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Klein–Gordon equation from the path integral formalism*

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Abstract. By using Feynman's path integral formalism in the second order for the relativistic Lagrangian for a spinless particle in a gauge field and applying the covariant derivative instead of the commonly used derivative, but without knowing the operator expressions for the momentum and energy, one can obtain the Klein–Gordon equation.

1 Introduction

Nowadays there is a general belief that there are several equivalent ways of describing nature, these, however, being totally inequivalent in trying to guess the new laws in physics [1]. Before testing the power of the predictability of one way or the other, one would want to find out in the first place the old well-known relativistic equations by using the path integral formalism [2–13] in the case of a relativistic Lagrangian. In this article we will treat the simple case of a spin 0 free particle, i.e. the classical Klein–Gordon equation, discovered in 1926 [14–16].

The authors suggest that for a particle in an external gauge field the simplest way of doing this is to replace the commonly used derivative with the covariant derivative in the Klein–Gordon equation for a free particle, as is well known, instead of dealing with a more complicated Lagrangian in the path integral formalism.

Moreover, one should use the relativistic Lagrangian in the first quantization approach, instead of trying to guess how the Lagrangian might look like, and introducing it in the Euler–Lagrange equations and obtaining eventually the well known relativistic equations, as in the quantum field theories.

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2 Basic formalism

We will apply the path integral formalism [2–13] for simplicity in the unidimensional case, and then we will make a 3D generalization.

As is well known, the wave function $\Psi_0(x_\mathrm{f}, t_\mathrm{f})$ for a particle to arrive at x_f from $x_\mathrm{i} = x_\mathrm{f} + \eta$ after a time $\varepsilon = t_\mathrm{f} - t_\mathrm{i}$ is given by

$$\Psi_0(x_\mathrm{f}, t_\mathrm{f}) = \int_{-\infty}^{\infty} K(x_\mathrm{f}, t_\mathrm{f}, x_\mathrm{i}, t_\mathrm{i})\, \Psi(x_i, t_\mathrm{i})\, \mathrm{d}x_\mathrm{i}, \qquad (1)$$

where $K(x_\mathrm{f}, t_\mathrm{f}, x_\mathrm{i}, t_\mathrm{i})$ is the kernel for the particle in an external gauge field which up to a normalization constant factor A is

$$K(x_\mathrm{f}, t_\mathrm{f}, x_\mathrm{i}, t_\mathrm{i}) = \frac{1}{A} \exp\left(\frac{\mathrm{i}S}{\hbar}\right). \qquad (2)$$

In the first order approximation, we will use the action S written as

$$S = \int L \mathrm{d}t \simeq L\varepsilon. \qquad (3)$$

The relativistic Lagrangian for a particle in a gauge field is given in the first quantization, by using the rest mass of the particle m_0, the gauge charge q, and a gauge field $\Phi_\mathrm{G} \equiv (\boldsymbol{A}, A_0)$, by

$$L = \sqrt{(\boldsymbol{p} + \boldsymbol{p}_\mathbf{G})^2 c^2 + m_0^2 c^4} - m_0 c^2 - V_\mathrm{G}, \qquad (4)$$

$$\boldsymbol{p}_\mathbf{G} = \frac{q\boldsymbol{A}}{c}, \qquad (5)$$

$$V_\mathrm{G} = qA_0. \qquad (6)$$

Now, one can notice that either one may choose to work with the above defined relativistic Lagrangian and consequently, to perform some long calculus when expanding the amplitude in the right hand side of (1) in the old fashion of the path integral formalism [7,12], or to use the relativistic Lagrangian for the free particle and then to introduce the covariant derivative instead of the commonly used derivative.

We use the relativistic expression for the particle momentum as usually defined:

$$\boldsymbol{p} = m\boldsymbol{v} = m_0\gamma\boldsymbol{v} = \frac{m_0}{\sqrt{1-\beta^2}}\boldsymbol{v}, \tag{7}$$

so we can rewrite the relativistic Lagrangian for a free particle in the following form:

$$L = m_0c^2\left(\frac{1}{\sqrt{1-\beta^2}} - 1\right). \tag{8}$$

For very small space-time intervals we can define as usually:

$$\beta^2 = \left(\frac{v}{c}\right)^2 = \frac{\eta^2}{c^2\varepsilon^2}. \tag{9}$$

