}_{\vec{k}}(x) \right] \checkmark$$

5.4. Scattering off a Potential Step

→ In nonrelativistic QM the number of massive particles participating at a process is not changing during the process.

$\hookrightarrow$ "n-particle Schrödinger equation" has explicit interpretation as the time evolution equation of a probability amplitude

Background: The non-relativistic situation is tied to the approximation

$$E_{kin},\ V(\vec{x}),\ |\vec{k}| \ll m \quad (\text{rest mass of the massive particles})$$

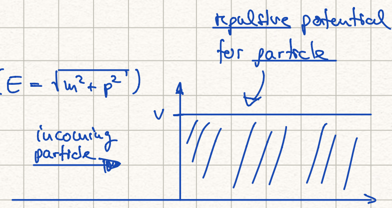
$\hookrightarrow$ If we apply the KG equation in exactly such a kinematic situation its solutions behave very similar to non-relat. QM. → No conceptual problems arise.

→ We consider the scattering of a <u>charged scalar particle</u> in 1 dimension off a potential step in analogy to Sec. 3.3. of the QM I lecture.

* particle with mass m and charge $q > 0$:
* $A^\mu = (\Phi, \vec{0})$, $\Phi(z) = \theta(z)\,\phi \longrightarrow V = q\,\phi$

↳ KG equation: $\left[-\left(i\partial_t - q\Phi(z)\right)^2 - \vec{\nabla}^2 + m^2\right]\psi(t,z) = 0$

We are looking for a <u>stationary particle energy eigensolution</u> $(E = \sqrt{m^2+p^2})$



→ $\boxed{\text{Ansatz: } \psi(t,z) = e^{-iEt}\,\psi(z)}$

↳ <u>$z<0$:</u> $\left[-E^2 - \frac{d^2}{dz^2} + m^2\right]\psi(z) = 0$

<u>$z>0$:</u> $\left[-(E-V)^2 - \frac{d^2}{dz^2} + m^2\right]\psi(z) = 0$

$\psi(z)$, $\frac{d}{dz}\psi(z)$ continuous at $z=0$ (because no $\delta(z)$, $\delta'(z)$ in KG equations)

→ We want to consider the case of an <u>incoming particle from the left side</u>

↳ $$\boxed{\begin{aligned} \psi_{<0}(z) &= I\,e^{ipz} + R\,e^{-ipz} \\ \psi_{>0}(z) &= T\,e^{ikz} \end{aligned}}$$

I incoming
R reflected
T transmitted

↳ <u>$z<0$:</u> $E^2 = p^2 + m^2 \implies p = \sqrt{E^2 - m^2}$ (incoming : $p>0$)

<u>$z>0$:</u> $(E-V)^2 = k^2 + m^2 \implies k = \pm\sqrt{(E-V)^2 - m^2}$ (sign not fixed yet)

<u>ψ continuous:</u> $I + R = T$

<u>ψ' continuous:</u> $pI - pR = kT$

$$\implies \boxed{\begin{aligned} T &= \frac{2p}{p+k}\,I \\ R &= \frac{p-k}{p+k}\,I \end{aligned}}$$

→ <u>Non-relativistic limit:</u> $E = m + E_{kin}$, $E_{kin}, V \ll m$

only + solution is relevant

We find the solutions we know from QM 1 : $\implies p = \sqrt{2mE_{kin}}$, $k = \sqrt{2m(E_{kin}-V)}$

(a) $E_{kin} > V$: $\psi_{>0}(z) = e^{ikz}$ (transmitted particle wave moving right)

We can exclude the solution for $k<0$, because we know that $E = m + E_{kin} > 0$, $E > V$ is positive, so that only particles can be present. (I, R, T are particles)

(b) $E_{kin} < V$: $\psi_{>0}(z) = e^{-\kappa z}$, $\kappa = \sqrt{2m(V-E_{kin})}$ (exponentially falling particle wave)

Particle cannot penetrate into $z>0$ region.

$\Rightarrow$ The KG equation provides relativistic corrections to the purely non-relativistic approximation treated in QM 1.

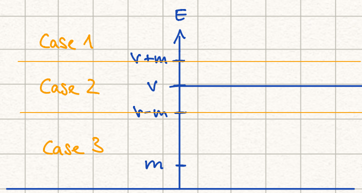
$\rightarrow$ Relativistic region: We consider the case $\boxed{E, V > m}$

Our knowledge from nonrel. QM I does not help us any more!
We need to distinguish 3 cases:

① $E > V + m$

② $|V - E| < m$

③ $E < V - m$



$\boxed{E > V+m}$ Particle has sufficient energy such that $E - V > m$ and it can still propagate for $z > 0$ $\Rightarrow$ $k = +\sqrt{(E-V)^2 - m^2} > 0$

$\hookrightarrow$ $j_<(z) = 2p\left(|I|^2 - |R|^2\right)$, $j_>(z) = 2k\,|T|^2$

$$|j_<^{refl}| + |j_>^{trans}| = 2p\,|R|^2 + 2k\,|T|^2 = 2p\left(\frac{p-k}{p+k}\right)^2 |I|^2 + 2k\left(\frac{2p}{p+k}\right)^2 |I|^2$$

$$= 2p\,|I|^2 = |j_<^{in}|$$

$\rightarrow$ Situation analogous to nonrel. case for $E_{kin} > V$.

$\boxed{|V-E| < m}$ $\rightarrow$ particle cannot propagate to $z > 0$ $(E - V < m)$
$\rightarrow$ antiparticle feels an attractive potential for $z < 0$ $(V - E < m)$ but it cannot gain sufficient energy > 0 to propagate for $z > 0$.

