

A special asymptotic limit of a Kampé de Fériet hypergeometric function appearing in nonhomogeneous Coulomb problems

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In the investigation of two-body Coulomb Schrödinger equations with some types of nonhomogeneities, the particular solution can be expressed in terms of a two-variable Kampé de Fériet hypergeometric function. The asymptotic limit of the latter—for both variables being large but their ratio being a bound constant—is required in order to extract relevant physical information from the solutions. In this report the mathematical limit is provided. For that purpose, a particular series representation of the hypergeometric function—in terms of products of Kummer and Gauss functions—is first derived. © 2011 American Institute of Physics. [doi:10.1063/1.3554698]

I. INTRODUCTION

Numerous physical and mathematical problems can be formulated in terms of nonhomogeneous differential equations. Those of second-order are of particular physical interest, and some of them have been studied in the mathematical book of Babister.¹ One example in physics is found in scattering theory within quantum mechanics, see, e.g., Refs. 2 and 3. In the study of the collision dynamics between two particles, the wave function satisfying the full Schrödinger equation may be written as the sum of a simplified and the scattering solution. This separation leads straightforwardly to a second-order nonhomogeneous equation where the source (the nonhomogeneity) is the product of the neglected interactions and the asymptotic solution.^{2,3} In Ref. 4 a nonhomogeneous Kummer-type Schrödinger equation which includes a Coulomb interaction has been investigated and solved in closed form. Its particular solution results to be expressed in terms of a two-variable hypergeometric function, named $\Theta^{(1)}$. Relevant physical information of the problem can be extracted from its asymptotic region where the distance between the interacting particles is large. This required to know the asymptotic limit of the wave function for large values of the radial coordinate, and hence the asymptotic limit of the mathematical hypergeometric function $\Theta^{(1)}$.

In this paper, we provide the mathematical details necessary to derive the asymptotic expression of the mentioned physical problem. More specifically, we are interested in the asymptotic limit of the Kampé de Fériet function,⁵

$$\Theta^{(1)} \left(\begin{matrix} a_1, a_2 | b_1, b_2 \\ c_1 | d_1, d_2 \end{matrix} ; x_1, x_2 \right) = \sum_{m_1=0}^{\infty} \sum_{m_2=0}^{\infty} \frac{(a_1)_{m_1} (a_2)_{m_2} (b_1)_{m_1} (b_2)_{m_1+m_2}}{(c_1)_{m_1} (d_1)_{m_1+m_2} (d_2)_{m_1+m_2}} \frac{x_1^{m_1} x_2^{m_2}}{m_1! m_2!}, \quad (1)$$

for large x_1 and x_2 but x_1/x_2 constant, and in the special case $d_1 = a_1 + a_2$. To obtain such limit a convenient series representation of the $\Theta^{(1)}$ function is needed, and this is presented in Sec. II. In

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Sec. III this representation is then used to derive the required asymptotic limit. Its application to the physical nonhomogeneous Coulomb problem mentioned above is described shortly in Sec. IV.

II. A TERM BY TERM SEPARABLE REPRESENTATION OF THE $\Theta^{(1)}$ FUNCTION FOR THE SPECIAL CASE $d_1 = a_1 + a_2$

The $\Theta^{(1)}$ function was studied in Ref. 6 in a different context, in relation with the solution of a nonhomogeneous Kummer-type equation, with equal variables $x_1 = x_2$. In Ref. 6 we have established a number of properties of the function $\Theta^{(1)}$ and provided series and integral representations. In the specific case of interest, we have found other series representations involving ${}_1F_1$ and ${}_2F_1$, or ${}_1F_2$ functions. None of them, however, uncouples sufficiently the variables x_1 and x_2 , making the study of the asymptotic limit particularly difficult. After a careful investigation, we realized that it was necessary to find an alternative, more adequate, series representation which we now establish.