One can now replace the kernel $K\left(x_{\mathrm{f}}, t_{\mathrm{f}}, x_{\mathrm{i}}, t_{\mathrm{i}}\right)$ for the free particle in (1) by corroborating (2), (3), (8), and (9), and by applying a cutoff on the integral limits implied by the second postulate of the special relativity [17]:

$$\begin{aligned}\Psi_0\left(x_{\mathrm{f}}, t_{\mathrm{i}}+\varepsilon\right) &= \frac{1}{A}\mathrm{e}^{-(im_0c^2\varepsilon)/\hbar} \qquad (10)\\ &\times \lim_{\delta\to 0}\int_{-c\varepsilon+\delta}^{c\varepsilon-\delta} \mathrm{e}^{(im_0c^3\varepsilon^2)/(\hbar\sqrt{c^2\varepsilon^2-\eta^2})}\Psi\left(x_{\mathrm{f}}+\eta, t_{\mathrm{i}}\right)\mathrm{d}\eta.\end{aligned}$$

After expanding the final wave function $\Psi_0\left(x_{\mathrm{f}}, t_{\mathrm{i}}+\varepsilon\right)$ in the right hand side, the initial wave function $\Psi(x_{\mathrm{f}} + \eta, t_{\mathrm{i}})$ and the exponential $\mathrm{e}^{-(im_0c^2\varepsilon)/\hbar}$ in the left hand side can be written

$$\begin{aligned}\Psi + \varepsilon\frac{\partial\Psi}{\partial t} + \frac{\varepsilon^2}{2!}\frac{\partial^2\Psi}{\partial t^2} &= \frac{1}{A}\left(1 - \frac{\mathrm{i}m_0c^2}{\hbar}\varepsilon - \frac{m_0^2c^4}{\hbar^2}\frac{\varepsilon^2}{2!}\right)\\ &\times \lim_{\delta\to 0}\int_{-c\varepsilon+\delta}^{c\varepsilon-\delta} \mathrm{e}^{(im_0c^3\varepsilon^2)/(\hbar\sqrt{c^2\varepsilon^2-\eta^2})}\\ &\times\left(\Psi + \frac{\partial\Psi}{\partial x}\eta + \frac{\partial^2\Psi}{\partial x^2}\frac{\eta^2}{2!}\right)\mathrm{d}\eta. \qquad (11)\end{aligned}$$

Taking into account that the factor $A\left(\varepsilon\right)$ is deduced from the normalization condition,

$$\frac{1}{A\left(\varepsilon\right)}\lim_{\delta\to 0}\int_{-c\varepsilon+\delta}^{c\varepsilon-\delta} \mathrm{e}^{(im_0c^3\varepsilon^2)/(\hbar\sqrt{c^2\varepsilon^2-\eta^2})}\mathrm{d}\eta = 1, \tag{12}$$

and also that $\left\{1, \varepsilon, \varepsilon^2, ...\right\}$ form a linear independent system, and finally that the odd integrand on symmetric intervals gives a zero contribution, we can identify the coefficient of ε^2 as follows [18]:

$$\left(\frac{\partial^2}{\partial t^2} - \frac{I_2\left(\varepsilon\right)}{\varepsilon^2}\frac{\partial^2}{\partial x^2} + \frac{m_0^2c^4}{\hbar^2}\right)\Psi = 0. \tag{13}$$

One can notice that after the evaluation of $I_2\left(\varepsilon\right)$, defined by

$$I_2\left(\varepsilon\right) = \frac{2}{A\left(\varepsilon\right)}\lim_{\delta\to 0}\int_0^{c\varepsilon-\delta} \mathrm{e}^{(im_0c^3\varepsilon^2)/(\hbar\sqrt{c^2\varepsilon^2-\eta^2})}\eta^2\mathrm{d}\eta, \tag{14}$$

only the terms in ε^2 should be preserved.

