

Calculating propagators for relativistic wave equations

Mingjie Li^{*} and S. A. R. Horsley[†]

Department of Physics and Astronomy, *University of Exeter*, Stocker Road, Exeter EX4 4QL, England



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Here we examine the propagation of relativistic fields in space-time using the viewpoint applied to derive the Rayleigh–Sommerfeld diffraction integral in three-dimensional space. We use this theory to find the propagators for both the Klein–Gordon equation and the Dirac equation. Based on these results, we highlight some apparently overlooked aspects of the Feynman checkerboard model as it is usually applied to the Dirac equation.

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I. INTRODUCTION

Inspired by Dirac’s discovery of a connection between the Lagrangian in classical mechanics and Heisenberg’s matrix mechanics [1], Feynman proposed the path-integral formulation [2] to describe the behavior of matter waves in terms of a sum over path-dependent phases, instead of a wave equation, providing an intuitive physical picture of how matter waves propagate through various paths. This approach has proven to be useful for calculating time evolution in quantum mechanics, both in single-particle theory and field theory [3–6]. The path integral shows that there is a contribution to the phase of a matter wave that is proportional to the Hamiltonian action of the particle, with the classical path dominating in the classical limit, $\hbar \rightarrow 0$.

There is a similar situation in optics, in diffraction theory, where Kirchhoff’s theory gives the optical wave in terms of a sum of source waves distributed across a wave front, which can be understood as a sum over paths. Although diffraction theory is usually applied in three-dimensional (3D) space—time being neglected through the assumption of time-harmonic fields—the same approach can be extended to space-time. This was first examined some time ago in, e.g., Ref. [7], where Kirchhoff diffraction theory was extended to treat propagation in $(3 + 1)$ dimensions. In this work, based on this connection between the path integral and diffraction theory, we use Rayleigh diffraction theory to construct the propagators for the Klein–Gordon [8] and Dirac equations [9]. We note that our work is connected to the application of diffraction theory, including time evolution, which has found wide-ranging applications in recent research [10–14].

In what follows we will compare the results of our approach to a different method for calculating the propagator,

given by Feynman [15], for the particular case of the $(1 + 1)$ D Dirac equation. This is known as the Feynman checkerboard model and differs from the sum over paths applied to the Schrödinger equation [16]. Note that this checkerboard approach has been extended to the full Dirac equation in $(3 + 1)$ dimensions, see, e.g., Ref. [17]. We shall show that, using our approach, we reclaim the checkerboard propagator but with additional terms that are nonzero only on the light cone, which are essential to reclaim the correct zero mass limit.

II. THE PROPAGATOR FOR THE KLEIN–GORDON EQUATION

We begin with a simple example of our approach, considering the $(3 + 1)$ dimensional Klein–Gordon equation [8,18]:

$$(\eta^{\mu\nu} \partial_\nu \partial_\mu + M^2)\Psi = 0, \quad (1)$$

with $\eta^{\mu\nu} = \text{diag}\{c^{-2}, -1, -1, -1\}$ and $M = mc/\hbar$. In the spirit of diffraction theory, we start from the following identity:

$$\Psi(x'^{\mu}) = \int_V \delta^{(4)}(x^{\mu} - x'^{\mu}) \Psi(x^{\mu}) dx dy dz dt, \quad (2)$$

where $\delta^{(4)}(x^{\mu} - x'^{\mu})$ is the four-dimensional δ function, and V is a four-dimensional volume containing the observation point (x', y', z', t') . Without loss of generality, let (x', y', z', t') be a space-time point in the future of time t , i.e., $t' > t$. The four-dimensional volume V is similarly chosen such that $t' \geq t$. To make use of the identity (2), the δ function needs to be expressed in terms of the Green function for the Klein–Gordon equation (1), which satisfies

$$(\eta^{\mu\nu} \partial_\nu \partial_\mu + M^2)G(x^{\xi} - x'^{\xi}) = \delta^{(4)}(x^{\xi} - x'^{\xi}). \quad (3)$$