For the present purpose, the following integral representation [see Eq. (51) of Ref. 6]

$$\begin{aligned} \Theta^{(1)} \left(\begin{matrix} a_1, a_2 | b_1, b_2 \\ c_1 | d_1, d_2 \end{matrix} ; x_1, x_2 \right) &= \frac{\Gamma(d_1) \Gamma(d_2)}{\Gamma(a_2) \Gamma(d_2 - b_2) \Gamma(b_2) \Gamma(d_1 - a_2)} \\ &\times \int_0^1 dt (1-t)^{d_1 - a_2 - 1} t^{a_2 - 1} \int_0^1 dv (1-v)^{d_2 - b_2 - 1} v^{b_2 - 1} \\ &\times e_2^{x_2 t v} F_2 \left(\begin{matrix} a_1, b_1 \\ c_1, d_1 - a_2 \end{matrix} ; x_1 (1-t) v \right) \end{aligned} \quad (2)$$

will be particularly useful; it is worth mentioning that this representation is also particularly efficient for its numerical evaluation for any value of the coordinates and parameters. In the physical problem mentioned in Sec. I and described in Sec. IV, it occurs that $d_1 = a_1 + a_2$ [see Eqs. (27a) and (27c)]. Under this condition the ${}_2F_2$ function appearing in the integral representation (2) reduces to a ${}_1F_1$ function, so that

$$\begin{aligned} \Theta^{(1)} &= \Theta^{(1)} \left(\begin{matrix} a_1, a_2 | b_1, b_2 \\ c_1 | a_1 + a_2, d_2 \end{matrix} ; x_1, x_2 \right) \\ &= \frac{\Gamma(a_1 + a_2) \Gamma(d_2)}{\Gamma(a_2) \Gamma(d_2 - b_2) \Gamma(b_2) \Gamma(a_1)} \\ &\times \int_0^1 dt (1-t)^{a_1 - 1} t^{a_2 - 1} \int_0^1 dv (1-v)^{d_2 - b_2 - 1} v^{b_2 - 1} \\ &\times e_1^{x_2 t v} F_1 \left(\begin{matrix} b_1 \\ c_1 \end{matrix} ; x_1 (1-t) v \right). \end{aligned} \quad (3)$$

This formulation will allow us to rewrite this function, noted simply $\Theta^{(1)}$ hereafter, as simple series in terms of Kummer and Gauss hypergeometric functions. To show this, we first use the Laplace representation of the ${}_1F_1$ function⁷

$${}_1F_1 \left(\begin{matrix} \alpha \\ \beta \end{matrix} ; z \right) = \frac{\Gamma(\beta)}{\Gamma(\alpha) \Gamma(\beta - \alpha)} \int_0^1 dt (1-t)^{\beta - \alpha - 1} t^{\alpha - 1} e^{zt}, \quad (4)$$

to get

$$\begin{aligned} \Theta^{(1)} &= \frac{\Gamma(a_1 + a_2) \Gamma(d_2) \Gamma(c_1)}{\Gamma(a_2) \Gamma(d_2 - b_2) \Gamma(b_2) \Gamma(a_1) \Gamma(b_1) \Gamma(c_1 - b_1)} \int_0^1 dv (1-v)^{d_2 - b_2 - 1} v^{b_2 - 1} \\ &\times \int_0^1 ds s^{b_1 - 1} (1-s)^{c_1 - b_1 - 1} \int_0^1 dt (1-t)^{a_1 - 1} t^{a_2 - 1} e^{x_2 t v + x_1 (1-t) v s}. \end{aligned} \quad (5)$$

By separating the argument of the exponential as follows:

$$x_2 t v + x_1 (1-t) v s = t(x_2 v - x_1 v s) + x_1 v s,$$

the integration over t can now be easily performed leading to

$$\Theta^{(1)} = \frac{\Gamma(d_2)\Gamma(c_1)}{\Gamma(d_2-b_2)\Gamma(b_2)\Gamma(b_1)\Gamma(c_1-b_1)} \int_0^1 dv (1-v)^{d_2-b_2-1} v^{b_2-1} \quad (6)$$

$$\times \int_0^1 ds s^{b_1-1} (1-s)^{c_1-b_1-1} e_1^{x_1vs} F_1\left(\begin{matrix} a_2 \\ a_1+a_2 \end{matrix} \middle| ; x_2v-x_1vs\right).$$