Before evaluating the $I_2\left(\varepsilon\right)$ integral, the authors wish to lay stress on another characteristic feature of the path integral formalism. We change the η variable, by choosing e.g. $\eta = c\varepsilon\sin p$. Thus, (12) and (14) become

$$\begin{aligned}I_0\left(\varepsilon\right) &= \frac{2c\varepsilon}{A\left(\varepsilon\right)}\lim_{\delta\to 0}\int_0^{(\pi/2)-\delta} \mathrm{e}^{(im_0c^2\varepsilon)/(\hbar\cos p)}\cos p\mathrm{d}p\\ &= 1, \qquad (15)\\ I_2\left(\varepsilon\right) &= \frac{2\left(c\varepsilon\right)^3}{A\left(\varepsilon\right)}\lim_{\delta\to 0}\int_0^{(\pi/2)-\delta} \mathrm{e}^{(im_0c^2\varepsilon)/(\hbar\cos p)}\cos p\sin^2 p\mathrm{d}p\\ &= \left(c\varepsilon\right)^2 - J_a\left(\varepsilon\right), \qquad (16)\end{aligned}$$

where

$$J_a\left(\varepsilon\right) = \frac{2\left(c\varepsilon\right)^3}{A\left(\varepsilon\right)}\lim_{\delta\to 0}\int_0^{(\pi/2)-\delta} \mathrm{e}^{(im_0c^2\varepsilon)/(\hbar\cos p)}\cos^3 p\mathrm{d}p. \tag{17}$$

3 The evaluation of the $I_2\left(\varepsilon\right)$ integral

The whole path integral formalism was developed on the assumption that the perturbative calculus for very small space-time intervals could be performed [1–13], and that consequently the greatest contribution of the above integral is given for small values of the phase $\theta = (m_0c^2\varepsilon)/(\hbar\cos p)$, i.e. in our case, for the nonrelativistic regime where $\cos p \approx 1$.

We give for comparison the representation of the nonrelativistic versus relativistic pionic real component of the propagator for different ε values (Fig. 1). The main contribution of the integral for higher ε values comes from the range of very small velocities $p \to 0$ as can be noticed from Figs. 1e,g.

In order to see the sensitivity to the rest mass of the particle m_0, in Fig. 2 we represent the real part of the kernel for a charged pion ($m_0 = 139\,\mathrm{MeV}$), a charged kaon ($m_0 = 494\,\mathrm{MeV}$), and a neutral η^0 ($m_0 = 548\,\mathrm{MeV}$) respectively, for a fixed time ε. In order to obtain the same shape of the kernel distribution for the same velocity of the particle, one needs to shift towards smaller ε as m_0 increases. Therefore, it has become a strong belief of the authors that the notion of the infinitesimal in physics could be very different from as it is nowadays understood in mathematics.

In order to evaluate the $I_2\left(\varepsilon\right)$ integral, one may derive $J_a\left(\varepsilon\right)$ as a function of the ε parameter:

$$\frac{\mathrm{d}J_a}{\mathrm{d}\varepsilon} = \left(\frac{3}{\varepsilon} - \frac{\mathrm{d}\ln A\left(\varepsilon\right)}{\mathrm{d}\varepsilon}\right)J_a + \left(\frac{\mathrm{i}m_0c^2}{\hbar}\right)J_b\left(\varepsilon\right), \tag{18}$$

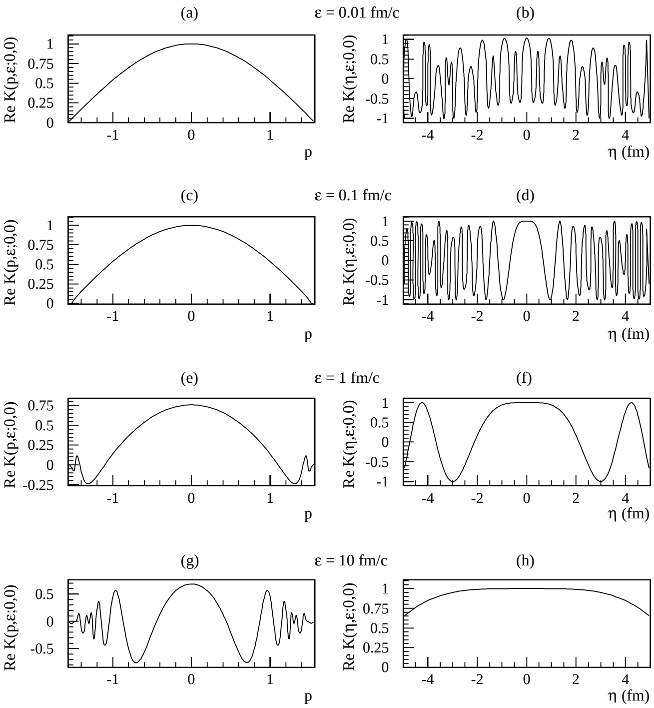

Fig. 1a–h. The relativistic (left panels) versus nonrelativistic pionic real part of the kernel for various small ε values

where

$$J_b\left(\varepsilon\right)=\frac{2\left(c\varepsilon\right)^3}{A\left(\varepsilon\right)}\lim_{\delta\to 0}\int_0^{(\pi/2)-\delta}\mathrm{e}^{(\mathrm{i}m_0c^2\varepsilon)/(\hbar\cos p)}\cos^2 p\mathrm{d}p. \tag{19}$$