In addition, we need to transform the space-time volume integral into a boundary integral. To achieve both of these aims, we should express the integrand of (2) as a four-dimensional divergence. By direct analogy with Kirchhoff’s approach to diffraction integrals, we observe that the integrand in Eq. (2) can—through application of Eq. (3)—be expressed as a four-divergence as follows:

$$-\eta^{\mu\nu} \partial_\mu [G \partial_\nu \Psi - \Psi \partial_\nu G] = \delta^{(4)}(x^{\mu} - x'^{\mu}) \Psi. \quad (4)$$

^{*}Contact author: ml813@exeter.ac.uk

[†]Contact author: S.Horsley@exeter.ac.uk

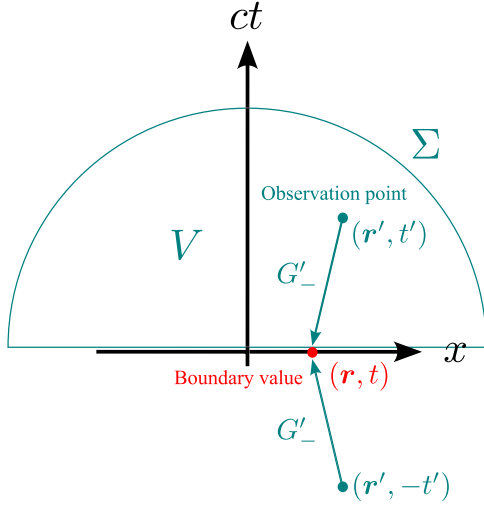


FIG. 1. Rayleigh's trick in space-time: The field at $(\mathbf{r}', t')$ is found through integrating an advanced Green function and its derivative (source point equals $(\mathbf{r}', t')$) over the boundary. The Green function can be made to vanish on the $t = 0$ boundary through including a mirrored (retarded) source outside V . This ensures that the field at the observation point depends only on the field values on the $t = 0$ boundary.

At this point we note that there are four different choices for the Green function. These are the retarded and advanced Green functions (vanishing for $t - t' < 0$ and $t - t' > 0$, respectively), which are given by

$$G_{\pm}(\mathbf{R}, \tau) = \frac{Mc}{4\pi s} \Theta\left(\pm\tau - \frac{R}{c}\right) J_1(Ms) - \frac{c}{2\pi} \delta\left(\tau \mp \frac{R}{c}\right), \quad (5)$$

and the noncausal Green functions (these are nonzero both for $t > t'$ and $t < t'$), which are defined by

$$G'_{\pm}(\mathbf{R}, \tau) = \frac{\mp ic}{(2\pi)^2 s} \frac{d}{ds} \left[\Theta(s^2) \frac{\pm i\pi}{2} H_0^{(\frac{3\mp 1}{2})}(\mu s) + \Theta(-s^2) K_0(\mu \sqrt{-s^2}) \right], \quad (6)$$

where in both Eqs. (5) and (6) we have now separated the time and space coordinates and used $s^2 = c^2 \tau^2 - R^2$ with $\tau = t - t'$, $R = |\mathbf{R}| = |\mathbf{r} - \mathbf{r}'|$, $\mathbf{r} = (x, y, z)$ and $\mathbf{r}' = (x', y', z')$. In these equations Θ is the Heaviside step function, J_n the n th-order Bessel function of the first kind, $H_n^{(3\mp 1)/2}$ is the n th-order Hankel function of the first or second kind (corresponding to $(3 \mp 1)/2 = 1, 2$), and K_n is the n th-order modified Bessel function of the second kind. Substituting Eq. (4) into Eq. (2) gives

$$\Psi(\mathbf{r}', t') = - \int_V \eta^{\mu\nu} \partial_{\mu} [G \partial_{\nu} \Psi - \Psi \partial_{\nu} G] dx dy dz dt. \quad (7)$$

Assuming the space-time volume indicated in Fig. 1 and applying the four-dimensional Gauss theorem to Eq. (7), the wave function at $(\mathbf{r}', t')$ becomes equal to a boundary

integral,

$$\Psi(\mathbf{r}', t') = \int_{t=0} \frac{1}{c^2} [G \partial_t \Psi - \Psi \partial_t G] dx dy dz + \int_{\Sigma} [\Psi \partial_{\mu} G - G \partial_{\mu} \Psi] d^3 S^{\mu}, \quad (8)$$

where Σ denotes the upper boundary shown in Fig. 1, and $d^3 S^{\mu}$ denotes the infinitesimal surface element in four-dimensional space along the upper boundary Σ .