Furthermore, using Kummer's transformation,⁷

$${}_1F_1\left(\begin{matrix} a_2 \\ a_1+a_2 \end{matrix} \middle| ; x_2v-x_1vs\right) = e_1^{x_2v-x_1vs} F_1\left(\begin{matrix} a_1 \\ a_1+a_2 \end{matrix} \middle| ; x_1vs-x_2v\right),$$

eliminates e^{x_1vs} in (6); expanding the remaining Kummer function as power series, we get

$$\Theta^{(1)} = \frac{\Gamma(d_2)\Gamma(c_1)}{\Gamma(d_2-b_2)\Gamma(b_2)\Gamma(b_1)\Gamma(c_1-b_1)} \sum_{m=0}^{\infty} \frac{1}{m!} \frac{(a_1)_m}{(a_1+a_2)_m} (-x_2)^m$$

$$\times \int_0^1 dv (1-v)^{d_2-b_2-1} v^{b_2+m-1} e^{x_2v} \int_0^1 ds s^{b_1-1} (1-s)^{c_1-b_1-1} \left(1 - \frac{x_1}{x_2}s\right)^m.$$

These transformations have uncoupled the integrations, which can be now evaluated analytically. Indeed, identifying the first integral with a Kummer hypergeometric function [see (4)] and the second using Euler integral representation of the Gauss function⁷

$${}_2F_1\left(\begin{matrix} \alpha, \beta \\ \gamma \end{matrix} \middle| ; z\right) = \frac{\Gamma(\gamma)}{\Gamma(\beta)\Gamma(\gamma-\beta)} \int_0^1 dt (1-t)^{\gamma-\beta-1} t^{\beta-1} (1-tz)^{-\alpha}, \quad (7)$$

we finally find

$$\Theta^{(1)} = \sum_{m=0}^{\infty} \frac{(a_1)_m (b_2)_m}{(a_1+a_2)_m (d_2)_m} \frac{(-x_2)^m}{m!} {}_1F_1\left(\begin{matrix} b_2+m \\ d_2+m \end{matrix} \middle| ; x_2\right) {}_2F_1\left(\begin{matrix} -m, b_1 \\ c_1 \end{matrix} \middle| ; \frac{x_1}{x_2}\right). \quad (8)$$

Note that, because of the negative integer as first parameter, the ${}_2F_1$ reduces to a polynomial of order m . This representation of the $\Theta^{(1)}$ function is one of the results of this paper. It has the particularity of being a series of product of functions depending—separately—on x_2 and the ratio x_1/x_2 ; the coupling between x_1 and x_2 , which was nontrivial in (1), was resumed in a particular manner that will be adequate for the asymptotic study given below.

III. THE ASYMPTOTIC LIMIT OF $\Theta^{(1)}$ FOR THE SPECIAL CASE $d_1 = a_1 + a_2$ AND $b_2 = c_1$

Consider now the asymptotic limit of the $\Theta^{(1)}$ function (8) for large x_1 and x_2 , but x_1/x_2 constant. Introducing the asymptotic ($z \rightarrow \infty$) form of the Kummer function⁷

$${}_1F_1\left(\begin{matrix} \alpha \\ \beta \end{matrix} \middle| ; z\right) \rightarrow \frac{\Gamma(\beta)}{\Gamma(\beta-\alpha)} (-z)^{-\alpha} + \frac{\Gamma(\beta)}{\Gamma(\alpha)} z^{\alpha-\beta} e^z \quad (9)$$

into expression (8), we get

$$\Theta^{(1)} \rightarrow \frac{\Gamma(d_2)}{\Gamma(d_2-b_2)} (-x_2)^{-b_2} T_1\left(\frac{x_1}{x_2}\right) + \frac{\Gamma(d_2)}{\Gamma(b_2)} x_2^{b_2-d_2} T_2(x_1, x_2), \quad (10)$$

where

$$T_1\left(\frac{x_1}{x_2}\right) = \sum_{m=0}^{\infty} \frac{(a_1)_m (b_2)_m}{m! (a_1+a_2)_m} F_1\left(\begin{matrix} -m, b_1 \\ c_1 \end{matrix} \middle| ; \frac{x_1}{x_2}\right), \quad (11)$$

$$T_2(x_1, x_2) = e^{x_2} \sum_{m=0}^{\infty} \frac{(a_1)_m}{(a_1+a_2)_m} \frac{(-x_2)^m}{m!} {}_2F_1\left(\begin{matrix} -m, b_1 \\ c_1 \end{matrix} \middle| ; \frac{x_1}{x_2}\right). \quad (12)$$

