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LETTER TO THE EDITOR

On the convergence of path integrals

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Abstract. We discuss the convergence of path integrals evaluating the quantum propagator of a particle under the action of a constant force by an iteration method.

Since Feynman introduced path integrals in quantum mechanics in 1948 [1], their use has increased in many areas of physics. Although their first applications were in the calculation of quantum propagators, it is in the formalism of quantum field theories that they have shown to be a very powerful tool. In the case of non-relativistic propagators the equivalence between the usual Schrödinger formalism and the Feynman one can be proved [2], at least for a Lagrangian of the form

$$L=\tfrac{1}{2}m(\mathrm{d}\boldsymbol{r}/\mathrm{d}t)^2-V(\boldsymbol{r}). \tag{1}$$

So we should be able to reproduce, in the Feynman formalism, the expressions for all propagators already obtained before from the Schrödinger one. However, even being sure of the equivalence of these two methods, only a few propagators have been obtained by path integrals. They are essentially those with quadratic actions (free particle, simple and forced harmonic oscillators, etc) or actions which, after some kind of transformation, reduce the problem to Gaussian integrals. For instance, the hydrogen atom can be reduced after a point canonical transformation and a time reparametrisation to the problem of a harmonic oscillator in four dimensions [3, 4].

From Feynman's postulates we can write, in one dimension [2],

$$K(a,b)=\int \mathrm{D}[x(t)]\exp(\mathrm{i}S(a,b)/\hbar) \tag{2}$$

where $K(a,b)=\langle x_b|U(t_b,t_a)|x_a\rangle$ is the usual propagator.

If one is not interested in the exact quantum results, but only in the first corrections to the classical theory or even in obtaining the classical limit, the Feynman formalism provides a very simple way of doing this.

In this letter we propose another approach for explicitly calculating path integrals. It can also be used in approximate calculations in more difficult problems and to put the question of convergence of path integrals in a more transparent form.

The formal relation (2) means in practice that

$$K(a,b)=\lim_{\substack{N\to\infty\\ \varepsilon\to 0}}\left(\frac{m}{2\pi\mathrm{i}\hbar\varepsilon}\right)^{N/2}\int_{-\infty}^{+\infty}\mathrm{d}x_1\ldots\int_{-\infty}^{+\infty}\mathrm{d}x_N$$
$$\times\exp\left[\frac{\mathrm{i}}{\hbar}\sum_{j=0}^{N}\left(\frac{m}{2\varepsilon}(x_{j+1}-x_j)^2-\tfrac{1}{2}\varepsilon V(x_j+x_{j+1})\right)\right] \tag{3}$$

where

$$x_a = x_0 \qquad t_a = t_0 \qquad (t_b - t_a)/(N+1) = \varepsilon$$
$$x_b = x_{N+1} \qquad t_b = t_{N+1}. \tag{4}$$

The usual technique of calculating explicitly the propagator via path integrals is to calculate the first of the infinite integrals in (3) and try to obtain a recurrence formula for the successive results for these integrals, without analysing the expression for the propagator at each stage. But only after all integrations does one obtain the expression for the propagator. In this way the convergence of the path integral is not transparent. In our approach we pay attention to this problem. We will be able to evaluate how rapidly the path integral converges to the final result. We will calculate the total expression for $K(a, b)$ when $N = 0$, called the zeroth approximation $K^{(0)}$, $N = 1$, called the first approximation $K^{(1)}$, etc, and try to find the expression for the general case $K^{(N)}$. The exact propagator will of course be given by

$$K(a, b) = \lim_{N\to\infty} K^{(N)}(a, b). \tag{5}$$

Note that in our approach we search for recurrence formulae between successive approximate expressions for the propagator.

We will illustrate our method performing the path integral explicitly for the propagator of a particle moving under the action of a constant force f. There are of course many other ways of calculating this propagator [2, 5, 6]. For this particular case, equation (3) reduces to

$$K(x_0, x_{N+1};\ \tau = t_{N+1} - t_0$$
$$= \lim_{\substack{N\to\infty \\ \varepsilon\to 0}} \left(\frac{1}{2\pi \mathrm{i}\hbar\varepsilon}\right)^{(N+1)/2} \int_{-\infty}^{+\infty} \mathrm{d}x_1 \ldots \int_{-\infty}^{+\infty} \mathrm{d}x_N$$
$$\times \exp\left[\frac{\mathrm{i}}{\hbar}\left(\sum_{j=0}^{N} \frac{1}{2\varepsilon}(x_{j+1} - x_j)^2 - \tfrac{1}{2}\varepsilon f(x_j + x_{j+1})\right)\right] \tag{6}$$

where we have set $m = 1$ for convenience.

