# PATH COLLAPSE IN FEYNMAN FORMULA. STABLE PATH INTEGRAL FORMULA FROM LOCAL TIME REPARAMETRIZATION INVARIANT AMPLITUDE ☆

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The Feynman formula, which expresses the time displacement amplitude $\langle x_b|\exp(-t\hat{H})|x_a\rangle$ in terms of a path integral $\prod_1^N(\int dx_n)\prod_1^{N+1}(\int dp_n/2\pi)\exp\{\sum_1^N[ip_n(x_n-x_{n-1})-\varepsilon H(p_n,x_n)]\}$ with large $N$, does not exist for systems with Coulomb $-1/r$ potential and gives incorrect threshold behaviours near centrifugal $1/r^2$ or angular $1/\sin^2\theta$ barriers. We discuss the physical origin of this failure and propose an alternative well-defined path integral formula based on a family of amplitudes that is invariant under arbitrary local time reparametrizations. The time slicing with finite $N$ breaks this invariance. For appropriate choices of the reparametrization function the fluctuations are stabilized and the new formula is applicable to all the above systems.

**1.** In 1938, Dirac [1] triggered the development of path integral physics by observing that the propagator for an infinitesimal time $\varepsilon$, $\langle x|\exp(-\varepsilon\hat{H})|x'\rangle$ [$\hat{H}=T(\hat{p})+V(\hat{x})$ is the hamiltonian operator, we shall work with imaginary time] is approximately given by

$$\langle x|\exp(-\varepsilon\hat{H})|x'\rangle\approx\exp\left(\int_0^\varepsilon dt\,[ip\dot{x}-H(p,x)]\right)\approx\int_{-\infty}^{\infty}\frac{dp}{2\pi}\exp[ip(x-x')-\varepsilon H(p,\bar{x})]\,, \tag{1}$$

where $\bar{x}=\frac{1}{2}(x+x')$. This observation expresses the fact that in the limit of high temperature $\varepsilon=1/T\to 0$, quantum statistics becomes classical. By decomposing in the finite-time propagator $\langle x't|x0\rangle\equiv\langle x'|\exp(-t\hat{H})|x\rangle$ the operator $\exp(-t\hat{H})$ into a large number $N+1$ of factors $\exp(-\varepsilon\hat{H})$ with $\varepsilon=t/(N+1)$ and inserting between each pair of these a completeness relation $\int dx_n|x_n\rangle\langle x_n|$ one finds the celebrated Feynman formula [2,3] [#1]

$$\langle x'|\exp(-t\hat{H})|x\rangle\approx\prod_{n=1}^{N}\left(\int dx_n\right)\int\prod_{n=1}^{N+1}\left(\int\frac{dp_n}{2\pi}\right)\exp\left(\sum_{n=1}^{N+1}[ip_n(x_n-x_{n-1})-\varepsilon H(p_n,\bar{x}_n)]\right). \tag{2}$$

The exponent can be viewed as the discrete approximation to the canonical action $\mathscr{A}[p,x]$ evaluated on an equally spaced time lattice $t_n=n\varepsilon$. The symbol $\approx$ denotes an equality up to terms of order $\varepsilon$ [this includes $\varepsilon^2(x_n-x_{n-1})^2$ terms since $\langle(x_n-x_{n-1})^2\rangle\sim\varepsilon^{-1}$ in the exponent]. A formula due to Trotter,

$$\exp[-t(\hat{T}+\hat{V})]=\lim_{N\to\infty}[\exp(-\varepsilon\hat{T})\exp(-\varepsilon\hat{V})]^{N+1}\,,$$

can be used to argue that no more than this order is necessary to obtain eventually, in the limit $N\to\infty$, the correct quantum mechanical amplitude. For sufficiently well-behaved potentials the argument can be made rigorous [4].

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[#1] Notice that going by history the name Wiener–Dirac–Feynman formula would be more appropriate.

