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Null Surfaces, Initial Values and Evolution Operators for Scalar Fields*

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ABSTRACT

We analyze the initial value problem for scalar fields obeying the Klein-Gordon equation. The standard Cauchy initial value problem for the second-order differential equation is to construct a solution function in a neighborhood of space and time form values of the function and its time derivative on a selected initial value surface. On the characteristic surfaces, the time derivative of the solution function may be discontinuous, so that the standard Cauchy construction breaks down. For the Klein-Gordon equation, the characteristic surfaces are null surfaces. An alternative version of the necessary initial data differs from that of the standard Cauchy problem, and in the case we discuss here the values of the function on an intersecting pair of null surfaces comprise the necessary initial value data. We also present an expression for the construction of a solution from null surface data; two analogues of the quantum mechanical Hamiltonian operator determine the evolution of the system.

I. Introduction

The standard Cauchy problem is to use a partial differential equation, with the values of the solution function, and some of its derivatives given on an initial value surface, to determine the values of the function in a neighborhood of the surface [1]. The derivatives needed for an n^{th} order partial differential equation in time are the first $n-1$ time derivatives; in applications to physics, a surface often used is three-space at some initial time. Solution of the standard Cauchy problem proceeds by showing how initial value data and the differential equation determine all the time derivatives of the function on the initial surface, and thus allow a power series development of the function for future times.

If the solution function has a discontinuity in its $n-1$ time derivative across some special surface, the the standard Cauchy problem cannot be solved using that surface for the initial value data. Such special surfaces, the characteristic surfaces or simply characteristics, have been studied extensively for many of the differential equations of physics. The physical significance of characteristics is that the solution or a derivative on one side may differ discontinuously from that on the other side, so that the characteristic can represent a physical discontinuity interpretable as a wave front or shock wave. For example, the characteristics of the Maxwell equations in free space are the wave fronts of light; that is, null surfaces [2]. The characteristics of the Einstein equations in free space are also null surfaces, so that gravity may be interpreted to propagate at the velocity of light [2], [3], [4].

The characteristics of the Klein-Gordon equation for free particles in flat space are easily shown to be null surfaces, as are the characteristics of a large class of interacting versions of the Klein-Gordon equation. Thus the derivative discontinuities of the solution functions propagate at the speed of light, independently of the mass parameter in the equations. Notice in particular that the discontinuities do not propagate at either the phase or group velocity of the wave solutions.

For many years, the use of null coordinates—coordinates lined up with the null surfaces—has been common in general relativity. For example, many problems involving black holes are conveniently studied with null coordinates since black hole surfaces are time-independent null surfaces [6],[7]. Interest has recently developed in using null coordinates in the study of quantum field theories, such as quantum electrodynamics and quantum chromodynamics. This is often referred to as light-cone quantization, although the planar surfaces $x = \pm t$ are usually used [8]. In quantum field theories, the behavior of the field operators is related to the behavior of the classical (c-number) fields. For example, the propagator may be interpreted as either the Green's function of the classical field or as the vacuum expectation value of the time-ordered field operators [10]. It is thus possible that our analysis may have implications for the study of black hole physics in curved space or quantum field theories in flat space. Regarding the latter topic, the transition from classical Green's functions to quantum vacuum expectation values is beset with subtleties stemming from the possible appearance of anomalies upon quantization [9].

We have studied the Klein-Gordon equation and its characteristics, in particular how the values of the solution function on characteristics determine the values of the fields in a neighborhood of space and time. Operators that determine how the solutions develop in time are usually called evolution operators. We use the same term *evolution operators* to include similar operators associated with null coordinates.

We briefly review the standard Cauchy problem for the Klein-Gordon equation and give an operator expression for developing the solution from a constant time surface using as initial value data the function and its first time derivative. We then obtain the characteristics, and solve the analogous problem for the planar null surfaces $x = \pm t$. Initial data for this situation consists of the value of the function on the **pair** of null surfaces, and does **not** include derivatives. We give a simple evolution expression in terms of null coordinates, which is a direct analogue to the usual expression of quantum theory, except that two analogues of the Hamiltonian operator determine the evolution solution [11], [12], [13], [14], [15].