$\hookrightarrow$ $k = i\sqrt{m^2 - (E-V)^2} = i\kappa$ $\Rightarrow$ transmitted wave falls off exponentially: $\psi_> = T e^{-\kappa}$

$$\left.\begin{aligned} R &= \frac{p - i\kappa}{p + i\kappa}\, I \quad \Rightarrow \quad |R|^2 = |I|^2 \\ j_<(z) &= 2p\left(|I|^2 - |R|^2\right) , \quad j_>(z) = 0 \end{aligned}\right\} \quad |j_<^{refl.}| = |j_<^{in}|$$

$\rightarrow$ Situation analogous to nonrel. case for $E_{kin} < V$.

$\boxed{V - E > m}$ $\rightarrow$ particle cannot propagate to $z > 0$ $(E - V < m$ still$)$
$\rightarrow$ antiparticle feels the attractive potential for $z > 0$ $(V - E > m\,!)$ and can gain sufficient energy (w.r. to energy level E where it did not yet exist) to be produced and to propagate to $z > 0$!

$\hookrightarrow$ $k = -|k|$, $\psi_{>0}(z) = T e^{-i|k|z}$ $\leftarrow$ antiparticle wave function has energy $V - E$

$T = \frac{2p}{p - |k|}\, I$, $R = \frac{p + |k|}{p - |k|}\, I > I$ (!)

$(p > |k|)$

$$|j_<^{refl}| + |j_>^{trans}| = 2p\left(\frac{p+|k|}{p-|k|}\right)^2|I|^2 - \underbrace{2|k|\left(\frac{2p}{p-|k|}\right)^2|I|^2}_{\text{negative norm flow}}$$

$$= 2p|I|^2 = |j_<^{in}|$$

But: $|j_<^{in}| < |j_<^{refl}|$! "Klein's Paradox"

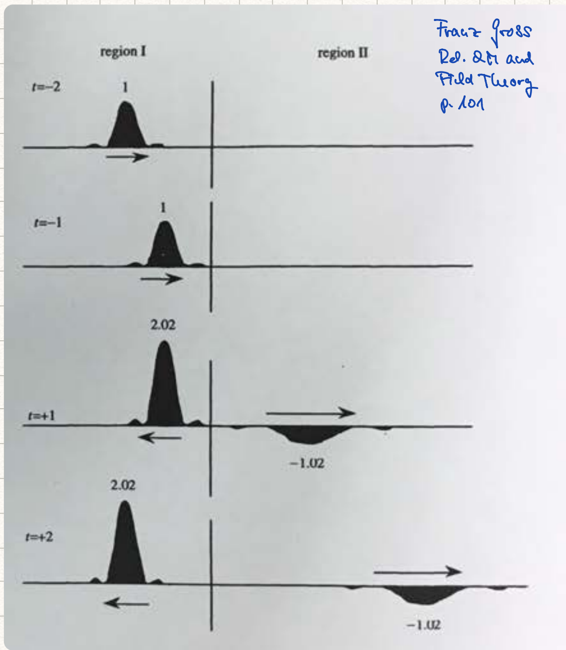
→ Klein's paradox is only a paradox if one interprets the conserved current as a probability current.

One then has a problem with negative probability and that the reflected particle has more probability than the incoming one.

→ There is no problem when one applies the electric current interpretation since antiparticles have opposite charge and the total charge before and after scattering are the same.

We have: $\boxed{V > E + m > 2m}$!

The potential step delivered sufficient energy so that a particle-antiparticle pair can be created.



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Klein's paradox indicates that the notion of a fixed particle number in general fails in the relativistic context.

But: For kinematic situations close to non-relativistic situations the fixed particle number concept still works reliably.

→ Nevertheless, using the KG equation for the potential step problem (and for any other potential) in cases where particle-antiparticle creation (or annihilation) is possible, does not provide a transparent treatment, because the concept of energy conservation is not obvious any more.

→ global energy is E $\left(\psi(t,z) = e^{-iEt}\psi(z)\right)$, but we have (incoming and outgoing) particles for $z<0$ that appear to be inconsistent with this assignment of energy.

KG equation is ok for problems where particle numbers are unchanged.
But we need a better formalism when particle creation/annihilation are possible.
→ Quantum Field Theory (QFT)

5.5 Propagator and Green's Function

Consider: $(\Box + m^2 + V(x))\,\psi(x) = 0 \iff (\Box + m^2)\,\psi(x) = -V(x)\,\psi(x)$

→ Propagator / Green's fct: Starting point of perturbative treatment of KG equation in the presence of an interaction.

⇝ Recall: As long as we do not consider particle-antiparticle creation/annihilation processes we can use the common interpretation of the Green's function, where we just need to account for the different time-evolution for particles and antiparticles.

But: For processes where particle/antiparticle creation or annihilation can take place we have to use QFT

$$\boxed{(\Box_x + m^2)\,\Delta_F(x,x') = (\partial_\mu \partial^\mu_x + m^2)\,\Delta_F(x,x') = -i\,\delta^{(4)}(x-x')} \qquad \Delta_F(x,x') = \Delta_F(x-x')$$

"F" for "Feynman propagator" (in honor for Feynman's contribution)

Form of a general solution: $\psi(x) = \underbrace{\psi_{free}(x)}_{\text{solution of free KG equation}} - i\underbrace{\int d^4x'\,\Delta_F(x,x')\,V(x')\,\psi(x')}_{\text{particular solution}}$ $\qquad x^\mu = (t,\vec{x}),\ x'^\mu = (t',\vec{x}')$

⇝ But: We will see eventually (→ Sec. 5.6) that this form of the general solution is only meaningful for particle solutions only. ⟶ This means for $t > t'$!