We apply the same procedure to the $J_b\left(\varepsilon\right)$ integral and obtain a first order linear differential equation:

$$\frac{\mathrm{d}J_b}{\mathrm{d}\varepsilon}=\left(\frac{3}{\varepsilon}-\frac{\mathrm{d}\ln A\left(\varepsilon\right)}{\mathrm{d}\varepsilon}\right)J_b+\frac{\mathrm{i}m_0c^4}{\hbar}\varepsilon^2=g\left(\varepsilon\right)J_b+h\left(\varepsilon\right), \tag{20}$$

having the following solution (see e.g. [19]):

$$J_b\left(\varepsilon\right)=\exp\left(\lim_{\varepsilon_0\to 0}\int_{\varepsilon_0}^{\varepsilon}g\left(\varepsilon^{'}\right)\mathrm{d}\varepsilon^{'}\right) \tag{21}$$
$$\times\lim_{\varepsilon_0\to 0}\int_{\varepsilon_0}^{\varepsilon}h\left(\varepsilon^{'}\right)\exp\left(-\lim_{\varepsilon_0\to 0}\int_{\varepsilon_0}^{\varepsilon^{'}}g\left(\varepsilon^{''}\right)\mathrm{d}\varepsilon^{''}\right)\mathrm{d}\varepsilon^{'}.$$

We have taken into account that

$$\lim_{\varepsilon_0\to 0}J_a\left(\varepsilon_0\right)=\lim_{\varepsilon_0\to 0}J_b\left(\varepsilon_0\right)=0. \tag{22}$$

As compared with the nonrelativistic case [7,12], we shall not be interested in how the normalization factor $A\left(\varepsilon\right)$ might look like, as long as for very small time intervals ε one can extend an analytical function into a power series, in our case from $\gamma=1$, as can be noticed from (15):

$$A\left(\varepsilon\right)=\sum_{\gamma=1}^{\infty}d_\gamma\varepsilon^\gamma, \tag{23}$$

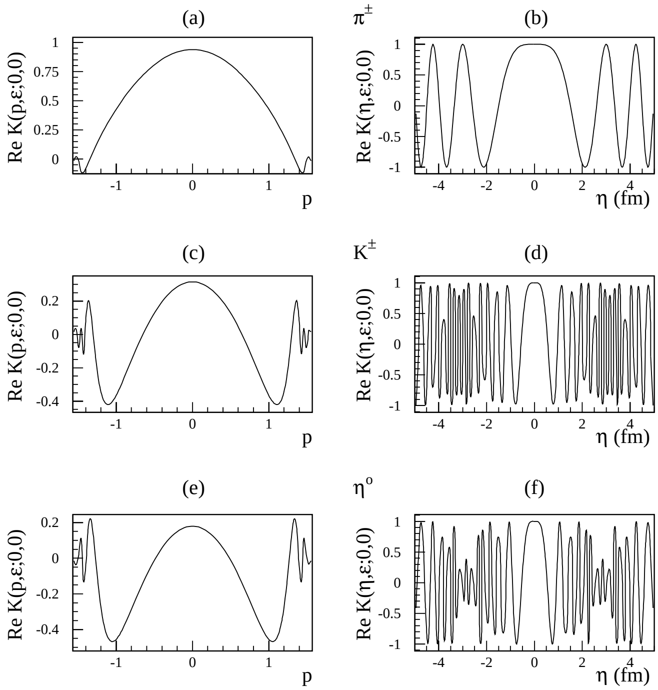

Fig. 2a–f. The real component of the propagator for several spinless particles from the ground-state pseudoscalar octet of SU(3): charged pions and kaons (upper and middle panels), and neutral η^0 respectively, for the chosen value of the time elapsed between the final and the initial state of the particle: $\varepsilon=0.5\,\mathrm{fm}/c$

and therefore, by using the absolute convergence of the above power series, to be able to switch it with the integral during our next calculations.