II. Development of a Scalar Function from a Constant Time Surface

The standard form of the Cauchy problem for the Klein-Gordon equation is to determine how a solution may be developed from the appropriate initial value data on a constant surface, which we take to be $t = 0$ (see Figure 1). The Klein-Gordon equation for the scalar function $\phi(\vec{x}, t)$ is

$$\phi_{|t|t}(\vec{x}, t) - \bigtriangledown^2\phi(\vec{x}, t) + m^2\phi(\vec{x}, t) \; = \; 0 \; . \tag{1}$$

We use the units in which $\hbar = c = 1$. The slash notation indicates differentiation with respect to the indicated variable; in this case, time t.

To solve the Cauchy problem, we use the Klein-Gordon equation with the value of the solution function and its first time derivative on the surface $t = 0$ to compute the value of the solution at future times. For this, we use a Taylor series expansion in t, which we write

$$\phi(\vec{x}, t) \; = \; \phi(\vec{x}, t)_{t=0} + \phi_{|t}(\vec{x}, t)_{t=0} t + \phi_{|t|t}(\vec{x}, t)_{t=0} \, \frac{t^2}{2!} + \ldots \; . \tag{2}$$

We specify the solution and its first time derivative at $t = 0$ as

$$\phi(\vec{x}, t)_{t=0} \; = \; h(\vec{x}) \quad \phi_{|t}(\vec{x}, t)_{t=0} = k(\vec{x}) \; . \tag{3}$$

The Klein-Gordon equation then allows us to calculate all the remaining time derivatives on the $t = 0$ surface needed in the series expansion; the second derivative is

$$\phi_{|t|t}(\vec{x},t)_{t=0} \;=\; [\bigtriangledown^2\phi(\vec{x},t) - m^2\phi(\vec{x},t)]_{t=0} \;=\; [\bigtriangledown^2 - m^2]h(\vec{x}) \;. \tag{4}$$

Higher derivatives are obtained in the same way,

$$\phi_{|2nt}(\vec{x},t)_{t=0} \;= [\bigtriangledown^2 - m^2]^n h(\vec{x}) \equiv (-1)^n E^{2n} h(\vec{x}) \quad \text{(even or } 2n\text{derivative)} \;,$$

$$\phi_{|(2n+1)t}(\vec{x},t)_{t=0} \;= [\bigtriangledown^2 - m^2]^n k(\vec{x}) \equiv (-1)^n E^{2n} k(\vec{x}) \quad \text{(odd or } 2n+1\text{derivative)} \;. \tag{5}$$

Here, E^2 is the Klein-Gordon energy squared operator, $E^2 = m^2 - \bigtriangledown^2$. The series (2) may now be written

$$\phi(\vec{x},t) \;=\; \sum_0^\infty (-1)^n \,\frac{(Et)^{2n}}{(2n)!}\, h(\vec{x}) + \sum_0^\infty (-1)^n \,\frac{(Et)^{2n+1}}{(2n+1)!}\, \frac{k(\vec{x})}{E} \;. \tag{6}$$

This may be formally summed to yield a concise result,

$$\phi(\vec{x},t) \;=\; \cos(Et)h(\vec{x}) + \frac{\sin(Et)}{E}k(\vec{x}) \;, \tag{7}$$

which displays the solution in terms of evolution operators acting on the initial value functions $h(\vec{x})$ and $k(\vec{x})$ given on the initial $t = 0$ surface.

The formal result (7) is directly usable if $h(\vec{x})$ and $k(\vec{x})$ are expressed as Fourier transforms; the operator E may then be replaced by the appropriate value $\pm\sqrt{m^2 + p^2}$, for the p-th Fourier component: $h(\vec{x})$ is $\exp\{i\vec{p}\cdot\vec{x}\}$, and $k(\vec{x})$ is $-iE\exp\{i\vec{p}\cdot\vec{x}\}$. Substituting these into (7) produces the correct function $\exp\{-iEt+i\vec{p}\cdot\vec{x}\}$ for the p-th component. It is thus clear that (7) indeed represents the general solution of the Klein-Gordon equation.

We have so far limited our discussion to the free Klein-Gordon equation (1). However, if there is an additional interaction term in the equation that is a function of the scalar field, time, and position, $F(\phi, \vec{x}, t)$, then it is evident that the same considerations allow determination of higher time derivatives, just as in (4) and (5), so that a power-series solution will also exist in this more general case.