Implication of the Feynman-Stückelberg interpretation for $\Delta_F(x,x') = \Delta_F(t,\vec{x};t',\vec{x}')$:

* Particle states propagate forward in time: $\Delta_F(x,x') \sim \theta(t-t')$ — particle time direction
* Antiparticle states propagate forward in time: $\Delta_F(x,x') \sim \theta(t'-t)$ — antiparticle time direction

⇝ The correct implementation of this interpretation implements causality into our formalism and is also the reason that all calculation we need to do involve only analytic functions (which means that we can do calculations without ambiguities).

→ Propagator in momentum space: $(\rightsquigarrow \Delta_F(x,x') \sim \langle x|\Delta_F|x'\rangle)$

$$\tilde{\Delta}_F(q,q') \equiv \int d^4x\, d^4x'\, e^{+iqx}\,\Delta_F(x,x')\,e^{-iq'x'}$$

$$\Delta_F(x,x') = \int \frac{d^4q}{(2\pi)^4}\frac{d^4q'}{(2\pi)^4}\, e^{-iqx}\,\tilde{\Delta}_F(q,q')\,e^{+iq'x'}$$

$$\longrightarrow\ (q^2 - m^2)\,\tilde{\Delta}_F(q,q') = i\,(2\pi)^4\,\delta^{(4)}(q-q')$$

↳ The correct form of the Feynman propagator is:

$$\boxed{\tilde{\Delta}_F(q,q') = \frac{i(2\pi)^4\delta^{(4)}(q-q')}{q^2-m^2+i\epsilon}}$$

($\epsilon > 0$, infinitesimal)

↳ To see that this is the correct propagator let us calculate the position space propagator

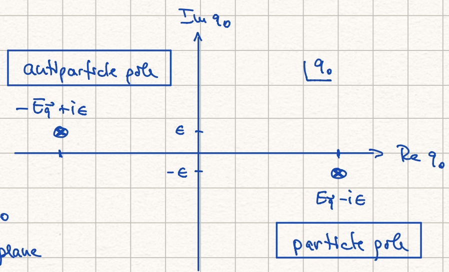
→ Propagator in position space

We have $q^2-m^2+i\epsilon = q_0^2-\vec{q}^2-m^2+i\epsilon = q_0^2 - E_{\vec q}^2 + i\epsilon = [q_0-(E_{\vec q}-i\epsilon)][q_0+(E_{\vec q}-i\epsilon)]$

$$= q_0^2 - E_{\vec q}^2 + i\epsilon(\cancel{q_0}+E_{\vec q} - \cancel{q_0}+E_{\vec q}) \qquad (E_{\vec q}>0) \quad \checkmark$$

$$\Rightarrow \frac{1}{q^2-m^2+i\epsilon} = \frac{1}{2E_{\vec q}}\frac{1}{q_0-E_{\vec q}+i\epsilon} - \frac{1}{2E_{\vec q}}\frac{1}{q_0+E_{\vec q}-i\epsilon}$$

$$\boxed{\begin{aligned}\Delta_F(x-x') &= \int\frac{d^4q}{(2\pi)^4}\frac{d^4q'}{(2\pi)^4}\, e^{-iqx}\,\frac{i(2\pi)^4\delta^{(4)}(q-q')}{q^2-m^2+i\epsilon}\, e^{+iq'x'} \\ &= \int\frac{d^4q}{(2\pi)^4}\, e^{-iq(x-x')}\,\frac{i}{q^2-m^2+i\epsilon}\end{aligned}}$$



particle contribution:

We must have $t>t'$ to close in lower half-plane

$$i\int\frac{d^4q}{(2\pi)^4}\, e^{-iq_0(t-t')}\, e^{i\vec q(\vec x-\vec x)}\,\frac{1}{2E_{\vec q}}\,\frac{1}{q_0-E_q+i\epsilon}$$

"pick up pole at $+E_{\vec q}-i\epsilon$"

We only get $\neq 0$ result if we close contour in lower half-plane.

$$= i(-2\pi i)\,\Theta(t-t')\int\frac{d^3q}{(2\pi)^4}\,\frac{1}{2E_{\vec q}}\, e^{-iE_{\vec q}(t-t')}\, e^{i\vec q(\vec x-\vec x)}$$

$$= \Theta(t-t')\int\frac{d^3\vec q}{(2\pi)^3}\,\frac{1}{2E_{\vec q}}\, e^{-iq(x-x')} \qquad q^\mu = (E_{\vec q},\vec q)$$

$$= \Theta(t-t')\int d^3\vec q\; \varphi^{(+)}_{\vec q}(x)\,\varphi^{(+)*}_{\vec q}(x')$$

← Correct forward particle time evolution!

antiparticle contribution:

We must have $t'>t$ to close in upper half-plane.

$$-i\int\frac{d^4q}{(2\pi)^4}\, e^{-iq_0(t-t')}\, e^{i\vec q(\vec x-\vec x')}\,\frac{1}{2E_{\vec q}}\,\frac{1}{q_0+E_{\vec q}-i\epsilon}$$

"pick up pole at $-E_{\vec q}+i\epsilon$"

We only get $\neq 0$ result if we close contour in upper half-plane.

$$= -i(2\pi i)\,\Theta(t'-t)\int\frac{d^3\vec q}{(2\pi)^4}\,\frac{1}{2E_{\vec q}}\, e^{+iE_{\vec q}(t-t')}\, e^{i\vec q(\vec x-\vec x')} \qquad (\vec q \to -\vec q)$$

$$= \Theta(t'-t)\int\frac{d^3\vec q}{(2\pi)^3}\,\frac{1}{2E_{\vec q}}\, e^{+iq.(x-x')}$$

$$= \Theta(t'-t)\int d^3\vec q\; \varphi^{(-)}_{\vec q}(x)\,\varphi^{(-)*}_{\vec q}(x')$$

← Correct forward anti-particle time evolution!

$$\boxed{\Delta_F(x,x') = \Theta(t-t')\int d^3\vec{q}\; \varphi^{(+)}_{\vec{q}}(x)\,\varphi^{(+)*}_{\vec{q}}(x') + \Theta(t'-t)\int d^3\vec{q}\; \varphi^{(-)}_{\vec{q}}(x)\,\varphi^{(-)*}_{\vec{q}}(x')}$$

5.6. S-matrix Elements for Scattering Processes

5.6.1 Particle Scattering

We use the formalism we have already developed for time-dependent perturbation theory in the non-relativistic context and just take care of the relativistic generalization.