**2.** Unfortunately, most physically relevant systems have potentials which do not fall into this class. As soon as they contain an abyss of the Coulomb type or a centrifugal barrier (or the similar Pöschl–Teller $1/\sin^2\theta$ barrier at the poles of a sphere at fixed azimuthal angular momentum $m$), the Dirac relation is not true uniformly enough in $x$ to allow for a Feynman formula. There is a simple physical reason for this. Consider the case of an attractive Coulomb potential. The path with $N+1$ time steps may be viewed as a random chain in space-time fluctuating in equilibrium in the neighbourhood of a $1/r$ hole. If the chain has only a finite number of links, $N+1$, it can easily stretch out and slide down into the hole, just as a single classical particle would do. Infinitely many links (which for a finite time require infinitely short time spacings) are obviously necessary to provide for enough configurational entropy to maintain a finite gyration radius which halts the collapse. A random chain in $D$ dimensions with $k$ links on a simple cubic lattice has $(2D)^k = \exp(k \ln 2D)$ configuration. If for a fixed chain length the number of links $k$ is increased near $r=0$ as $1/r$, the exponent develops a repulsive potential of the Coulomb type which prevents the collapse.

By the same token the Feynman formula cannot explain correctly the small $r$ behaviour of radial wave functions near a centrifugal barrier. A finite path slides down the barrier too easily. An infinite increase in entropy is needed to convert the classical radial amplitude $\propto \exp(1/r^2)$ into the correct threshold behaviour $r^l$.

In the past there have been two attempts to circumvent this problem.

(i) In the Coulomb potential one has smeared out the singularity, used the Feynman formula, taken the limit of large $N$, and gone back to the limit of a singular potential at the end. This procedure was followed in Monte Carlo simulations [5]. In analytic work it is hard to implement.

(ii) In many so-called solutions of path integrals one uses the non-existing Feynman formula (2) as a starting point and repairs this by ensuing illegal operations [#2], made possible by the knowledge of the solutions $\psi_k(x)$ of the Schrödinger equation $\hat{H}\psi_k = E_k\psi_k$. This knowledge suggests the replacement of the infinitesimal integrands in (2) by

$$\int \frac{dp_n}{2\pi} \exp[ip_n(x_n - x_{n-1}) - \varepsilon H(p_n, \bar{x}_n)] \to \int dk\, \psi_k(x_n)\psi_k^\dagger(x_{n-1}) \exp(-\varepsilon E_k) . \tag{3}$$

At fixed $\varepsilon$ this is justified if $x$ stays sufficiently far away from any singularity. With the right-hand side of (3) it is trivial to integrate out all $x_n$ using the orthogonality relations for $\psi_k(x)$. Since $\hat{H}$ is diagonal, this procedure replaces the fluctuating path in $x$ space by a completely stiff (i.e. time independent) path in $k$ space thereby converting the path integral into an ordinary integral over $k$, $\langle x_b | \exp(-t\hat{H}) | x_a \rangle = \int dk\, \psi_k(x_b)\psi_k^\dagger(x_a) \exp(-tE_k)$. While the result is obviously correct, the initial step is not. The wave function replacement (3) has introduced a specific and correct regularization of the integrals $\int dx_n$ near the singularity, Its knowledge, however, was borne out of the Schrödinger equation, not of the non-existing Feynman formula.

As an example, consider a free particle in radial coordinates. By using the well-known radial Schrödinger wave functions for an azimuthal angular momentum $m$, a simpler, by projecting the cartesian $D=2$ result into a fixed $m$, $\langle x_b | \exp[-t(\frac{1}{2}\hat{p}^2)] | x_a \rangle = \sum_m (1/\sqrt{r_b r_a})(r_b; r_a t)_m \exp[m(\varphi_b - \varphi_a)/2\pi]$, we find that the radial amplitude can be written in a certainly valid path integral representation as