III. Characteristics of the Klein Gordon Equation

Surfaces other than $t = 0$ may be used for the series development of the Klein-Gordon solutions; indeed, only a limited class of surfaces (the characteristic surfaces)does not allow such a series development. On these surfaces, the standard Cauchy problem breaks down.

We attempt to develop a solution of the Klein-Gordon equation from a surface S, given by $t = T(\vec{x})$. We suppose that the solution and its first time derivative are given on S by initial value functions

$$\phi(\vec{x}, T(\vec{x})) \;=\; \phi(\vec{x}, t)_{t=T} \;=\; h(\vec{x}) \;, \qquad \phi_{|t}(\vec{x}, t)_{t=T} \;=\; k(\vec{x}) \;. \tag{8}$$

For brevity, we write $t = T$ to denote $t = T(\vec{x})$. We then represent the solution as a Taylor series in the form

$$\begin{aligned} \phi(\vec{x}, t) \;=\; & \phi(\vec{x}, t)_{t=T} + [t - T(\vec{x})]\phi_{|t}(\vec{x}, t)_{t=T} \\ & + \frac{[t - T(\vec{x})]^2}{2}\, \phi_{|t|t}(\vec{x}, t)_{t=T} \quad + \; \ldots \;. \end{aligned} \tag{9}$$

A critical step is to find the second time derivative in this expansion. To do this, we first relate derivatives of the initial data functions to derivatives of the solution function ϕ on S. From (8), we immediately obtain

$$\begin{aligned} \bigtriangledown h(\vec{x}) \;&=\; \bigtriangledown\, \phi(\vec{x}, t)_{t=T} + \phi_{|t}(\vec{x}, t)_{t=T} \bigtriangledown T(\vec{x}) \;, \\ \bigtriangledown k(\vec{x}) \;&=\; \bigtriangledown\, \phi_{|t}(\vec{x}, t)_{t=T} + \phi_{|t|t}(\vec{x}, t)_{t=T} \bigtriangledown T(\vec{x}) \;, \end{aligned} \tag{10}$$

where the gradient on ϕ represents the partial with respect to the three spatial variables. We differentiate this again , and rearrange terms using (10) to obtain

$$\begin{aligned} \bigtriangledown^2 h(\vec{x}) \; &= \; \bigtriangledown^2 \phi(\vec{x},t)_{t=T} \; + \phi_{|t}(\vec{x},t)_{t=T} \bigtriangledown^2 T(\vec{x}) \\ & -\phi_{|t|t}(\vec{x},t)_{t=T} \bigtriangledown T(\vec{x})^2 + 2 \bigtriangledown k(\vec{x}) \cdot \bigtriangledown T(\vec{x}) \end{aligned} \quad . \tag{11}$$

Using (11), the Klein-Gordon equation, and the definitions (8) for the initial value functions, we get the desired equation for the second time-derivative of ϕ on S,

$$\begin{aligned} (1 - \bigtriangledown T(\vec{x})^2)\phi_{|t|t}(\vec{x},t)_{t=T} \; &= (\bigtriangledown^2 - m^2) h(\vec{x}) \\ & - \, k(\vec{x}) \bigtriangledown^2 T(\vec{x}) - 2 \bigtriangledown k(\vec{x}) \cdot \bigtriangledown T(\vec{x}) \; . \end{aligned} \tag{12}$$

If the square of the gradient of T is not equal to one, we may solve this as in Section 2, and develop a power series solution in a similar manner. Indeed, the previous case corresponds to the function T having zero gradient and Laplacian. However, If the gradient squared *is* equal to one, then the equation cannot be solved for the second time derivative, and the surface is a characteristic. Thus, the equation for the characteristics of the Klein-Gordon equation is

$$\bigtriangledown T(\vec{x})^2 = 1 \; . \tag{13}$$

To see that this is the equation of a null surface—that is, the normal to S is a null vector—we write the equation of S as

$$t - T(\vec{x}) \; = \; G(x^\alpha) \; . \tag{14}$$

The normal to S is the 4-gradient of G, or

$$n_\alpha = G_{|\alpha} = (1, - \bigtriangledown T(\vec{x})) \; . \tag{15}$$

Thus, n is a null vector by (13), and S is a null surface.