In the zeroth approximation we have

$$K^{(0)}(x_0, x_{N+1} = x_1;\ \tau = \varepsilon) = \left(\frac{1}{2\pi \mathrm{i}\hbar\varepsilon}\right)^{1/2} \exp\left[\frac{\mathrm{i}}{\hbar}\left(\frac{(x_1 - x_0)^2}{2\tau} - \tfrac{1}{2}\tau f(x_1 + x_0)\right)\right]. \tag{7}$$

In this case only one trajectory contributes to the propagator since there is no integration to be performed (see figure 1). This approximation becomes exact only for the free particle case. That is, in this particular case the propagator has the same form, independent of the length of the time interval.

The reason is that the only trajectory which contributes in the zeroth approximation coincides with the classical one and, as is well known, for quadratic actions the propagators can always be written as

$$K = F(\tau)\exp(\mathrm{i}/\hbar)S_{\text{clas}} \tag{8}$$

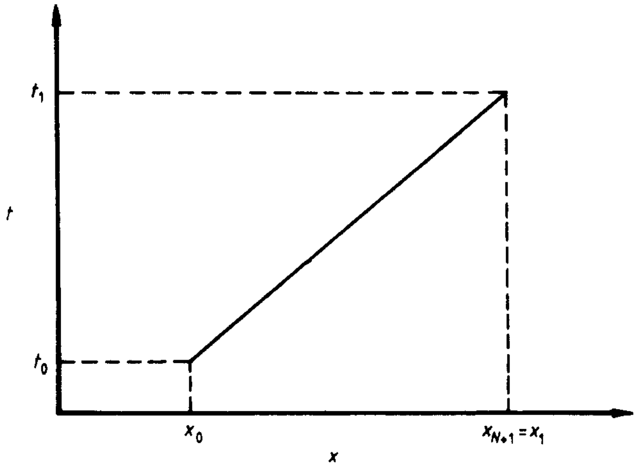

Figure 1. In this case just one trajectory contributes.

where $F(\tau)$ is the pre-exponential factor [2].

In the first approximation we write

$$K^{(1)}(x_0, x_{N+1}=x_2, \tau=2\varepsilon) = \left(\frac{1}{\pi \mathrm{i}\hbar\tau}\right)\int_{-\infty}^{+\infty} \mathrm{d}x_1 \exp\left[\frac{\mathrm{i}}{2\hbar}\left(\frac{(x_2-x_1)^2+(x_1-x_0)^2}{\varepsilon} - \varepsilon f(x_0+x_1) - \varepsilon f(x_1+x_2)\right)\right]. \tag{9}$$

Here, infinite trajectories contribute, but all of them are of the same type. They are polygonals with just one 'vertex' because we still have to integrate over the intermediate variable x_1 (see figure 2). Completing squares in (9) we obtain

$$K^{(1)} = \left(\frac{1}{\pi \mathrm{i}\hbar\tau}\right)\exp\left[\frac{\mathrm{i}}{\hbar}\left(\frac{1}{\varepsilon}[(x_0^2+x_2^2)-\varepsilon^2 f(x_0+x_2)] - \frac{2}{\varepsilon}(c_1^1)^2\right)\right] \times \int_{-\infty}^{+\infty}\mathrm{d}x_1 \exp\left(\frac{\mathrm{i}}{\hbar}\frac{2}{\varepsilon}(x_1-c_1^1)^2\right) \tag{10}$$

where

$$c_1^1 = \tfrac{1}{2}(x_2+x_0) + \tfrac{1}{2}\varepsilon^2 f. \tag{11}$$

We will use a particular nomenclature for the constants $c_i^{(N)}$ which will appear from now on in the process of completing squares in the Fresnel integrals. In this notation the upper index indicates the number of intermediate integrations and the lower index means that this constant was introduced to complete squares in the ith integration.