In view of the physical application presented in Sec. IV, we shall assume that $b_2 = c_1$ hereafter. Since the factor $T_1(\frac{x_1}{x_2})$ depends only on the coordinates ratio x_1/x_2 , it remains constant. This factor can be easily evaluated by noting that it corresponds to a formulation of an Appell function F_1 as a sum of polynomials [Eq. (8), p. 34; Ref. 5]

$$T_1\left(\frac{x_1}{x_2}\right) = F_1\left(a_1, b_1, c_1 - b_1, a_1 + a_2; 1 - \frac{x_1}{x_2}, 1\right), \tag{13}$$

Moreover, as one of the arguments equals unity, the F_1 reduces to a ${}_2F_1$ function [Eq. (23), p. 22; Ref. 5], so that

$$T_1\left(\frac{x_1}{x_2}\right) = \frac{\Gamma(a_1 + a_2)\Gamma(a_2 + b_1 - c_1)}{\Gamma(a_2)\Gamma(a_1 + a_2 + b_1 - c_1)} {}_2F_1\left(a_1, b_1 \middle| a_1 + a_2 + b_1 - c_1 \middle| 1 - \frac{x_1}{x_2}\right). \tag{14}$$

Let us now look at the term $T_2(x_1, x_2)$. We start by recalling one of the series representations of $\Theta^{(1)}$ [see Eq. (46a) of Ref. 6]

$$\begin{aligned} \Theta^{(1)}\left(a_1, a_2 \middle| b_1, b_2 \middle| c_1 \middle| d_1, d_2 \middle| x_1, x_2\right) \\ = \sum_{m_1=0}^{\infty} \frac{(a_1)_{m_1} (b_1)_{m_1} (b_2)_{m_1}}{(c_1)_{m_1} (d_1)_{m_1} (d_2)_{m_1}} \frac{x_1^{m_1}}{m_1!} {}_2F_2\left(a_2, b_2 + m_1 \middle| d_1 + m_1, d_2 + m_1 \middle| x_2\right). \end{aligned} \tag{15}$$

Equalling the $\Theta^{(1)}$ obtained from (15) and (8), in the particular subcase $b_2 = d_2$, provides the following relation:

$$\begin{aligned} T_2(x_1, x_2) &= \sum_{m_1=0}^{\infty} \frac{(a_1)_{m_1} (b_1)_{m_1}}{(c_1)_{m_1} (a_1 + a_2)_{m_1}} \frac{x_1^{m_1}}{m_1!} {}_1F_1\left(a_2 \middle| a_1 + a_2 + m_1 \middle| x_2\right) \\ &= e^{x_2} \sum_{m=0}^{\infty} \frac{(a_1)_m}{(a_1 + a_2)_m} \frac{(-x_2)^m}{m!} {}_2F_1\left(-m, b_1 \middle| c_1 \middle| \frac{x_1}{x_2}\right). \end{aligned} \tag{16}$$

The asymptotic limit of $T_2(x_1, x_2)$ can be easily obtained from this result. Indeed, by using the asymptotic formula (9) in the first equality of (16), the summation may be easily performed

$$\begin{aligned} T_2(x_1, x_2) \longrightarrow \frac{\Gamma(a_1 + a_2)}{\Gamma(a_2)} e^{x_2} x_2^{-a_1} {}_2F_1\left(b_1, a_1 \middle| c_1 \middle| \frac{x_1}{x_2}\right) \\ + \frac{\Gamma(a_1 + a_2)}{\Gamma(a_1)} (-x_2)^{-a_2} {}_1F_1\left(b_1 \middle| c_1 \middle| x_1\right). \end{aligned} \tag{17}$$

Using again the asymptotic formula (9), one finally finds

$$\begin{aligned} T_2(x_1, x_2) \longrightarrow \frac{\Gamma(a_1 + a_2)}{\Gamma(a_2)} e^{x_2} x_2^{-a_1} {}_2F_1\left(b_1, a_1 \middle| c_1 \middle| \frac{x_1}{x_2}\right) \\ + \frac{\Gamma(a_1 + a_2)}{\Gamma(a_1)} (-x_2)^{-a_2} \left[\frac{\Gamma(c_1)}{\Gamma(b_1)} e^{x_1} x_1^{b_1 - c_1} + \frac{\Gamma(c_1)}{\Gamma(c_1 - b_1)} (-x_1)^{-b_1} \right]. \end{aligned} \tag{18}$$