To avoid problems we do not consider any process with particle/antiparticle creation or annihilation at this point. → See however Chap. 6.7!

As in the non-relativ. context we see that the Feynman propagator again acts as a time-evolution operator:

$$\int d^3\vec{x}'\, \Delta_F(x,x')\, i\overleftrightarrow{\partial}_{t'}\, \varphi^{(+)}_{\vec{k}}(x') = \Theta(t-t')\,\varphi^{(+)}_{\vec{k}}(x)$$

and also
$$\int d^3\vec{x}'\, \varphi^{(+)*}_{\vec{k}}(x')\, i\overleftrightarrow{\partial}_{t'}\, \Delta_F(x',x) = \Theta(t'-t)\,\varphi^{(+)*}_{\vec{k}}(x)$$

Recall: S-matrix element $\hat{=}$ Amplitude that a free incoming particle at $t_i \to -\infty$ with momentum $\vec{k}_i$ is later at $t_f \to +\infty$ detected as a free outgoing particle with momentum $\vec{k}_f$.

Time-evolved in-particle state ($t \gg t_i$): $x' = (t_i, \vec{x}')$, $x = (t, \vec{x})$, $\varphi^{(+)}_{in}$ is free plane wave!

with interaction included

$$\tilde{\varphi}^{(+)}_{in}(t,\vec{x}) = \int d^3\vec{x}'\, \Delta_F(x,x')\, i\overleftrightarrow{\partial}_{t_i}\, \varphi^{(+)}_{in}(t_i,\vec{x}') - i\int_{t_{in}}^{t} dt' \int d^3\vec{x}'\, \Delta_F(x,x')\, V(t',\vec{x}')\, \tilde{\varphi}^{(+)}_{in}(t',\vec{x}')$$

$$= \varphi^{(+)}_{in}(t,\vec{x}) - i\int_{t_{in}}^{t} dt' \int d^3\vec{x}'\, \Delta_F(x,x')\, V(t',\vec{x}')\, \tilde{\varphi}^{(+)}_{in}(t',\vec{x}')$$

$$= \varphi^{(+)}_{in}(t,\vec{x})$$
$$- i\int_{t_{in}}^{t} dt' \int d^3\vec{x}'\, \Delta_F(x,x')\, V(t',\vec{x}')\, \varphi^{(+)}_{in}(t',\vec{x}')$$
$$+ (-i)^2 \int_{t'>t_{in}} d^4x' \int_{t''>t_{in}} d^4x''\, \Delta_F(x,x')\, V(x')\, \Delta_F(x',x'')\, V(x'')\, \varphi^{(+)}_{in}(x'') + \dots$$

takes care of time-ordering automatically

S-matrix element in configuration space:

not written out in the following any more

$$S_{\vec{k}_f \vec{k}_i} = \lim_{\substack{t_f \to +\infty \\ t_i \to -\infty}} \int d^3\vec{x}\; \varphi^{(+)*}_{\vec{k}_f}(t_f,\vec{x})\, i\overleftrightarrow{\partial}_{t_f}\, \tilde{\varphi}^{(+)}_{\vec{k}_i}(t_f,\vec{x})$$

$$= \int d^3\vec{x}\; \varphi^{(+)*}_{\vec{k}_f}(t_f,\vec{x})\, i\overleftrightarrow{\partial}_t\, \varphi^{(+)}_{\vec{k}_i}(t_f,\vec{x})$$

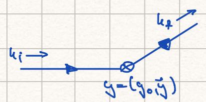
$\varphi^{(+)*}_{\vec{k}_f}(y)$

$$- i \int d^3\vec{x}\, d^4y\, \left(\varphi^{(+)*}_{\vec{k}_f}(t_f,\vec{x})\, i\overleftrightarrow{\partial}_t\, \Delta_F(t_f,\vec{x},y)\right) V(y)\, \varphi^{(+)}_{\vec{k}_i}(y)$$

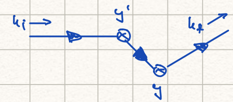
$$+ (-i)^2 \int d^3x\, d^4y\, d^4y'\; \varphi^{(+)*}_{\vec{k}_f}(t_f,\vec{x})\, i\overleftrightarrow{\partial}_t\, \Delta_F(t_f,\vec{x},y)\, V(y)\, \Delta_F(y,y')\, \varphi^{(+)}_{\vec{k}_i}(y') + \ldots$$

$$= \delta^{(3)}(\vec{k}_f - \vec{k}_i)$$

$$- i \int d^4y\; \varphi^{(+)*}_{\vec{k}_f}(y)\, V(y)\, \varphi^{(+)}_{\vec{k}_i}(y) \quad \leftarrow \text{Born approx.}$$



$$+ (-i)^2 \int d^4y\, d^4y'\; \varphi^{(+)*}_{\vec{k}_f}(y)\, \underbrace{V(y)\, \Delta_F(y,y')\, V(y')}\, \varphi^{(+)}_{\vec{k}_i}(y') \quad \leftarrow \text{2nd order}$$