To eliminate the temporal derivative term of Ψ in Eq. (8), we can define the Green function as arising from two sources, one of which is outside of the space-time integration region V , as shown in Fig. 1. Being outside of the integration region, this second source does not modify the left-hand side of Eq. (8). Mirroring these two sources in time, we can thus choose the Green function in Eq. (8) to vanish on the $t = 0$ boundary, defining

$$G_R(\mathbf{r}, \mathbf{r}'; t, t') = G'_-(\mathbf{R}, t - t') - G'_-(\mathbf{R}, t + t'), \quad (9)$$

where G'_- is the Green function defined in Eq. (6), which we refer to as the “Rayleigh–Green function.” As noted in the caption to Fig. 1, this approach is formally identical to that used by Rayleigh in the theory of diffraction, where the $t = 0$ boundary is, in that case, a spatial boundary.

As it stands, Eq. (8) requires us to specify the field Ψ on both the $t = 0$ and the infinite future (Σ space-time surfaces). In diffraction theory, the contribution of the analogous spatial boundary at infinity is eliminated using the Sommerfeld condition [19], which is equivalent to the statement that all energy travels outward to infinity. We now give the boundary condition necessary to eliminate the contribution of the field on the boundary Σ in space-time to eliminate the upper boundary integral in Eq. (8).

Performing the Fourier transformation with respect to 3D spatial coordinates and replacing the Green function in Eq. (9) with the Rayleigh–Green function Eq. (9) yields

$$\Psi(\mathbf{k}, t') = \frac{1}{c^2} [\Psi(\mathbf{k}, t) \partial_t G_R(t - t'; \mathbf{k}) - G_R(t - t'; \mathbf{k}) \partial_t \Psi(\mathbf{k}, t)]_{t=0}^{\infty}, \quad (10)$$

where Σ is now the upper $t = \infty$ boundary on the square brackets. Since by definition the “Rayleigh–Green function” G_R vanishes at $t = 0$, Eq. (10) simplifies to

$$\Psi(\mathbf{k}, t') = - \frac{1}{c^2} \Psi(\mathbf{k}, t) \partial_t G_R(t - t'; \mathbf{k})|_{t=0} + \frac{1}{c^2} [\Psi(\mathbf{k}, t) \partial_t G_R(t - t'; \mathbf{k}) - G_R(t - t'; \mathbf{k}) \partial_t \Psi(\mathbf{k}, t)]_{t \rightarrow \infty}. \quad (11)$$

The corresponding Fourier transformation of the Rayleigh–Green function Eq. (9), $G_R(t - t'; \mathbf{k})$, in Eq. (11) is then given by

$$G_R(t - t'; \mathbf{k}) = - \frac{i\pi}{\omega k} (e^{-i\omega k |t - t'|} - e^{-i\omega k |t + t'|}). \quad (12)$$

Note we have here chosen the negative exponential, the positive sign also being admissible provided we modify the boundary condition in Eq. (13), below. Substituting Eq. (12)

into Eq. (11), we find that in order to eliminate the second term corresponding to the upper boundary $t \rightarrow \infty$, the wave function must satisfy the following condition:

$$\lim_{T \rightarrow \infty} i\omega_k \Psi(\mathbf{k}, T) + \partial_t \Psi(\mathbf{k}, T) = 0, \quad (13)$$

where $\omega_k = c\sqrt{|\mathbf{k}|^2 + M^2} > 0$. We observe that Eq. (13) is the space-time analog of the usual Sommerfeld condition discussed above and is equivalent to the requirement that each Fourier component of the field evolves in time with a positive frequency, i.e., as $\exp(-i\omega_k t)$. Therefore, applying condition Eq. (13), the Rayleigh–Sommerfeld diffraction integral for the Klein–Gordon equation is given by the simple expression

$$\Psi(\mathbf{r}', t') = -\frac{1}{c^2} \int_{t=0} \Psi(\mathbf{r}, 0) \partial_t G_R(\mathbf{r}, \mathbf{r}'; t, t') d\mathbf{x} d\mathbf{y} d\mathbf{z}. \quad (14)$$

From our simple argument, we can thus see that the propagator (for positive frequency fields) for the Klein–Gordon equation is given by

$$K(\mathbf{r}, \mathbf{r}'; t, t') = -\frac{1}{c^2} \partial_t G_R(\mathbf{r}, \mathbf{r}'; t, t'), \quad (15)$$

where the Green function is the “Rayleigh–Green function” defined in Eq. (9).