Performing the Fresnel integral in (10) and rearranging terms we obtain

$$K^{(1)} = \left(\frac{1}{2\pi \mathrm{i}\hbar\tau}\right)^{1/2}\exp\left[\frac{\mathrm{i}}{\hbar}\left(\frac{(x_2-x_0)^2}{2\tau} - \frac{\tau}{2}f(x_0+x_2) - \frac{\tau^2 f^2}{32}\right)\right]. \tag{12}$$

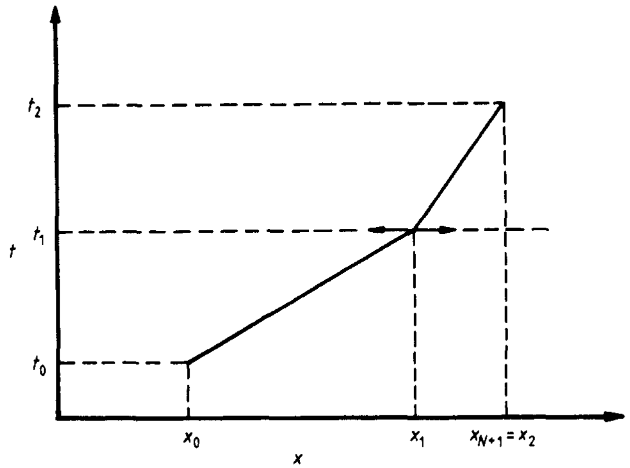

Figure 2. Polygonals which contribute in the first-order approximation.

In the second approximation we have

$$K^{(2)}(x_0, x_{N+1}=x_3;\ \tau=3\varepsilon)$$
$$=\left(\frac{1}{2\pi \mathrm{i}\hbar\varepsilon}\right)^{3/2}\int_{-\infty}^{+\infty}\mathrm{d}x_1\int_{-\infty}^{+\infty}\mathrm{d}x_2$$
$$\times\exp\left(\frac{\mathrm{i}}{2\hbar\varepsilon}\left[(x_3-x_2)^2+(x_2-x_1)^2+(x_1-x_0)^2-\varepsilon^2 f(x_0+2x_1+2x_2+x_3)\right]\right). \tag{13}$$

Here all the trajectories which contribute to K have two 'vertices', because there are just two intermediate integrations (see figure 3).

Completing squares to integrate over the variable x_2 we write

$$K^{(2)}=\left(\frac{1}{2\pi\mathrm{i}\hbar\varepsilon}\right)^{3/2}\exp\left(\frac{\mathrm{i}}{2\hbar\varepsilon}(x_0^2+x_3^2-\varepsilon^2 f(x_0+x_3))\right)$$
$$\times\int_{-\infty}^{+\infty}\mathrm{d}x_1\exp\left(\frac{\mathrm{i}}{2\hbar\varepsilon}\{-2c_1^2+2[x_1^2-x_1(x_0+\varepsilon^2 f)]\}\right)$$
$$\times\int_{-\infty}^{+\infty}\mathrm{d}x_2\exp\left(\frac{\mathrm{i}}{\hbar\varepsilon}(\bar{x}_2-C_1^2)^2\right) \tag{14}$$

where

$$c_1^2=\tfrac{1}{2}(x_1+x_3)+\tfrac{1}{2}\varepsilon^2 f. \tag{15}$$

Performing the Fresnel integral in (14) and completing squares to integrate over the variable x_1 we have

$$K^{(2)}=\left(\frac{1}{2\sqrt{2}\,\pi\mathrm{i}\hbar\varepsilon}\right)\exp\left(\frac{\mathrm{i}}{2\hbar\varepsilon}[(x_0^2+\tfrac{1}{2}x_3^2)-\varepsilon^2 f(x_0+2x_3)-\tfrac{1}{2}\varepsilon^4 f^2-\tfrac{3}{2}(c_2^2)^2]\right)$$
$$\times\int_{-\infty}^{+\infty}\mathrm{d}x_1\exp\left[\left(\frac{\mathrm{i}}{2\hbar\varepsilon}\right)\tfrac{3}{2}(x_1-c_2^2)^2\right] \tag{16}$$