In the next sections, we study the particular null surfaces for T taken as $\pm x$ or in terms of the commonly used null coordinates u and v,

$$\begin{aligned} u &= t - x = 0 \qquad u \text{ characteristic or null surface },\\ v &= t + x = 0 \qquad v \text{ characteristic or null surface }. \end{aligned} \tag{16}$$

It is interesting that the characteristics are independent of the mass m. This is an example of a more general fact, that if there is an interaction term of the form $F(\phi, \vec{x}, t)$ in the Klein-Gordon equation, then an equation analogous to (12) is obtained, with the same left- hand side. The equation for the characteristics is thus independent of the extra term, and the characteristics are again null surfaces.

Equation (12) gives the equation of the characteristics, but it also tells us that the functions h and k on the characteristics are constrained if the solution is regular, since the right-hand side of (12) is zero. Such constraints are typical of characteristics; in this case, there is a simple physical interpretation. To see this, consider the characteristic $t = x$, and let ϕ be a plane wave of the form $\exp\{-iEt + kx\}$. Then setting the right-hand side of (12)to zero, we see that $E^2 = k^2 + m^2$, the usual energy-momentum or mass-shell relation.

IV. Construction of a Solution Function from Null Surface Data

We now show how to construct solutions to the Klein-Gordon equations using initial data on null surfaces from the pair of null surfaces $u = t - x = 0$ and $v = x + t = 0$. In terms of the null coordinates u and v, the Klein-Gordon equation is

$$4\phi_{|u|v}(u, v, x_\perp) + \nabla_\perp^2 \phi(u, v, x_\perp) + m^2 \phi_{|u|v}(u, v, x_\perp) \;=\; 0\;. \tag{17}$$

Here, the perpendicular symbol $\bigtriangledown_\perp$ refers to the y,z subspace; in the remainder of this paper, we suppress this subspace dependence, writing the Klein-Gordon equation in the form

$$\phi_{|u|v}(u,v) \;=\; -\mu^2\phi(u,v) \;, \qquad\qquad \mu^2 = \frac{m^2}{4} \;. \tag{18}$$

For the case where $\mu = 0$, this is the wave equation and has particularly simple solutions: any differentiable function of u or v. We accordingly expand about this special massless case by setting up a solution as a power series in μ^2, written explicitly as

$$\phi(u,v) \;=\; \phi^{(0)}(u,v) + \mu^2\phi^{(1)}(u,v) + \mu^4\phi^{(2)}(u,v) + \ldots \;. \tag{19}$$

We substitute this into (18) and equate powers of μ^2 to obtain a perturbative solution. The zeroth-order equation and solution are

$$\phi^{(0)}_{|u|v} = 0 \;, \qquad\qquad \phi^{(0)}(u,v) = f(u) + g(v) \;, \tag{20}$$

where f and g are differentiable functions. The first-order equation is

$$\phi^{(1)}_{|u|v} = -\phi^{(0)}(u,v) = -[f(u) + g(v)] \;. \tag{21}$$

This is an inhomogeneous linear equation, so the solution is composed of a homogeneous part and a particular part. But the homogeneous part is of the same form as the solution of the zeroth-order equation (20), and can be absorbed into that solution. We thus need only obtain a particular solution to (21), which is elementary. We write it in the form

$$\phi^{(1)}(u,v) \;=\; -\left[\;,\int_{u_0}^{u} f(u')du'\right](v-v_0) \;-\; \left[\;\int_{v_0}^{v} g(v')dv'\right](u-u_0) \;. \tag{22}$$

The parameters u_0 and v_0 are arbitrary constants and correspond to arbitrariness in the functions f and g.