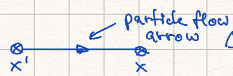
$$+ \ldots$$

New aspect: There are 2 time orderings possible:

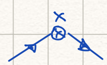
$y_0 > y_0'$: exists as for non-relat. QM

$y_0 < y_0'$: does not exist in non-rel. QM

Configuration space Feynman rules:



$\Delta_F(x,x')$ propagator



$-i\,V(x)$ vertex factor

$\varphi^{(+)}_{in}(x)$ incoming particle

$\varphi^{(-)*}_{in}(x)$ incoming antiparticle

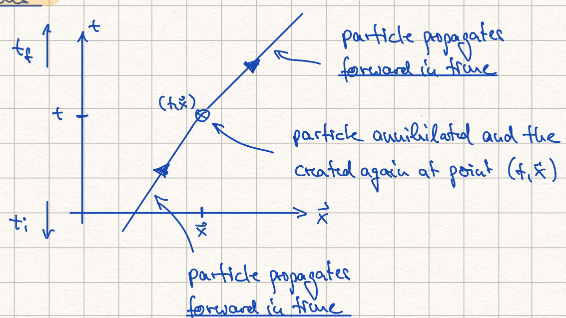
$\varphi^{(+)*}_{out}(x)$ outgoing particle

$\varphi^{(-)}_{out}(x)$ outgoing antiparticle

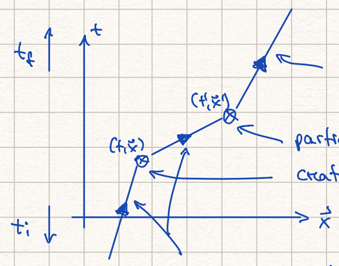
Additional rules:
- * Write down all terms against the particle flow arrow
- * Integrate over all intermediate vertex factor locations x : $\int d^4x$

Space-time diagrams

Born approximation:



2nd order: (A)



particle propagates forward in time

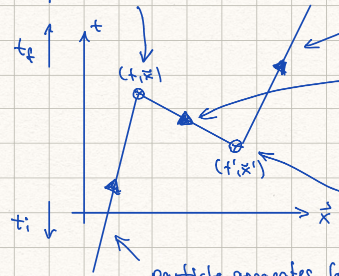
particle annihilated and the created again at points $(t,\vec{x})$ and $(t',\vec{x}')$

particle propagates forward in time

particle-antiparticle pair annihilated at point $(t,\vec{x})$

(B)

Obvious question: Why was this contribution not important for non-rel. QM? →



particle propagates forward in time

antiparticle propagates forward in time (described by particle that propagates backward in time)

virtual particle-antiparticle pair created at point $(t',\vec{x}')$

particle propagates forward in time

S-matrix element in momentum space

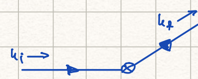
We use: $\Delta_F(x,x') = \int \frac{d^4q}{(2\pi)^4}\, e^{-iqx} \frac{i}{q^2-m^2+i\epsilon}\, e^{+iqx'}$

$$\int d^4x\, e^{+iqx} V(x) e^{-iq'x} =: \tilde{V}(q,q') = \tilde{V}(q-q')$$

outgoing mom. → q, q' ← incoming momentum

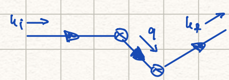
$$S^{(1)}_{k_f,k_i} = -i \int d^4y\, \psi^{(+)*}_{k_f}(y)\, V(y)\, \psi^{(+)}_{k_i}(y)$$

$$= \frac{1}{(2\pi)^{3/2}} \frac{1}{\sqrt{2E_{k_f}}} \left[-i\,\tilde{V}(k_f,k_i)\right] \frac{1}{(2\pi)^{3/2}} \frac{1}{\sqrt{2E_{k_i}}}$$

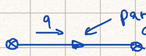


$$S^{(2)}_{k_f k_i} = (-i)^2 \int d^4y\, d^4y'\, \psi^{(+)*}_{k_f}(y)\, V(y)\, \Delta_F(y,y')\, V(y')\, \psi^{(+)}_{k_i}(y')$$

$$= \int \frac{d^4q}{(2\pi)^4}\, \frac{1}{(2\pi)^{3/2}} \frac{1}{\sqrt{2E_{k_f}}} \left[-i\,\tilde{V}(k_f,q)\right] \frac{i}{q^2-m^2+i\epsilon} \left[-i\,\tilde{V}(q,k_i)\right] \frac{1}{(2\pi)^{3/2}} \frac{1}{\sqrt{2E_{k_i}}}$$

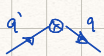


Momentum space Feynman rules



particle flow arrow

$\frac{i}{q^2-m^2+i\epsilon}$ propagator



$-i\,\tilde{V}(q,q')$ vertex factor

$\frac{1}{(2\pi)^{3/2}} \frac{1}{\sqrt{2E_{k_i}}}$ incoming particle

$\frac{1}{(2\pi)^{3/2}} \frac{1}{\sqrt{2E_{k_i}}}$ incoming antiparticle

$\frac{1}{(2\pi)^{3/2}} \frac{1}{\sqrt{2E_{k_f}}}$ outgoing particle

$\frac{1}{(2\pi)^{3/2}} \frac{1}{\sqrt{2E_{k_f}}}$ outgoing antiparticle

Additional rules:
* Write down all terms against the particle flow arrow
* Integrate over all virtual (propagator) momenta q_i : $\int \frac{d^4q}{(2\pi)^4}$