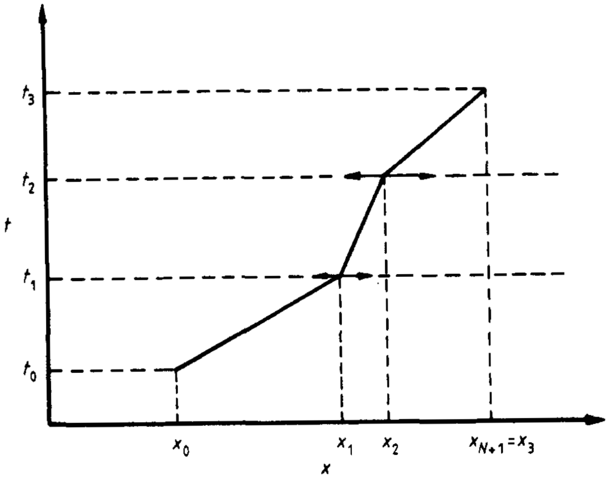

Figure 3. Polygonals which contribute in the second-order approximation.

where

$$c_2^2=\tfrac{1}{3}(2x_0+x_3)+\varepsilon^2 f. \tag{17}$$

Performing the integration in (16) and rearranging terms in the exponential we obtain for this approximation the result

$$K^{(2)}=\left(\frac{1}{2\pi \mathrm{i}\hbar\varepsilon}\right)\exp\left[\frac{\mathrm{i}}{\hbar}\left(\frac{(x_3-x_0)^2}{2\tau}-\frac{\tau}{2}f(x_0+x_3)-\frac{\tau^3 f^2}{27}\right)\right]. \tag{18}$$

In the third approximation we have

$$\begin{aligned}K^{(3)}&(x_0, x_{N+1}=x_4;\ \tau=4\varepsilon)\\ &=\left(\frac{1}{2\pi\hbar \mathrm{i}\varepsilon}\right)^2\int_{-\infty}^{+\infty}\mathrm{d}x_1\ldots\int_{-\infty}^{+\infty}\mathrm{d}x_3\\ &\quad\times\exp\left(\frac{\mathrm{i}}{2\hbar\varepsilon}[(x_4-x_3)^2+\ldots+(x_1-x_0)^2\varepsilon f(x_0+2x_1+2x_2+2x_3+x_4)]\right).\end{aligned} \tag{19}$$

In this case all trajectories which contribute to the propagator are polygonals with three 'vertices', because there are three intermediate integrations.

With an entirely analogous procedure to the one used before, we obtain, after the first integration in the variable x_3,

$$\begin{aligned}K^{(3)}=\frac{1}{4}\left(\frac{1}{\pi \mathrm{i}\hbar\varepsilon}\right)^{3/2}&\exp\left(\frac{\mathrm{i}}{2\hbar\varepsilon}[(x_4^2+x_0^2)-\varepsilon^2 f(x_0+x_4)]\right)\int_{\infty}^{\infty}\mathrm{d}x_1\int_{\infty}^{\infty}\mathrm{d}x_2\\ &\times\exp\left(\frac{\mathrm{i}}{2\hbar\varepsilon}\{-2(c_1^3)^2+2[x_2^2-x_2(x_1+\varepsilon^2 f)]+2[x_2^2-x_1(x_0+\varepsilon^2 f)]\}\right)\end{aligned} \tag{20}$$

where

$$c_1^3=\tfrac{1}{2}(x_4+x_2+\varepsilon^2 f). \tag{21}$$

Completing squares in the variable x_2 and integrating in this variable we have

$$K^{(3)}=\left(\frac{1}{3}\right)^{1/2}\left(\frac{1}{2\pi i\hbar\varepsilon}\right)\exp\left(\frac{i}{2\hbar\varepsilon}[(x_0^2+\tfrac{1}{2}x_4^2)+\varepsilon^2f(x_0+2x_4)-\tfrac{1}{2}\varepsilon^4f^2]\right)$$
$$\times\int_{-\infty}^{+\infty}dx_1\exp\left(\frac{i}{2\hbar\varepsilon}\{-\tfrac{3}{2}(c_2^3)^2+2[x_1^2-x_1(x_0+\varepsilon^2f)]\}\right) \tag{22}$$