Higher orders are handled in the same way. The second-order solution is

$$
\begin{aligned}
\phi^{(2)}(u,v) \;=\; & -\left[\,,\int_{u_0}^{u} du' \int_{u_0}^{u'} \; f(u'')du''\right] \frac{(v-v_0)^2}{2} \\
& -\left[\,,\int_{v_0}^{v} dv' \int_{v_0}^{v'} g(v'')dv''\right] \;\frac{(u-u_0)^2}{2}\ .
\end{aligned}
\tag{23}
$$

The series solution can be written

$$
\begin{aligned}
\phi(u,v) \;=\; & \sum_{n=0}^{\infty} \frac{[-\mu^2(v-v_0)\Gamma_u]^n}{n!}\; f(u) \\
& + \sum_{m=0}^{\infty} \frac{[-\mu^2(u-u_0)\Gamma_v]^m}{m!}\; g(v)\ ,
\end{aligned}
\tag{24}
$$

where the multiple integral operator Γ_u^n on f is defined

$$
\Gamma_u^n f(u) \;=\; \int_{u_0}^{u} du' \int_{u_0}^{u'} du'' \;\ldots\; \int_{u_0}^{u^{n-1}} du^n f(u^n)\ . \tag{25}
$$

The operators $\Gamma_{u,v}^n$ are linear, and the series (24) may be summed to give a remarkably concise result in terms of a pair of exponential evolution operators,

$$
\phi(u,v) = \exp\{-\mu^2(v-v_0)\Gamma_v\}\; f(u) + \exp\{-\mu^2(u-u_0)\Gamma_u\}\; g(v)\ . \tag{26}
$$

This shows explicitly how the solution is given in terms of the two generating functions $f(u)$ and $g(v)$, right-moving and left-moving waves, which are related to initial value data, as discussed below.

We illustrate the simplest case, using (26), and consider the evolution operator acting on a constant $f(u) = 1$. The terms in the series (24) are trivially obtained by integration, and give

$$\phi(u,v) \;=\; \sum_{n=0}^{\infty} \frac{(-\mu^2 uv)^2}{(n!)^2} \;=\; F_c(uv) \;, \tag{27}$$

where we have taken $u_0 = v_0 = 0$ for convenience without loss of generality. This is easily verified to be a solution of the Klein-Gordon equation by substitution; moreover, we recognize the series as the Bessel function

$$F_c(uv) \;=\; J_0\,(2\mu\sqrt{uv}\,) \;. \tag{28}$$

This special solution will be useful in the discussion of exponential solutions below.

Consider the values of ϕ on the null surfaces $u = u_0 = 0$ and $v = v_0 = 0$. We see that

$$\phi_0(u,0) \;=\; f(u) + g(0) \;, \qquad \phi_0(0,v) \;=\; f(0) + g(v) \;. \tag{29}$$

Thus, up to a constant, the generating functions are the initial values on the pair of null surfaces, representing right- and left-moving plane waves. The value of either of the generating functions at 0 may be chosen arbitrarily. We choose for convenience both equal to $\phi_0/2$ at the intersection of the surfaces, so that

$$f(u) \;=\; \phi_0(u,0) - \frac{\phi_0(0,0)}{2} \;, \qquad g(v) \;=\; \phi_0(0,v) - \frac{\phi_0(0,0)}{2} \;. \tag{30}$$

We emphasize that the initial value data needed for the null surface development consists of the function on a pair of null surfaces; this is not the same as the data needed in the standard Cauchy problem, which is the function and its first time-derivative on an initial surface [14],[15].

V. Plane Wave Solutions

We next discuss plane-wave solutions of the Klein-Gordon equation, which form a convenient set for the expansion of a general solution. We display the appropriate generating functions and verify that the evolution operators in (26) give a correct solution. Plane-wave solutions of energy E and momentum k may be written in terms of t and x or u and v coordinates,

$$\phi(t,x) \ = \ \exp\{-iEt + ikx\} \ = \ \exp\{-i\lambda u - i\tau v\} \ , \tag{31}$$

where the null momenta λ and τ are related to E and k and to the mass parameter μ^2 by

$$\lambda = \frac{E+k}{2} \ , \qquad \tau = \frac{E-k}{2} \ , \quad \text{and} \quad \lambda\tau \ = \ \frac{E^2-k^2}{4} \ = \ \frac{m^2}{4} = \mu^2 \ . \tag{32}$$

For the plane waves, the appropriate generating functions are thus

$$f(u) \ = \ \exp\{-i\lambda u\} - \frac{1}{2} \ , \quad g(v) \ = \exp\{-i\tau v\} - \frac{1}{2} \ , \quad \text{and} \quad \lambda\tau \ = \ \mu^2 \ . \tag{33}$$

