

HOW TO DO THE TIME SLICED PATH INTEGRAL OF THE H ATOM

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In response to criticism concerning the formal nature of the Duru–Kleinert transformation of the path integral of the H atom, we perform this transformation explicitly in the time sliced form and arrive, of course, at the desired product of gaussian factors which yield the harmonic oscillator. We also point out where previous attempts to do the same thing went wrong.

In 1976, H. Duru and the author [1] proposed a procedure of how to transform the path integral of the H atom into that of a harmonic oscillator. The transformation involved two key steps: a change of the time variable and taking the “square root of the coordinates” via a Kustaanheimo–Stiefel transformation. The paper was structural in character and the transformation was done formally in the continuum version of the path integral. This has given rise to justified criticism [2,3] and prompted Inomata [4] and Ho and Inomata [5], in 1981 (2) to attempt going through the Duru–Kleinert procedure in the time sliced form of the path integral. After some manipulations they did arrive at the same result as ref. [1]. Unfortunately, their manipulations contain two essential mistakes, such that their arrival at the known answer was fortuitous and the problem they set out to do remained unsolved. Since their work has been quoted in numerous publications [7] in conjunction with refs. [1,7], the mistake has obviously gone unnoticed (it has reappeared in a number of these papers). Since it concerns an elementary problem of quantum mechanics, we feel that it is worth clarifying the situation by giving a correct application of the Duru–Kleinert procedure to the time sliced version of the path integral, arriving at the desired product of gaussian integrals of a harmonic oscillator. Along the way, we shall point out where the previous attempts [4,5] to do the same thing went wrong.

For simplicity, we shall consider only the case of the two-dimensional H atom. The starting point is the observation that the Fourier transformed amplitude

$$\begin{aligned}
 G(\mathbf{x}_b, \mathbf{x}_a | E) &= \int_0^\infty dt e^{iEt} \langle \mathbf{x}_b | t | \mathbf{x}_a 0 \rangle = \int_0^\infty dt \int \mathcal{D}^D x \exp \left(i \int_0^t dt' [\mathbf{p} \cdot \dot{\mathbf{x}} - H(\mathbf{p}, \mathbf{x})] \right) \\
 &= \int_0^\infty dt e^{iEt} \langle \mathbf{x}_b | e^{-i\hat{H}t} | \mathbf{x}_a \rangle = \langle \mathbf{x}_b | i(E - \hat{H})^{-1} | \mathbf{x}_a \rangle, \tag{1}
 \end{aligned}$$

can also be rewritten in any of the three following ways

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$$G(\mathbf{x}_b, \mathbf{x}_a | E) = f(r_a) \int_0^\infty ds \langle \mathbf{x}_b | \exp[-isf(r)(\hat{H}-E)] | \mathbf{x}_a \rangle \quad (2a)$$

$$= f(r_b) \int_0^\infty ds \langle \mathbf{x}_b | \exp[-is(\hat{H}-E)f(r)] | \mathbf{x}_a \rangle \quad (2b)$$

$$= f^{1/2}(r_b) f^{1/2}(r_a) \int_0^\infty ds \langle \mathbf{x}_b | \exp[-isf^{1/2}(r)(\hat{H}-E)f^{1/2}(r)] | \mathbf{x}_a \rangle, \quad (2c)$$

where $f(r)$ is a rather arbitrary function of r . By grating the s axis with $s_n = \epsilon n$, $n=0, \dots, N+1$, $\epsilon \equiv s/(N+1)$ and inserting a complete set of states at each s_n , (2b) and (2c) become

$$G(\mathbf{x}_b, \mathbf{x}_a | E) \approx f(r_{N+1}) \int_0^\infty ds \prod_{n=1}^N \left(\int d^D x_n \right) \prod_{n=1}^{N+1} \langle \mathbf{x}_n | \exp[-i\epsilon(\hat{H}-E)f(r_{n-1})] | \mathbf{x}_{n-1} \rangle, \quad (3a)$$

$$G(\mathbf{x}_b, \mathbf{x}_a | E) \approx f^{1/2}(r_{N+1}) f^{1/2}(r_0) \int_0^\infty ds \prod_{n=1}^N \left(\int d^D x_n \right) \langle \mathbf{x}_n | \exp[-i\epsilon f^{1/2}(r_n)(\hat{H}-E)f^{1/2}(r_{n-1})] | \mathbf{x}_{n-1} \rangle, \quad (3b)$$

where $\mathbf{x}_a = \mathbf{x}_0$, $\mathbf{x}_b = \mathbf{x}_{N+1}$, and this can be rewritten as

$$\begin{aligned} \mathcal{G}(\mathbf{x}_b, \mathbf{x}_a | E) &\approx f(r_{N+1}) \int_0^\infty ds \prod_{n=1}^N \left(\int d^D x_n \right) \\ &\times \prod_{n=1}^{N+1} \int d\mathbf{p}_n \exp\left(i \sum_{n=1}^{N+1} [\mathbf{p}_n \cdot (\mathbf{x}_n - \mathbf{x}_{n-1}) - \epsilon(H_n - E)f^{1/2}(r_{n-1})] \right), \end{aligned} \quad (4a)$$