where

$$c_2^3=\tfrac{1}{3}(2x_1+x_4+3\varepsilon^2f). \tag{23}$$

To perform the last integration we rewrite (22) in the form

$$K^{(3)}=\left(\frac{1}{3}\right)^{1/2}\left(\frac{1}{2\pi i\hbar\varepsilon}\right)\exp\left(\frac{i}{2\hbar\varepsilon}[(x_0^2+\tfrac{1}{3}x_4^2)-\varepsilon^2f(x_0+3x_4)-2\varepsilon^4f^2]-\tfrac{4}{3}(c_3^3)^2\right)$$
$$\times\int_{\infty}^{\infty}dx_1\exp\left(\frac{i}{2\hbar\varepsilon}[\tfrac{4}{3}(x_1-c_3^3)^2]\right) \tag{24}$$

where

$$c_3^3=\tfrac{1}{4}(3x_0+x_4)+\tfrac{3}{2}\varepsilon^2f. \tag{25}$$

Evaluating the integral in (24) and using (25) we finally obtain

$$K^{(3)}=\left(\frac{1}{2\pi i\hbar\tau}\right)^{1/2}\exp\left[\frac{i}{\hbar}\left(\frac{(x_4-x_0)^2}{2\tau}-\frac{\tau}{2}f(x_0+x_4)-\frac{\tau^3f^2}{25.6}\right)\right]. \tag{26}$$

We could go on to the next approximation, but it is really not necessary. As we will see, with the previous results we will be able to obtain the expression for the Nth approximation for the propagator.

Let us have a look at the successive approximate expressions for the propagator before the last integration is performed in the variable x_1. In order to do this, we will write the respective expressions appearing in the exponential arguments in (10), (16) and (24) (apart from a factor $(i/2\hbar\varepsilon)$) as

$$N=1\qquad[(x_0^2+x_2^2)-\varepsilon^2f(x_0+x_2)-a_1\varepsilon^4f^2]-2(x_1-c_1^1)^2-2(c_1^1)^2\qquad a_1=0 \tag{27a}$$
$$N=2\qquad[(x_0^2+\tfrac{1}{2}x_3^2)-\varepsilon^2f(x_0+2x_3)-a_2\varepsilon^4f^2]+\tfrac{3}{2}(x_1-c_2^2)^2-\tfrac{3}{2}(c_2^2)^2\qquad a_2=\tfrac{1}{2} \tag{27b}$$
$$N=3\qquad[(x_0^2+\tfrac{1}{3}x_4^2)-\varepsilon^2f(x_0+3x_4)-a_3\varepsilon^4f^2]+\tfrac{4}{3}(x_1-c_3^3)^2-\tfrac{4}{3}(c_3^3)^2\qquad a_3=2 \tag{27c}$$

where we have introduced the coefficients a_j for convenience.

Generalising equations (27) we write

$$\text{general } N\qquad\left[\left(x_0^2+\frac{x_{N+1}^2}{N}\right)-\varepsilon^2f(x_0+Nx_{N+1})-a_N\varepsilon^4f^2\right]$$
$$+\frac{(N+1)}{N}(x_1-c_N^N)^2-\left(\frac{N+1}{N}\right)(c_N^N)^2. \tag{28}$$

Note that in (28) we still have to identify the expressions for c_N^N and the coefficients a_N.

Looking at equations (11), (17) and (25) we see clearly that

$$c_N^N=\frac{1}{N+1}(Nx_0+x_{N+1})+\frac{N}{2}\varepsilon^2f. \tag{29}$$

With the aim of finding a_N, observe that this is the total coefficient of the term $\varepsilon^4 f^2$ in the exponential argument for the $K^{(N)}$ before the last integration in the variable x_1 is performed. When we make this last integration, completing squares in the variable x_1, new terms in $\varepsilon^4 f^2$ will appear which are present in $(N+1/N)(c_N^N)^2$ (see for example equations (27)). The coefficient of these new terms will be defined by α_N and using (29) we find

$$\alpha_N = \tfrac{1}{4}N(N+1). \tag{30}$$

Then, in the final result for $K^{(N)}$, the total coefficient of the term in $\varepsilon^4 f^2$ will be $a_N + \alpha_N$. Thus, in calculating $K^{(N+1)}$, we expect some kind of relation between a_{N+1}, a_N and α_N.