We substitute these generating functions into (26), abbreviating for convenience $B = -i\lambda$, $C = -i\tau$, $\mu^2 = -BC$, and find

$$\begin{aligned} \phi(u,v) \ &= \big(\exp\{BCv\Gamma_u\} \ \exp\{Bu\} + \exp\{BCu\Gamma_v\} \ \exp\{Cv\}\big) \\ &- \ \frac{1}{2} \ \big(\exp\{BCv\Gamma_u\} + \exp\{BCu\Gamma_v\}\big) \ . \end{aligned} \tag{34}$$

We recognize the last term as F_c, which we obtained as the series in (28). The first two terms are readily evaluated by expanding in double series,

$$\begin{aligned} &\big(\exp\{BCv\Gamma_u\} \exp\{Bu\} \ + \ \exp\{BCu\Gamma_v\} \exp\{Cv\}\big) \\ &= \sum_{n=0,j=0}^{\infty} \frac{(BCv\Gamma_u)^n}{n!} \ \frac{(Bu)^j}{j!} \ + \sum_{m=0,k=0}^{\infty} \frac{(BCu\Gamma_v)^m}{m!} \ \frac{(Cv)^k}{k!} \ . \end{aligned} \tag{35}$$

It is easy to obtain the operation of Γ^n on powers of u,

$$\Gamma_u^n u^j \;=\; \frac{u^{j+n}}{(j+1)(j+2)\;\ldots\;(j+n)}\;. \tag{36}$$

We substitute this into (35) and rearrange summation indices to find

$$(e^{BCv\Gamma_u}e^{Bu}+e^{BCu\Gamma_v}e^{Cv})=\sum_{n\le j}^{\infty}\frac{(Cv)^n}{n!}\frac{(Bu)^j}{j!}+\sum_{m\ge k}^{\infty}\frac{(Cv)^m}{m!}\frac{(Bu)^k}{k!}$$

$$=\sum_{n=0,j=0}^{\infty}\frac{(Cv)^n}{n!}\frac{(Bu)^j}{j!}+\sum_{n=0}^{\infty}\frac{(-\mu^2uv)^2}{(n!)^2}=e^{Bu+Cv}+F_c(uv) \tag{37}$$

Thus the F_c part cancels and in summary of (34) to (37) we have

$$\phi(u,v)=e^{Bu+Cv}=e^{-i\lambda u-i\tau v} \tag{38}$$

which is the correct plane wave solution. It follows that the evolution operator equation (26) will produce the correct solution in any case that may be expanded as a Fourier transform.

VI. Relation to Null Surface Quantization

The form of the solution in (26) is suggestive of the quantum mechanical time evolution operator e^{-iHt}. In fact the analogy can be made complete and is the basis of "light cone" quantization schemes [8], [14], [15]. In terms of the momenta λ and τ associated with the null coordinates u and v, the energy-momentum relation is $\lambda\tau = \mu^2 = \frac{m^2}{4}$ from (32). If we use the standard operator replacements for these momenta,

$$\Lambda \equiv i\frac{\partial}{\partial u} \quad \Sigma \equiv i\frac{\partial}{\partial v} \ , \tag{39}$$

then the the integral operators $\Gamma_{u,v}$ can be written symbolically in terms of the momentum operators as follows:

$$\Gamma_u = \frac{i}{\Lambda}, \quad \Gamma_v = \frac{i}{\Sigma}, \tag{40}$$

The expression (26)giving the solution can then be written as

$$\phi(u,v) = e^{-iv\frac{\mu^2}{\Lambda}} f(u) + e^{-iu\frac{\mu^2}{\Sigma}} g(v)$$

$$= e^{-iv\frac{\mu^2}{\Lambda}}[\phi_0(u,0) - \frac{1}{2}] + e^{-iu\frac{\mu^2}{\Sigma}}[\phi_0(0,v) - \frac{1}{2}] \tag{41}$$

The operators μ^2/Λ and μ^2/Σ are equal to Σ and Λ by (32)and play the role of Hamiltonian operators relative to v and u; equation (41)thus represents the operation of a pair of Hamiltonians evolving a solution from the initial values on the pair of null surfaces [11], [12], [13], [14], [15].

Note from the above discussion that initial value data on both null surfaces are necessary for the evolution of a solution. From the discussion of the exponential solutions it is also clear that the constant term in the generating functions plays an important role in the evolution.

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