$$(r_b; r_a | t)_m = \prod_{n=1}^{N} \left( \int \frac{dr_n}{\sqrt{2\pi\varepsilon}} \right) \exp(\tilde{\mathscr{A}}_m^N) , \tag{4a}$$

where $\tilde{\mathscr{A}}_m^N$ is an effective action ($I_m$ is the modified Bessel function)

$$\tilde{\mathscr{A}}_m^N = -\sum_{n=1}^{N+1} \left( \frac{(r_n - r_{n-1})^2}{2\varepsilon} - \ln[\sqrt{2\pi r_n r_{n-1}/\varepsilon}\, I_m(r_n r_{n-1}/\varepsilon)] \right) . \tag{4b}$$

Each term in the sum corresponds to the right-hand side of (3). Now, for $r_n$, $r_{n-1}$ far enough away from the

[#2] A good sample of such illegal operations can be found in table 1 of the recent review article by Bernido, Carpio-Bernido and Inomata. Also many other papers which should have been quoted in that table fall into this class.

singularity at the origin, $r_n, r_{n-1} \gg \varepsilon$, the asymptotic expansion of the Bessel function $I_m$ gives indeed the classical action of the Feynman type

$$\mathscr{A}_m^N = -\sum_{n=1}^{N+1}\left(\frac{(r_n-r_{n-1})^2}{2\varepsilon}+\varepsilon\frac{m^2-1/4}{2r_n r_{n-1}}\right) \tag{4c}$$

so that (3) is correct. Unfortunately, this is not true uniformly enough in $r$ to allow for this replacement in the path *integral*. For smaller $r$, the effective action can only be expanded in an asymptotic power series in $\varepsilon^k/r^{2k}$ which does not converge for any $\varepsilon/r^2$ and cannot be used at all near $r=0$. The short-time amplitude cannot be approximated by the classical one. In fact, the partition function with the free system subtracted reads $Z=-\frac{1}{2}m$ while the classical partition function is $Z_{\mathrm{cl}}=-[\frac{1}{2}(m^2-\frac{1}{4})]^{1/2}$. More dramatically, with (4c) the path integrand of the Feynman type (4a) would blow up for $m=0$, i.e. the path would collapse into the origin. The path integral (4a) is only correct with the action (4b). But this information stems from the Schrödinger equation, not from the Feynman formula.

A similar situation holds for $1/\sin^2\theta$ potentials if one makes use of the limit $P_l^m(\cos\theta)\to J_m(\theta l)/l^m$, $l\to\infty$ ($J_m$ is the Bessel function).

**3.** This suggests one possibility of salvaging a correct path integral formula for quantum mechanical amplitudes in the presence of a centrifugal barrier. We separate the barrier out of the potential and write $V=V_{\mathrm{c}}+V_{\mathrm{sm}}$, where $V_{\mathrm{sm}}$ is smooth in $x$. Now the Trotter formula *is* valid for the splitting $\{\exp[-\varepsilon(T+V_{\mathrm{c}})]\exp[-\varepsilon V_{\mathrm{sm}}]\}^{N+1}$. Hence a correct path integral valid for an arbitrary smooth $V_{\mathrm{sm}}$ reads

$$(r_{\mathrm{b}}; r_{\mathrm{a}}\,|\,t)_m=\prod_{n=1}^{N}\left(\int\frac{\mathrm{d}r_n}{\sqrt{2\pi\varepsilon}}\right)\exp\left(\mathscr{A}_m^N-\varepsilon\sum_{n=1}^{N+1}V_{\mathrm{sm}}(r_n)\right), \tag{5}$$

i.e. the classical free particle *plus* barrier part in the Feynman formula, $\mathscr{A}_m^N$, has to be replaced by the *full quantum mechanical* $\tilde{\mathscr{A}}_m^N$ of (4b). Only $V_{\mathrm{sm}}$ enters classically the short-time amplitude.