From (30) we can write the first α_N:

$$\alpha_1 = \tfrac{1}{2} \qquad \alpha_2 = \tfrac{3}{2} \qquad \alpha_3 = 3 \tag{31}$$

and so on. Comparing (31) with the values for a_1, a_2, a_3, written in (27*a*), (27*b*) and (27*c*) respectively, we conclude that

$$a_{N+1} = a_N + \alpha_N. \tag{32}$$

In other words we have

$$a_{N+1} = \sum_{i=0}^{N} \alpha_i \tag{33}$$

where $\alpha_0 = 0$ because in the zeroth approximation we do not have any integration to perform. Substituting (20) in (33) we have

$$a_{N+1} = \tfrac{1}{4}\sum_{i=0}^{N} i(i+1). \tag{34}$$

Now we are ready to compute the exact propagator.

As we have seen in equations (7), (12), (18) and (26), the pre-exponential factor and the first two terms of the exponential argument in the expression for the propagator are always the same. So when $N\to\infty$ they will remain with the same values (this can be confirmed by direct calculation using (28)). The problem in question becomes essentially how to find the limiting value of the last term in the exponential argument of $K^{(N)}$.

To obtain this limiting value, let us look at equation (28). All we have to do is calculate the total coefficient of the term $\varepsilon^4 f^2$, which is given after the last integration in the variable x_1 by $(a_N + \alpha_N) = a_{N+1}$, apart from a negative sign. Therefore

$$\left(\frac{\mathrm{i}}{\hbar}\right)\frac{a_{N+1}}{2\varepsilon}\,\varepsilon^4 f^2 = \left(\frac{\mathrm{i}}{\hbar}\right)\frac{\tau^3 f^3}{8(N+1)^3}\sum_{i=0}^{N} -i(i+1) \tag{35}$$

where we have used (34) and $\tau = (N+1)\varepsilon$. Taking $\lim_{N\to\infty}$ on both sides of (35) we have

$$\lim_{N\to\infty}\frac{1}{(N+1)^3}\sum_{i=0}^{N} i(i+1) = \lim_{N\to\infty}\left[\left(\frac{1}{N+1}\right)^3\left(\sum_{i=0}^{N} i^2 + \sum_{i=0}^{N} i\right)\right]. \tag{36}$$

Using the well known results for these series [5]

$$\sum_{i=0}^{N} i^2 = \tfrac{1}{6}N(N+1)(2N+1) \qquad \sum_{i=0}^{N} i = \tfrac{1}{2}N(N+1) \tag{37}$$

we have

$$\lim_{N\to\infty}\left(\frac{1}{N+1}\right)^3\sum_{i=0}^{N} i(i+1)=\frac{1}{3}. \tag{38}$$

Substituting (38) in (35) we obtain

$$\lim_{N\to\infty}\frac{\mathrm{i}}{\hbar}\frac{a_{N+1}}{2\varepsilon}\varepsilon^4 f^2=\frac{\mathrm{i}}{\hbar}\frac{\tau^3 f^2}{24}. \tag{39}$$

Therefore the exact propagator is given by

$$K(x_0, x_N; t_0, t_N)$$
$$= \lim_{N\to\infty} K^{(N)}$$
$$=\left(\frac{1}{2\pi\mathrm{i}\hbar\tau}\right)^{1/2}\exp\left[\frac{\mathrm{i}}{\hbar}\left(\frac{(x_{N+1}-x_0)^2}{2\tau}-\frac{\tau f(x_0+x_{N+1})}{2}+\frac{\tau^3 f^2}{24}\right)\right] \tag{40}$$

which is the exact result for the propagator of a particle moving under the action of a constant force. One interesting property of this approach is that in each stage we have an explicit approximate expression for the propagator. In the case treated previously, this succession converges rapidly (see equations (7), (12), (18) and (26)). We expect that this will occur whenever we have a quadratic action, where the propagator is given correctly by (3), because the convergence depends essentially on how well the classical trajectory can be approximated by a polygonal one. Of course this method is not practical for quadratic actions because the semiclassical approximation (2) provides an exact result. But it not only illustrates the procedure of convergence in the path integral method, but also gives an alternative method for approximate calculations. It would be very interesting to compare this method with the semiclassical approximation in problems where non-quadratic actions are involved.

We are indebted to I C Moreira for helpful discussions.

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