III. THE DIFFRACTION INTEGRAL FOR THE DIRAC EQUATION

Having found the propagator from the Klein–Gordon equation using an argument analogous to Rayleigh’s, we apply the idea to the Dirac equation [9]:

$$(i\gamma^\mu \partial_\mu - M\mathbb{1})\Psi = 0, \quad (16)$$

where $\mathbb{1}$ is the identity matrix and the γ^μ are the four Dirac γ matrices obeying $\{\gamma^\mu, \gamma^\nu\} = 2\eta^{\mu\nu}$, and M is defined as in the previous section. We again start from the δ function identity Eq. (2) and introduce the (matrix) Green function, obeying $(i\gamma^\mu \partial_\mu - M)G = \delta^{(4)}(x^\nu - x'^\nu)$. Similar to Eq. (4), we find that

$$\partial_\mu (-i\bar{G}\gamma^\mu \Psi) = \delta^{(4)}(x^\nu - x'^\nu) \Psi, \quad (17)$$

where $\bar{G}$ denotes the Dirac adjoint of the Green function, i.e., $\bar{G} = \gamma^0 G^\dagger \gamma^0$, with $\dagger$ denoting the Hermitian conjugate. Again, as in the previous example, there are four different choices for the Green function. By contrast, here we choose the *causal* (advanced) Green function:

$$G = -(i\gamma^\mu \partial_\mu + M\mathbb{1})G_-, \quad (18)$$

where G_- is the advanced Green function defined in Eq. (5). Integrating Eq. (17) over the same space-time domain as shown in Fig. 1, i.e., $t > 0$, we again obtain a Rayleigh-like diffraction integral for the Dirac equation:

$$\Psi(\mathbf{r}', t') = \int_{t=0} \frac{i}{c} \gamma^0 G^\dagger(\mathbf{r} - \mathbf{r}', t - t') \Psi(\mathbf{r}, t) d\mathbf{x} d\mathbf{y} d\mathbf{z}. \quad (19)$$

In this case, the integration over the upper boundary Σ vanishes since the Green function itself vanishes there. The propagator for the Dirac equation is therefore given by

$$K(\mathbf{r} - \mathbf{r}', t - t') = \frac{i}{c} \gamma^0 G^\dagger(\mathbf{r} - \mathbf{r}', t - t'). \quad (20)$$

In the special case of the $(1+1)$ -dimensional Dirac equation with $\gamma^0 = \sigma_x$ and $\gamma^1 = -i\sigma_y$, the integral Eq. (19) reduces to 1 over a single spatial coordinate x , and the advanced Green function appearing in Eq. (18) is given by (see Appendix for derivation)

$$G_-(x - x', \tau) = \frac{c}{2} \Theta\left(-\tau - \frac{|x - x'|}{c}\right) J_0(Ms), \quad (21)$$

where τ was defined in the previous section. Combining Eqs. (18), (20), and (21), the propagator Eq. (20) for the $(1+1)$ -dimensional Dirac equation becomes

$$\begin{aligned} K = & -\frac{1}{2} \left\{ i\sigma_x M \Theta\left(-\tau - \frac{|x - x'|}{c}\right) J_0(Ms) \right. \\ & - \mathbb{1} \Theta\left(-\tau - \frac{|x - x'|}{c}\right) \frac{Mc\tau}{s} J_1(Ms) \\ & - \sigma_z \Theta\left(-\tau - \frac{|x - x'|}{c}\right) \frac{M(x - x')}{s} J_1(Ms) \\ & - \frac{1}{c} \mathbb{1} \delta\left(-\tau - \frac{|x - x'|}{c}\right) \\ & \left. + \sigma_z \frac{1}{c} \delta\left(-\tau - \frac{|x - x'|}{c}\right) \sin(x - x') \right\}. \end{aligned} \quad (22)$$

where $s = \sqrt{c^2\tau^2 - |x - x'|^2}$. Note in the special case when the mass is zero, the propagator Eq. (22) is simply a sum of two δ functions, indicating free propagation at the speed of light. As we shall see, these δ functions arise from propagation along the light cone, which appear to have been overlooked in previous treatments of the Feynman checkerboard model.