Collecting results (14) and (18) into (10), we obtain the mathematical result sought after, i.e., the asymptotic limit of the $\Theta^{(1)}$ function for the special case $d_1 = a_1 + a_2$ and $b_2 = c_1$. In view of the physical parameters appearing in Sec. IV, we also have $a_2 = 1$ and $d_2 = b_1 + 1$; in this case, easy algebraic simplifications lead to

$$\begin{aligned} \Theta^{(1)} \longrightarrow (-x_2)^{-c_1} \frac{\Gamma(a_1 + 1)\Gamma(b_1 + 1)}{\Gamma(a_1 + 1 + b_1 - c_1)} {}_2F_1\left(a_1, b_1 \middle| a_1 + 1 + b_1 - c_1 \middle| 1 - \frac{x_1}{x_2}\right) \\ + \frac{\Gamma(a_1 + 1)\Gamma(b_1 + 1)}{\Gamma(c_1)} e^{x_2} x_2^{c_1 - b_1 - 1 - a_1} {}_2F_1\left(b_1, a_1 \middle| c_1 \middle| \frac{x_1}{x_2}\right) \\ - \frac{a_1 b_1}{x_2^2} \left[e^{x_1} \left(\frac{x_1}{x_2}\right)^{b_1 - c_1} + \frac{\Gamma(b_1)}{\Gamma(c_1 - b_1)} (-x_1)^{-b_1} x_2^{c_1 - b_1} \right]. \end{aligned} \tag{19}$$

IV. APPLICATION: RADIAL TWO-BODY COULOMB NONHOMOGENEOUS SCHRÖDINGER EQUATIONS

Consider the following non-homogeneous Coulomb Schrödinger equation (in atomic units, $\hbar = e = 1$)

$$[H - E] \Psi(\mathbf{r}) = \Phi_0(\mathbf{r}), \quad (20)$$

where the Hamiltonian $H = -\frac{1}{2\mu}\nabla^2 + \frac{z_1 z_2}{r}$ includes the kinetic energy (reduced mass μ) and a Coulomb potential for two charges z_1 and z_2 (Sommerfeld parameter $\alpha = z_1 z_2 \mu / k$). Hereafter, the energy $E = k^2 / (2\mu)$ will be taken as positive (scattering states); for bound states ($E < 0$), an analytic continuation $k \rightarrow ik$ has to be applied. We expand the wave function $\Psi(\mathbf{r})$, as well as the driven term $\Phi_0(\mathbf{r})$, in terms of spherical harmonics $Y_l^m(\theta, \varphi)$, and consider the rather general source

$$\Phi_0(\mathbf{r}) = \sum_{l,m} c_{lm} Y_l^m(\theta, \varphi) \frac{1}{r} \left(e^{-\lambda r} r^l \sum_{\sigma=0}^{\infty} a_{l,\sigma} r^\sigma \right), \quad (21)$$

where λ is a parameter, and $a_{l,\sigma}$ and c_{lm} are expansion coefficients [note that the nonhomogeneity (21) is general enough to be used as the basic brick for almost any source]. This leads to solving the radial nonhomogeneous equation (in atomic units, $\hbar = e = 1$)

$$\left[-\frac{1}{2\mu} \left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} \right) + \frac{z_1 z_2}{r} - E \right] h_{l,\sigma}(r) = a_{l,\sigma} e^{-\lambda r} r^{l+\sigma}. \quad (22)$$

The radial part of the solution $\Psi(\mathbf{r})$ will be given by a linear combination of the solutions $h_{l,\sigma}(r)$.⁴ With the change of function

$$h_{l,\sigma}^P(r) = \frac{(-2\mu)a_{l,\sigma}}{(-2ik)^{\sigma+1}} e^{ikr} r^{l+1} f_{l,\sigma}(r), \quad (23)$$

the change of variable $u = -2ikr$, and defining $a = i\alpha + l + 1$, $c = 2l + 2$, and $\rho = \frac{1}{2} \left(1 + \frac{\lambda}{ik} \right)$, we get the mathematical Kummer-type equation to be studied⁷

$$\left[u \frac{d^2}{du^2} + (c - u) \frac{d}{du} - a \right] f_{l,\sigma}(u) = e^{\rho u} u^\sigma. \quad (24)$$