↳ Let us have a closer look at contributions A and B

$$\frac{i}{q^2-m^2+i\epsilon} = \underbrace{\frac{1}{2E_{\vec q}}\frac{i}{q_0-E_{\vec q}+i\epsilon}}_{\text{A virtual particle propagation}} - \underbrace{\frac{1}{2E_{\vec q}}\frac{i}{q_0+E_{\vec q}-i\epsilon}}_{\text{B virtual antiparticle propagation}}$$

We consider the non-relativistic limit:

$$E_{\vec q} = m + \frac{\vec q^2}{2m} + \dots$$

nonrel. expression (see Chap. 2.8)

$$\tilde V(k_f,q) = \tilde V(k_f-q) = \tilde V(E_{\vec k_f}-q_0,\vec k_f-\vec q) \approx \tilde V\left(\frac{\vec k_f^2}{2m}+m-q_0,\vec k_f-\vec q\right) = (2\pi)^3\,\tilde V_{NR}\left(\frac{\vec k_f^2}{2m}+m-q_0,\vec k_f-\vec q\right)$$

$$\tilde V(q,k_i) = \dots \approx (2\pi)^3\,\tilde V_{NR}\left(q_0-m-\frac{\vec k_i^2}{2m},\vec q-\vec k_i\right)$$

To recover the momentum definition used for the nonrelativistic calculation we have to do the variable change: $q_0-m \longrightarrow q_0$ $\quad(q_0\longrightarrow q_0+m)$

$$S^{(2)}_{\vec k_f\vec k_i} = \int\frac{d^4q}{(2\pi)^4}\frac{1}{(2\pi)^{3/2}\sqrt{2E_{\vec k_f}}}\left[-i\tilde V(k_f,q)\right]\frac{i}{q^2-m^2+i\epsilon}\left[-i\tilde V(q,k_i)\right]\frac{1}{(2\pi)^{3/2}}\frac{1}{\sqrt{2E_{\vec k_i}}}$$

$$\approx \frac{1}{(2\pi)}\frac{1}{(2m)^2}\int d^4q\left[-i\tilde V\left(\frac{\vec k_f^2}{2m}+m-q_0,\vec k_f-\vec q\right)\right]\left(\frac{i\;\text{A}}{q_0-m_0-\frac{\vec q^2}{2m}+i\epsilon}-\frac{i\;\text{B}}{q_0+m_0+\frac{\vec q^2}{2m}+i\epsilon}\right)$$

$$*\left[-i\tilde V_{NR}\left(q_0-m-\frac{\vec k_i^2}{2m},\vec q-\vec k_i\right)\right] \quad \Big\downarrow\; q_0\to m+q_0$$

$$= \frac{1}{(2\pi)}\frac{1}{(2m)^2}\int d^4q\left[-i\tilde V\left(\frac{\vec k_f^2}{2m}-q_0,\vec k_f-\vec q\right)\right]\left(\frac{i\;\text{A}}{q_0-\frac{\vec q^2}{2m}+i\epsilon}-\underbrace{\frac{i\;\text{B}}{2m+q_0+\frac{\vec q^2}{2m}+i\epsilon}}_{\approx\frac{i}{2m}\left(1-\frac{q_0}{2m}-\frac{\vec q^2}{4m^2}+\dots\right)}\right)$$

$$*\left[-i\tilde V_{NR}\left(q_0-\frac{\vec k_i^2}{2m},\vec q-\vec k_i\right)\right]$$

↳ We see: A exactly reproduces the nonrelativistic limit (up to the norm) and provides relativistic corrections

B is suppressed in the nonrelativistic limit and thus represents a relativistic correction

⟹ In the nonrelativistic limit is the virtual antiparticle contribution for particle scattering strongly suppressed.

Relativistic QM is more general than nonrelat. QM.

<u>But:</u> For this argument to work one has to assume that $q_0,\frac{\vec q^2}{2m}\ll m$. This assumption is implicit for nonrelativistic QM.

<u>However:</u> How can this be reconciled with the integration $\int d^4q$, which goes over all momenta? How can one justify to expand the integrant for $q\ll m$, even though one integrates over all q?

→ The answer is that nonrel. QM is an <u>effective quantum theory</u>.
Even though $\int d^4q$ in nonrel. QM is an integration over all momenta the states that are summed over only describe realistic nonrel. states for $q\ll m$. The states for $q\gtrsim m$ are contributions the

effective quantum theory needs for consistency reasons, but whether they are physically correct cannot be answered from within the effective quantum theory itself. This can only be judged from the point of view of a more complete theory.

Still the effective quantum theory provides the correct results in <u>the limit of its validity.</u>

↳ Nonrelativistic limit for nonrelativistic QM.

5.6.2 Antiparticle Scattering

↳ Everything works as for the particle scattering, but with opposite time-ordering.

Again we see that the Feynman propagator acts as a time-evolution operator:

$$\int d^3\vec{x}'\, \varphi_{\vec{k}}^{(-)*}(x')\, i\overleftrightarrow{\partial}_{t'}\, \Delta_F(x',x) = -\theta(t-t')\, \varphi_{\vec{k}}^{(-)*}(x) \quad \longleftarrow \text{time evolved } \underline{\text{in-state}}$$

$$\int d^3\vec{x}'\, \Delta_F(x,x')\, i\overleftrightarrow{\partial}_{t'}\, \varphi_{\vec{k}}^{(-)}(x') = -\theta(t'-t)\, \varphi_{\vec{k}}^{(-)}(x) \quad \longleftarrow \text{time evolved } \underline{\text{out-state}}$$

Time-evolved in-antiparticle state ($t \gg t_i$): $\quad x' = (t_i, \vec{x}')$, $\varphi_{in}^{(-)*}$ is free plane wave!