**4.** A much more powerful formula is obtained by allowing for the above described increase in entropy by means of position dependent time intervals which shorten to zero near a singularity. The inspiration for this comes from the Duru–Kleinert solution [7] of the Coulomb path integral and its explicit time sliced form [8]. Generalizing this we consider an infinite family of amplitudes, some members of which will be seen to possess a bona fide finite step path integral representation. This family is given by

$$K(x_{\mathrm{b}}t_{\mathrm{b}}; x_{\mathrm{a}}t_{\mathrm{a}}\,|\,s)=f(x_{\mathrm{b}},t_{\mathrm{b}})^{1-\lambda}\langle x_{\mathrm{b}}t_{\mathrm{b}}|\exp[-sf(\hat{x},\hat{t})^{\lambda}(\hat{H}-\hat{E})f^{1-\lambda}(\hat{x},\hat{t})]\,|x_{\mathrm{a}}t_{\mathrm{a}}\rangle f(x_{\mathrm{a}},t_{\mathrm{a}})^{\lambda} \tag{6}$$

with an arbitrary pseudo-time $s$ and parameter $\lambda$ (preferably $\lambda=\frac{1}{2}$). Here $|xt\rangle$ are states localized in space and time on which the operators $\hat{p}$, $\hat{E}$ have the differential matrix elements $\langle xt|\hat{p}=-\mathrm{i}\partial_x\langle xt|$, $\langle xt|\hat{E}=\mathrm{i}\partial_t\langle xt|$. For the sake of generality we shall allow $\hat{H}$ to depend explicitly on $t$. The integral over $s$ in (5) is obviously the usual quantum mechanical amplitude

$$\langle x_{\mathrm{b}}t_{\mathrm{b}}|x_{\mathrm{a}}t_{\mathrm{a}}\rangle=\int_0^\infty \mathrm{d}s\,K(x_{\mathrm{b}}t_{\mathrm{b}}; x_{\mathrm{a}}t_{\mathrm{a}}\,|\,s)=(\hat{H}-\hat{E})^{-1}\delta(x_{\mathrm{b}}-x_{\mathrm{a}})\delta(t_{\mathrm{b}}-t_{\mathrm{a}})\,. \tag{7}$$

It is remarkable that this is true for *any* function $f(x,t)$ and we shall call this property of (7) *local time reparametrization invariance*. In order to calculate this amplitude we decompose $s$ into $N_s+1$ pieces $\varepsilon_s=s/(N_s+1)$ and insert the $N_s+1$ completeness relations $\int\mathrm{d}x_n\int\mathrm{d}t_n\,|x_n t_n\rangle\langle x_n t_n|=1$ thus obtaining a product of integrals over small-$s$ amplitudes:

$$\langle x_n t_n|\exp(-\{\varepsilon_s f(\hat{x},\hat{t})^{\lambda}[H(\hat{p},\hat{x},\hat{t})-\hat{E}]f(\hat{x},\hat{t})^{1-\lambda}\})\,|x_{n-1}t_{n-1}\rangle\,. \tag{8}$$

Notice that the time reparametrization invariance of (7) is *broken* by the finite $-\varepsilon_s$ "time" slicing. The Feynman formula would be retrieved for the special choice $f(x,t)\equiv 1$. In the presence of a singularity in $H$ the invariance is broken so badly that it is impossible to obtain the correct amplitude for $f(x,t)\equiv 1$. Exploiting the new "gauge" degree of freedom we may, however, choose the function $f(x,t)$ to vanish appropriately at each singularity. In this way we can shorten the local time intervals $\varepsilon=\varepsilon_s f(x,t)$ so that the chain entropy prevents a collapse.