After applying the well known formula

$$\mathrm{e}^{k\ln u}=u^k, \tag{24}$$

we get the following expression for $J_b\left(\varepsilon\right)$:

$$J_b\left(\varepsilon\right)=\frac{\mathrm{i}m_0c^4}{\hbar}\lim_{\varepsilon_0\to 0}\left(\frac{\varepsilon}{\varepsilon_0}\right)^3\frac{A\left(\varepsilon_0\right)}{A\left(\varepsilon\right)}$$
$$\times\lim_{\varepsilon_0\to 0}\int_{\varepsilon_0}^{\varepsilon}\left(\frac{\varepsilon_0}{\varepsilon^{'}}\right)^3\frac{A\left(\varepsilon^{'}\right)}{A\left(\varepsilon_0\right)}\varepsilon^{'2}\mathrm{d}\varepsilon^{'}. \tag{25}$$

One can easily perform the whole calculus and finally obtain

$$J_b\left(\varepsilon\right)=\frac{\mathrm{i}m_0c^4}{\hbar}\frac{\sum_{\gamma=1}^{\infty}\dfrac{d_\gamma\varepsilon^{\gamma+3}}{\gamma}}{\sum_{\gamma=1}^{\infty}d_\gamma\varepsilon^\gamma}. \tag{26}$$

We shall now go to the result in (18), and repeating the whole procedure one easily gets the final expression for $I_2\left(\varepsilon\right)$:

$$I_2\left(\varepsilon\right)=\left(c\varepsilon\right)^2+\left(\frac{m_0c^3}{\hbar}\right)^2\frac{\sum_{\gamma=1}^{\infty}\dfrac{d_\gamma\varepsilon^{\gamma+4}}{\gamma\left(\gamma+1\right)}}{\sum_{\gamma=1}^{\infty}d_\gamma\varepsilon^\gamma}. \tag{27}$$

4 Final results and conclusions

One can also notice that the terms containing ε^4 will not contribute to (13), so we can rewrite after introducing (27) and dividing by c^2

$$\sum_{\gamma=1}^{\infty} d_\gamma \varepsilon^\gamma \left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2} + \frac{m_0^2 c^2}{\hbar^2} \right) \Psi = 0. \quad (28)$$

After we generalize to 3D the above equation, by using the d'Alembertian operator

$$\Box \equiv g^{\mu\nu}\partial_\mu \partial_\nu = \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2}, \quad (29)$$

where the spacetime metric $g^{\mu\nu}$ in an inertial coordinate system has only diagonal elements:

$$g^{11} = g^{22} = g^{33} = -g^{00} = -1, \quad (30)$$

we finally obtain the Klein–Gordon equation for a free particle:

$$\left(\Box + \frac{m_0^2 c^2}{\hbar^2} \right) \Psi = 0 \; . \quad (31)$$

Moreover, because the path integral formalism does not impose any constraints on how the derivative might look like, one can finally substitute the commonly used derivative with the covariant derivative:

$$D_\mu = \partial_\mu + \frac{\mathrm{i}q}{\hbar c} A_\mu, \quad (32)$$

and obtain the Klein–Gordon equation for a particle in a gauge field:

$$\left(\Box + \frac{2\mathrm{i}q}{\hbar c} A^\mu \partial_\mu + \frac{\mathrm{i}q}{\hbar c} \partial_\mu A^\mu - \frac{q^2}{\hbar^2 c^2} A_\mu A^\mu + \frac{m_0^2 c^2}{\hbar^2} \right) \Psi = 0, \quad (33)$$

which is usually written as

$$\left(D_\mu D^\mu + \frac{m_0^2 c^2}{\hbar^2} \right) \Psi\left(x,t\right) = 0, \quad (34)$$

or, by using the coupling constant g and the source of the scalar field $\rho\left(x,t\right)$:

$$\left(\Box + \frac{m_0^2 c^2}{\hbar^2} \right) \Psi\left(x,t\right) = g\rho\left(x,t\right). \quad (35)$$

One may notice that the Klein–Gordon equation for a particle, subject to no external influence, naturally emerged from the path integral formalism without even knowing the operator expressions for the momentum and energy. Also, we performed the calculus in the first quantization approach, with a Lorentz invariant Lagrangian that one should not be forced to guess by starting from the form of the field equation itself and then applying the Euler–Lagrange equation.

The path integral formalism, which represents an extension of the principle of minimum action, could be the most satisfactory way to find the old equations of physics and maybe also to predict new ones.

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