The two solutions, regular and irregular at the origin, of the corresponding homogeneous Coulomb differential equation are well known functions.^{7,8} On the other hand, by expanding the exponential on the right-hand side, a closed form of the particular solution of Eq. (24) is given by Eq. (4.219) of Ref. 1

$$f_{l,\sigma}(u) = u^{\sigma+1} \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{\Gamma(\sigma+1+a+m+n) \Gamma(\sigma+1+n) \Gamma(\sigma+c+n)}{\Gamma(\sigma+1+a+n) \Gamma(\sigma+2+m+n) \Gamma(\sigma+1+c+m+n)} \frac{u^{n+m} \rho^n}{n!}. \quad (25)$$

This double series is related to the series representation of the two variables hypergeometric function $\Theta^{(1)}$, defined by (1) and studied in Ref. 6. The particular solution $h_{l,\sigma}^P(r)$ of the physical Eq. (22) is expressed in terms of $\Theta^{(1)}$ as follows:⁴

$$h_{l,\sigma}^P(r) = (-2\mu) a_{l,\sigma} \frac{e^{ikr} r^{l+\sigma+2}}{(\sigma+1)(2l+2+\sigma)} \Theta^{(1)} \left(\begin{matrix} a_1, a_2 | b_1, b_2 \\ c_1 | d_1, d_2 \end{matrix} ; x_1, x_2 \right), \quad (26)$$

where the parameters a_i, b_i, c_1, d_i , and the variables x_i ($i = 1, 2$) read

$$a_1 = \sigma + 1, \quad a_2 = 1, \quad (27a)$$

$$b_1 = \sigma + c = 2l + 2 + \sigma, \quad b_2 = c_1 = a + \sigma + 1 = i\alpha + l + 2 + \sigma, \quad (27b)$$

$$d_1 = \sigma + 2, \quad d_2 = \sigma + c + 1 = 2l + 3 + \sigma. \quad (27c)$$

$$x_1 = \rho u = -(ik + \lambda)r, \quad x_2 = u = -2ikr. \quad (27d)$$

Although not at all obvious from formula (26), for real values of λ and $a_{l,\sigma}$, i.e., a real source, the particular solution $h_{l,\sigma}^P(r)$ is a real definite function⁴ as it should be.

In order to investigate the physical behavior of such particular solutions for large values of the coordinate r , use is made of the asymptotic limit (19) of the $\Theta^{(1)}$ function for large x_1 and x_2 but constant finite ratio $x_1/x_2 = \rho$; indeed, from relations (27a)–(27d) we have that $d_1 = a_1 + a_2$, $b_2 = c_1$, $a_2 = 1$ and $d_2 = b_1 + 1$. For positive energies and for sources with real positive values of λ , the physical variables and parameters (27a)–(27d) are such that the third and fourth terms of (19) vanish faster than the first two. Moreover, the first two asymptotic terms are related (complex conjugated) so that the particular solution is real. The large coordinate limit can be shown⁴ to have the following cosine behavior:

$$h_{l,\sigma}^P(r) \longrightarrow N_{source} \cos(kr - \alpha \ln(2kr) + \delta), \quad (28)$$

where δ and N_{source} are functions of all the parameters l , σ , λ , α , and $a_{l,\sigma}$. The asymptotic behavior described by the scattering solution corresponds then to a superposition of incoming and outgoing waves. On the other hand, for negative energy, bound states can be constructed for any value of λ . Through an analytic continuation of the momentum, imaginary values of k can be found in such a way to enforce the scattering solution to decrease exponentially at large distances. In both bound and scattering cases, the solutions are real definite functions as long as the source is real.

V. SUMMARY

In this report we gave basically two main results. We obtained a term-by-term separable representation of the Kampé de Fériet hypergeometric function appearing in nonhomogeneous Coulomb problems. We also derived a special asymptotic limit necessary to extract the relevant physical information for those problems.

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