IV. COMMENTS ON THE FEYNMAN CHECKERBOARD MODEL

The propagator for the Dirac equation was first discussed by Feynman [15], via the Feynman checkerboard model, which we have described in Fig. 2. This calculation of the propagator is notably different from the approach applied to the Schrödinger equation. In Feynman’s original calculation of the propagator (22), the particle can only move forward or backward in one dimension at the speed of light, c . The particle occasionally reverses its direction at a rate proportional to the rest mass, m . This generates a random walk, as sketched in Fig. 2. The corresponding wave function of the particle is assumed to change its amplitude by a factor $iMc\epsilon$ after each reversal, where ϵ is the small time step into which the path is discretized (also shown in Fig. 2). Combining these assumptions, the propagator K for the Dirac equation is equal to [15]

$$K = \sum_R N(R) (iMc\epsilon)^R, \quad (23)$$

where R is the number of corners on the path illustrated in Fig. 2 (i.e., the number of times the trajectory switches between left-going and right-going), and $N(R)$ is the total number of paths with R corners. The sum in the propagator Eq. (23) can, after an evaluation of $N(R)$ using combinatorics and an application of the Stirling formula for a large number

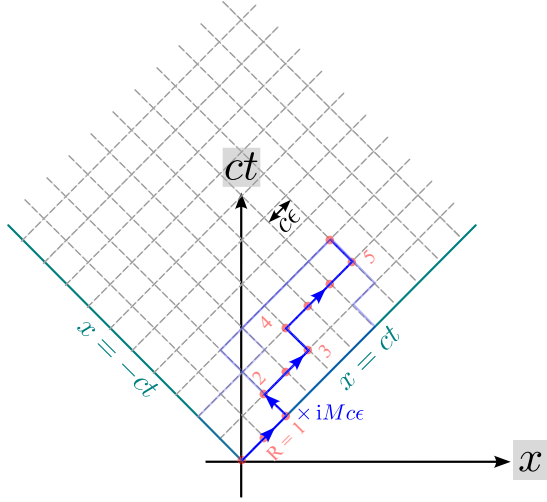


FIG. 2. The Feynman checkerboard model: The propagator for the $(1+1)$ -dimensional Dirac equation can be constructed according to Eq. (23), as a sum over paths, each traveling at the speed of light $x = \pm ct$. Here we show one such path as the dark-blue zigzag line (other contributions represented as faded blue lines), which has $R = 5$ corners in this example. This trajectory illustrates that the particle occasionally moves forward or backward at light speed, with the rate of interchange determined by M , defined below Eq. (1). At each corner the contribution to the propagator from the chosen path gains a factor of iMc .

of time steps [20], be evaluated as

$$K = \sigma_x J_0(Ms) + i \frac{c\tau}{s} J_1(Ms) + i \frac{(x - x')}{s} \sigma_z J_1(Ms). \quad (24)$$

The Pauli matrices in the propagator Eq. (24) assume the representation of the γ matrices in the $(1+1)$ D Dirac equation with $\gamma^0 = \sigma_x$ and $\gamma^1 = -i\sigma_y$. We should also note that, in Feynman's model, all paths are confined inside the light cone, as shown in Fig. 2. To ensure zero propagation outside of the light cone and to confine ourselves to propagation into the future, $t' > t$, we should thus multiply Eq. (24) by the Heaviside step functions, $\Theta(-\tau)\Theta(s^2) = \Theta(-\tau - |x - x'|/c)$, as we have in Eq. (22).