There is then no problem in obtaining a well-defined finite-$N_s$ path integral formula for this amplitude which reads

$$K^{N_s}(x_b t_b; x_a t_a|s)=f(x_b,t_b)^{1-\lambda}f(x_a,t_a)^{\lambda}\prod_{n=1}^{N}\left(\int dx_n\int dt_n\right)\prod_{n=1}^{N+1}\left(\int\frac{dp_n}{2\pi}\int\frac{dE_n}{2\pi}\right)\exp(\mathscr{A}_s^{N_s}), \tag{9a}$$

where $\mathscr{A}_s^{N_s}$ is the $N_s^{+1}$ step decomposition

$$\mathscr{A}_s^{N_s}=\sum_{n=1}^{N+1}\{ip_n(x_n-x_{n-1})-iE_n(t_n-t_{n-1})-\varepsilon_s f(x_n,t_n)^{\lambda}[H(p_n,\bar{x}_n,\bar{t}_n)-E_n]f(x_{n-1},t_{n-1})^{1-\lambda}\} \tag{9b}$$

of the classical action

$$\mathscr{A}_s[x,p,t,E]\equiv\int_0^s ds'\ [px'-Et'-f(x,t)(H-E)] \tag{9c}$$

in the phase space of spacetime paths $x(s)$, $t(s)$, $p(s)$, $E(s)$ parametrized by $s('\equiv d/ds)$. The energy integrations can be performed. This forces the fluctuating time intervals to be equal to the space dependent ones $\Delta t_n=\varepsilon_s f(x_n,t_n)$, resulting in the alternative formula

$$K^{N_s}(x_b t_b; x_a t_a|s)=f(x_b,t_b)^{1-\lambda}f(x_a,t_a)^{\lambda}\prod_{n=1}^{N_s}\left(\int dx_n\right)\prod_{n=1}^{N_s+1}\left(\int\frac{dp_n}{2\pi}\right)$$

$$\times\delta\left(t_b-t_a-\varepsilon_s\sum_{n=1}^{N_s+1}f(x_n,t_n)^{\lambda}f(x_{n-1},t_{n-1})^{1-\lambda}\right)\exp(\mathscr{A}_{s2}^{N_s}), \tag{10a}$$

where

$$\mathscr{A}_{s2}^{N_s}=\sum_{n=1}^{N_s+1}[ip_n(x_n-x_{n-1})-\varepsilon_s f(x_n,t_n)^{\lambda}H(p_n,\bar{x}_n,\bar{t}_n)f(x_{n-1},t_{n-1})^{1-\lambda}]. \tag{10b}$$

In the common case that the energy is independent of $t$ we can restrict ourselves also to $t$ independent slicing functions $f(x)$. Then the amplitude depends only on the time difference and we may conveniently integrate (10a) over $\int dt_b \exp[iE(t_b-t_a)]$ obtaining

$$\int_{t_a}^{\infty}dt_b\exp[iE(t_b-t_a)]K^{N_s}(x_b t_a; x_a t_a|s)=f(x_b)^{1-\lambda}f(x_a)^{\lambda}\prod_{n=1}^{N_s}\left(\int dx_n\right)\prod_{n=1}^{N_s+1}\left(\frac{dp_n}{2\pi}\right)\exp(\mathscr{A}_{s3}^{N_s}) \tag{11a}$$

with

$$\mathscr{A}_{s3}^{N_s}=\sum_{n=1}^{N_s+1}\{ip_n(x_n-x_{n-1})-\varepsilon_s f(x_n)^{\lambda}[H(p_n,\bar{x}_n)-E]f(x_{n-1})^{1-\lambda}\}. \tag{11b}$$

This is the path integral representation of the auxiliary amplitude

$$f(x_b)^{1-\lambda}\langle x_b|\exp[-sf(\hat{x})^{\lambda}(\hat{H}-E)f(\hat{x})^{1-\lambda}]|x_a\rangle f(x_a)^{\lambda}. \tag{11c}$$

Integration over $s$ approximately by performing the sum $\varepsilon_s \sum_{N_s=1}^{\infty}$ and doing the energy integral $\mathrm{d}E \exp[-\mathrm{i}E(t_\mathrm{b}-t_\mathrm{a})]$ gives again, in the limit $\varepsilon_s \to 0$, the usual Green's function (7).