with interaction included

$$\tilde{\varphi}_{in}^{(-)*}(t,\vec{x}) = \int d^3\vec{x}'\, \varphi_{in}^{(-)*}(t_i,\vec{x}')\, i\overleftrightarrow{\partial}_{t'}\, \Delta_F(x',x) - i\int_{t_{in}}^{t} dt' \int d^3\vec{x}'\, \tilde{\varphi}_{in}^{(-)*}(t',\vec{x}')\, V(t',\vec{x}')\, \Delta_F(x',x)$$

$$= -\varphi_{in}^{(-)*}(t,\vec{x})$$

$$-(-i)\int_{t_{in}}^{t} dt' \int d^3\vec{x}'\, \varphi_{in}^{(-)*}(t',\vec{x}')\, V(t',\vec{x}')\, \Delta_F(x',x) \qquad \text{takes care of time-ordering automatically}$$

$$-(-i)^2 \int_{t'>t_{in}} d^4x' \int_{t''>t_{in}} d^4x''\, \varphi_{in}^{(-)*}(x'')\, V(x'')\, \Delta_F(x'',x')\, V(x')\, \Delta_F(x',x)$$

<u>S-matrix element in configuration space:</u>

$$S_{\vec{k}_f\vec{k}_i} = \lim_{\substack{t_f\to+\infty \\ t_i\to-\infty}} \int d^3\vec{x}\, \tilde{\varphi}_{\vec{k}_i}^{(-)*}(t_f,\vec{x})\, i\overleftrightarrow{\partial}_{t_f}\, \varphi_{\vec{k}_f}^{(-)}(t_f,\vec{x})$$

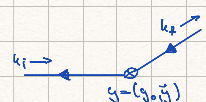
$$= -\int d^3\vec{x}\, \varphi_{\vec{k}_i}^{(-)*}(t_f,\vec{x})\, i\overleftrightarrow{\partial}_{t}\, \varphi_{\vec{k}_f}^{(-)}(t_f,\vec{x})$$

$$-(-i)\int d^3\vec{x}\, d^4y\, \varphi_{\vec{k}_i}^{(-)*}(y)\, V(y)\, \Delta_F(y;t_f,\vec{x})\, i\overleftrightarrow{\partial}_{t}\, \varphi_{\vec{k}_f}^{(-)}(t_f,\vec{x})$$

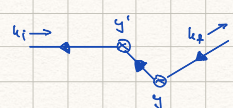
$$-(-i)^2\int d^3x\, d^4y\, d^4y'\, \varphi_{\vec{k}_i}^{(-)*}(y')\, V(y)\, \Delta_F(y,y')\, V(y')\, \Delta_F(y';t_f,\vec{x})\, i\overleftrightarrow{\partial}_{t}\, \varphi_{\vec{k}_f}^{(-)}(t_f,\vec{x}) + \dots$$

$$= \delta^{(3)}(\vec{k}_f - \vec{k}_i)$$

$$-i\int d^4y\, \varphi_{\vec{k}_i}^{(-)*}(y)\, V(y)\, \varphi_{\vec{k}_f}^{(-)}(y) \quad \longleftarrow \text{Born}$$



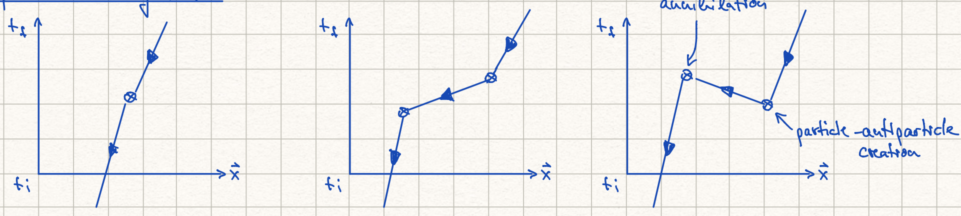
$$+(-i)^2\int d^4y\, d^4y'\, \varphi_{\vec{k}_i}^{(-)*}(y')\, V(y')\, \Delta_F(y',y)\, V(y)\, \varphi_{\vec{k}_f}^{(-)}(y) \quad \longleftarrow \text{2nd order}$$



↳ The configuration space Feynman rules we already formulated are still valid, just with an extension concerning the external antiparticle wave functions.

Again particle and antiparticle propagation is contained in $\Delta_F(y', y)$.

Space-time diagrams:



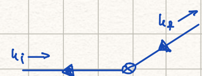
S-matrix element in momentum space

We use again: $\Delta_F(x, x') = \int \frac{d^4q}{(2\pi)^4} e^{-iqx} \frac{i}{q^2 - m^2 + i\epsilon} e^{+iqx'}$

$$\int d^4x \, e^{+iqx} V(x) e^{-iq'x} =: \tilde{V}(q, q') = \tilde{V}(q - q')$$

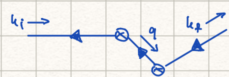
$$\bar{S}^{(1)}_{\vec{k}_f, \vec{k}_i} = -i \int d^4y \, \varphi^{(-)*}_{\vec{k}_i}(y) V(y) \varphi^{(-)}_{\vec{k}_f}(y)$$

$$= \frac{1}{(2\pi)^{3/2}} \frac{1}{\sqrt{2E_{\vec{k}_i}}} \left[-i \hat{V}(k_i, k_f)\right] \frac{1}{(2\pi)^{3/2}} \frac{1}{\sqrt{2E_{\vec{k}_f}}}$$



$$\bar{S}^{(2)}_{\vec{k}_f \vec{k}_i} = (-i)^2 \int d^4y \, d^4y' \, \varphi^{(-)*}_{\vec{k}_i}(y') V(y') \Delta_F(y', y) V(y) \varphi^{(-)}_{\vec{k}_f}(y)$$

$$= \frac{1}{(2\pi)^{3/2}} \frac{1}{\sqrt{2E_{\vec{k}_i}}} \left[-i \hat{V}(k_i, q)\right] \frac{i}{q^2 - m^2 + i\epsilon} \left[-i \hat{V}(q, k_f)\right] \frac{1}{(2\pi)^{3/2}} \frac{1}{\sqrt{2E_{\vec{k}_i}}}$$



↳ The momentum space Feynman rules we already formulated are still valid, just with an extension concerning the external antiparticle wave functions.