The propagator given in Eq. (24) is very closely related to the expression we found above but neglects two terms, which are the δ functions in Eq. (22). The three nonsingular terms in propagator Eq. (24), derived from the Feynman checkerboard model in, e.g., Ref. [20], are identical to those in our result Eq. (22) except for a normalization factor $-iM/2$ (we note that this factor is required to give the propagator the correct units of inverse length and thus does not alter the units of the field!). We note also that our propagator Eq. (22) becomes a δ function when the evolution time τ vanishes (as required to give back the original field distribution when taking the limit of zero time evolution). In contrast, the propagator Eq. (24) does not. Furthermore, when the mass vanishes, namely, $m = 0$ —a case not obviously considered by Feynman—the propagator Eq. (23) is 1 on the light cone and 0 elsewhere. But in this case, the Dirac equation is identical to the $(1+1)$ D Maxwell equations in free space. These δ terms in the propagator Eq. (22) simply mean that the wave

propagates freely with a retarded time $\tau = |x - x'|/c$. This fact is excluded from the propagator Eq. (24), which tends to unity when $m = 0$. In fact, the additional $\delta(\tau - |x - x'|/c)$ terms originate from those paths on the light cone which have no corner in the Feynman checkerboard model, illustrated as the teal line in Fig. 2. These discrepancies arise because the Feynman checkerboard model is a discrete model. For paths lying on the light cone, the amplitude computed from Eq. (23) is always 1, which, in fact, we can understand as a Kronecker δ , equivalent to zero in the continuous limit, thus eliminating the required δ -function terms from Eq. (24).

In addition, in the $(3+1)$ D Feynman checkerboard model, the $(3+1)$ D Dirac propagator Eq. (20) also differs from the one given in earlier works (e.g., Ref. [17]), as evident from the presence of Bessel and δ functions in Eq. (5). Furthermore, when $\tau = 0$ the propagator should be a δ function, whereas the one in Ref. [17] is 1, which arises again from a Kronecker δ —the same issue discussed above, arising from the discrete nature of the Feynman checkerboard model. We should emphasize that our propagator, Eq. (20), is correct, being derived directly from the wave equation itself without relying on any particular model.

V. SUMMARY AND CONCLUSIONS

We have developed an approach analogous to the Rayleigh–Sommerfeld diffraction integral, applied in space-time, to find the propagators of both the Klein–Gordon and Dirac equations. Specifically, we have compared our $(1+1)$ D Dirac propagator Eq. (22) with the propagator given by the Feynman checkerboard model [15,20], finding that these previous results are missing terms required to give the correct limit for both zero mass and the limit of zero time evolution. We find that this problem results from the amplitude having been assigned as unity for those paths lying on the light cone, which, from our results, should actually be singular, i.e., a contribution of $\delta(\tau - |x - x'|/c)$ to the propagator in the continuous limit. We found that the same problem is present in the $(3+1)$ -dimensional propagator for the Dirac equation and that previous propagators derived from the $(3+1)$ D Feynman checkerboard model in Ref. [17] have the same problem in the zero mass and null evolution limits. Not only does our method provide a means to check and correct these previous results, but it also gives a way to derive the time evolution of wave fields.

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DATA AVAILABILITY

No data were created or analyzed in this study.

APPENDIX

Here we derive the Green function for (1 + 1)D Klein–Gordon equation. The Green function should satisfy

$$\left(\frac{1}{c^2}\partial_t^2 - \partial_x^2 + M^2\right)G(x - x', t - t') = \delta(x - x')\delta(t - t'), \quad (\text{A1})$$

which can, using the Fourier transformation, be solved as

$$G = \frac{-1}{4\pi^2} \iint_{-\infty}^{+\infty} \frac{\exp[i(k(x - x') - \omega(t - t'))]}{\frac{\omega^2}{c^2} - k^2 - M^2} d\omega dk. \quad (\text{A2})$$

There are two singular points, $\omega = \pm c\sqrt{k^2 + M^2}$, on the integral path $k = \text{constant}$. To avoid them, we should choose a contour going clockwise over (anticlockwise under) both poles to give the retarded (advanced) Green function. Integrate Eq. (A2) over ω and replace k with $M \sinh \eta$, giving

$$G_{\pm} = \frac{\Theta(\pm(t - t'))\Theta(s^2)}{2\pi} \int_{-\infty}^{\infty} \sin(Ms \cosh(\eta)) d\eta. \quad (\text{A3})$$

Using the integral representation of Bessel function [21], Eq. (A3) yields Eq. (21).

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