The integration of eqs. (11) can proceed after a convenient variable change. This needs some care since it is usually a non-holonomic transformation [9] which brings the kinetic term $f(\hat{x})^{\lambda}(\frac{1}{2}\hat{p}^2)f(\hat{x})^{1-\lambda}$ to the standard form $\frac{1}{2}\hat{p}^2$.

**5.** As an example, we write down an existing path integral for the radial motion with a centrifugal barrier. Take the above discussed case of a free particle in two dimensions. The regularizing function $f(x)$ has to remove the barrier, i.e. the proper choice is $f(x)=r^2$. After a change from $r$ to $\exp(\xi)$, this implies the space dependent time intervals $\Delta t = \varepsilon_s \exp(2\xi)$, we have

$$(r_\mathrm{b}; r_\mathrm{a} | t)_m = \int_{-\infty}^{\infty} \mathrm{d}E \exp(-\mathrm{i}Et)\, \varepsilon_s \sum_{N_s=1}^{\infty} \prod_{n=1}^{N_s} \left( \int \mathrm{d}\xi_n \right) \prod_{n=1}^{N_s+1} \left( \int \frac{\mathrm{d}p_n^{\xi}}{2\pi} \right) \exp(\mathscr{A}_{s3}^{N_s}) \tag{12a}$$

with

$$\mathscr{A}_{s3}^{N_s} = \sum_{n=1}^{N_s+1} \{\mathrm{i}p_n^{\xi}(\xi_n - \xi_{n-1}) - \varepsilon_s[\tfrac{1}{2}(p_n^{\xi})^2 + \tfrac{1}{2}m^2 - E\exp(2\bar{\xi}_n)]\}\,. \tag{12b}$$

We may add a further Coulomb potential. This introduces a term $-e^2\exp(\bar{\xi}_n)$ and the action (12b) becomes that of the Morse potential. The same thing happens to the radial path integral for the Coulomb potential in any dimension $D$ with angular momentum $l$, in which case $m = \frac{1}{2}D - 1 + l$. Likewise for a radial harmonic oscillator. After a change of variables $\xi_\mathrm{C} = 2\xi_\mathrm{O}$, $m_\mathrm{C} = \frac{1}{4}m_\mathrm{O}$ the last two amplitudes are the same [apart from a trivial normalization factor $(r^\mathrm{C}; r^\mathrm{C} | t)^\mathrm{C} = \frac{1}{2}\sqrt{r_\mathrm{b}^\mathrm{O} r_\mathrm{a}^\mathrm{O}}\,(r_\mathrm{b}^\mathrm{O}; r_\mathrm{a}^\mathrm{O} | t)_m^\mathrm{O}$]. This operation proves the path integral equivalence of a Coulomb system with $D$, $l$ and a harmonic oscillator with $D^\mathrm{O} = 2D-2$, $l^\mathrm{O} = 2l$. A previous attempt [10] based on the two weak regulator function $f(x) = r$ must be considered as failed (in spite of the author's claim to the contrary) since it only manipulates non-existing time-sliced expressions with collapsing paths.

Notice that the Morse path integral (12) must be integrated as it stands and not in the reversed fashion found in the literature [11], where it is transformed into the meaningless Feynman path integral of the Coulomb plus centrifugal potential.

**6.** Similarly, the action with the angular barrier $1/\sin^2\theta$, must first be transformed with $f = \sin^2\theta$, $\mathrm{d}t = \mathrm{d}s \sin^2\theta$, $\sin^2\theta = 1/\mathrm{ch}^2 x$ to the modified Pöschl–Teller action before it possesses a time-sliced path integral.

**7.** Let us finally remark that there is no way, in principle, of *deducing* the time reparametrization invariant amplitude (7) and the ensuing path integral formulas (9)–(11) from the non-existing finite-$N$ Feynman formula just as one cannot construct an analytic function from the knowledge of its value at one singular point.

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