Here the antiparticle part of the propagator gives the dominant contribution in the nonrelativistic limit.

5.6.3 Particle - Antiparticle Creation and Annihilation

Even though we do not yet have a full conceptual framework to systematically describe processes with particle - antiparticle creation and annihilation, we can see that some elements to do that are already contained in the present framework. $\longrightarrow$ Need: QFT

The framework of the KG equation is not capable to do it, but we can guess part of the answer from the Feynman rules!

Particle - antiparticle annihilation

$$\mathcal{M}_{\vec{k},\vec{k}'} = \int dt_f\, d^3\vec{x}\; \tilde{\varphi}^{(-)*}_{\vec{k}}(x,t_f)\, \hat{O}^a(t_f,\vec{x})\, \tilde{\varphi}^{(+)}_{\vec{k}'}(x,t_f)$$

$\longleftarrow$ There is some external process that causes the matrix element and is encoded in the external operator $\hat{O}^a(t_f,\vec{x})$

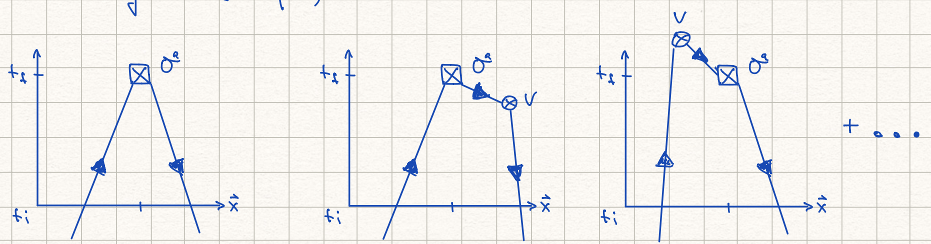
$\mathcal{M}_{\vec{k},\vec{k}'}$: only a part of the full amplitude

$\tilde{\varphi}^{(-)*}_{\vec{k}}$: incoming antiparticle time-evolved from $t_i \to -\infty$ to t_f

$\tilde{\varphi}^{(+)}_{\vec{k}'}$: incoming particle time evolved from $t_i \to -\infty$ t_f

$\hookrightarrow$ We can describe the effects of the interaction V within our available formalism.

Space-time diagrams: (examples)



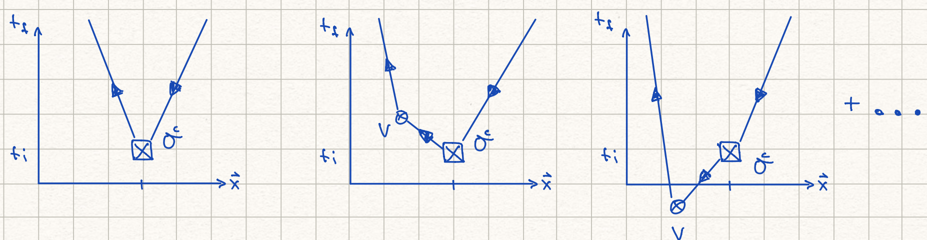
Particle - antiparticle creation

$$\mathcal{M}_{\vec{k},\vec{k}'} = \int dt_i\, d^3\vec{x}\; \tilde{\varphi}^{(+)*}_{\vec{k}}(x,t_i)\, \hat{O}^c(t_i,\vec{x})\, \tilde{\varphi}^{(-)}_{\vec{k}'}(x,t_i)$$

$\tilde{\varphi}^{(+)*}_{\vec{k}}$: outgoing particle time evolves into free particle at $t_f \to +\infty$

$\tilde{\varphi}^{(-)}_{\vec{k}'}$: outgoing particle time evolves into free particle at $t_f \to +\infty$

Space-time diagrams: (examples)



5.7. Charge Conjugation Transformation (C)

→ Which kind of particle we call particle and which antiparticle is in principle a convention.

C turns particle into antiparticle and vice versa.

Can be used for active and passive transformations

→ Here for a scalar particle:

$$C\,|\varphi_k^{(+)}\rangle = \eta\,|\varphi_k^{(-)}\rangle \;,\quad C\,|\varphi_k^{(-)}\rangle = \eta'\,|\varphi_k^{(+)}\rangle \;,\qquad |\eta|^2 = |\eta'|^2 = 1$$

↳ We propose: $\boxed{(\varphi(x))^c = \eta\,(\varphi(x))^* \,,\; |\eta| = 1}$ ← appears to work

But C has to be consistent to change the sign of the charge of a particle.

We can check this by applying C to the KG equation in the presence of an e.m. field:

$$(\Box + m^2 + iq\,(\partial_\mu A^\mu + A_\mu \partial^\mu) - q^2 A_\mu A^\mu)\,\varphi(x) = 0 \qquad \Big\downarrow (\;)^*$$

$$(\Box + m^2 - iq\,(\partial_\mu A^\mu + A_\mu \partial^\mu) - q^2 A_\mu A^\mu)\,\varphi^*(x) = 0 \qquad \leftarrow \text{Works!}$$