$$\begin{aligned} G(\mathbf{x}_b, \mathbf{x}_a | E) &\approx f^{1/2}(r_{N+1}) f^{1/2}(r_0) \int_0^\infty ds \prod_{n=1}^N \left(\int d^D x_n \right) \\ &\times \prod_{n=1}^{N+1} \int d\mathbf{p}_n \exp\left(i \sum_{n=1}^{N+1} [\mathbf{p}_n \cdot (\mathbf{x}_n - \mathbf{x}_{n-1}) - \epsilon f^{1/2}(r_n)(H_n - E)f^{1/2}(r_{n-1})] \right), \end{aligned} \quad (4b)$$

where $H_n \equiv \frac{1}{2}p_n^2 + V(\mathbf{x}_n)$. We can now integrate out the momenta, thereby obtaining

$$\begin{aligned} G(\mathbf{x}_b, \mathbf{x}_a | E) &\approx \frac{f(r_{N+1})}{(2\pi\epsilon)^{D/2} f^{D/2}(r_0)} \int_0^\infty ds \prod_{n=1}^N \left(\int \frac{d^D \mathbf{x}_n}{(2\pi\epsilon)^{D/2} f^{D/2}(r_n)} \right) \\ &\times \exp\left[-i \sum_{n=1}^{N+1} \left(\frac{(\mathbf{x}_n - \mathbf{x}_{n-1})^2}{2\epsilon f(r_{n-1})} - 2[V(\mathbf{x}_n) - E]f^{1/2}(r_{n-1}) \right) \right], \end{aligned} \quad (5a)$$

$$G(\mathbf{x}_b, \mathbf{x}_a | E) \approx \frac{f^{1/2}(r_{N+1})f^{1/2}(r_0)}{(2\pi\epsilon)^{D/2}f^{D/4}(r_{N+1})f^{D/4}(r_0)} \int_0^\infty ds \prod_{n=1}^N \left(\int \frac{d^D \mathbf{x}_n}{(2\pi\epsilon)^{D/2}f^{D/2}(r_n)} \right) \times \exp \left[-i \sum_{n=1}^{N+1} \left(\frac{(\mathbf{x}_n - \mathbf{x}_{n-1})^2}{2\epsilon f^{1/2}(r_n)f^{1/2}(r_{n-1})} - \epsilon [V(\mathbf{x}_n) - E]f^{1/2}(r_n)f^{1/2}(r_{n-1}) \right) \right]. \tag{5b}$$

In refs. [1,2] eq. (5a) was written directly in the continuum as

$$G(\mathbf{x}_b, \mathbf{x}_a | E) = \int_0^\infty ds \int \frac{\mathcal{D}^D x}{f(r)} \exp \left[i \int_0^s ds' \left(\frac{\dot{x}^2}{2f(r)} - [V(x) - E]f(r) \right) \right], \tag{6}$$

and no attention was paid to the time slicing.

In the case of interest, $V(\mathbf{x})$ is the Coulomb potential, the function $f(r)$ is chosen as $f(r) = r$ and a two-dimensional Kustaanheimo–Stiefel transformation (also called Levi-Civita transformation)

$$x_1 = u_1^2 - u_2^2, \quad x_2 = 2u_1 u_2, \tag{7}$$

(i.e. $x_1 + ix_2 = (u_1 + iu_2)^2$ such that u_1, u_2 may be viewed as “square roots of the coordinates” x_1, x_2) was used to reexpress

$$r = \mathbf{u}^2, \quad \dot{\mathbf{x}}^2 = \mathbf{u}\mathbf{u}^2 \dot{\mathbf{u}}^2, \quad d^2 x/r = d^2 u, \tag{8, 9}$$

such that the path integral (6) became that of a harmonic oscillator in two dimensions with mass $M=4$ and frequency $\omega = \sqrt{-2E/M}$

$$\frac{1}{4} \sum_{\pm} \left[\int_0^\infty ds e^{ie^{2s}} \int_{\substack{\mathbf{u}(0) = \sqrt{\mathbf{x}_a} \\ \mathbf{u}(s) = \pm \sqrt{\mathbf{x}_b}}} \mathcal{D}^2 u \exp \left(i \int_0^s ds' \left(\frac{1}{8} \dot{\mathbf{u}}^2 + E\mathbf{u}^2 \right) \right) \right]. \tag{10}$$

The square roots of $\mathbf{x}_{a,b}$ denote the inverse transformation (7). For each \mathbf{x}_b there are two solutions $\mathbf{u}(s)$ and it was shown that one has to sum over the two solutions $\pm \sqrt{\mathbf{x}_b}$ to include all paths in \mathbf{x} space.

The closed form of this expression is well known and leads to

$$G(\mathbf{x}_b, \mathbf{x}_a | E) = \frac{1}{4} \int_0^\infty ds e^{ie^{2s}} \frac{\omega M}{2\pi i \hbar \sin(\omega s)} \times \left[\exp \left(\frac{i M}{\hbar} \frac{1}{2 \sin(\omega s)} [(\mathbf{u}_b^2 + \mathbf{u}_a^2) \cos(\omega s) - 2\mathbf{u}_b \cdot \mathbf{u}_a] \right) + (\mathbf{u}_b \rightarrow -\mathbf{u}_b) \right],$$

which are the results stated in refs. [1,2].

The main point of ref. [3] (and ref. [4]) was to attempt the direct integration in eq. (5). They correctly observed that if (7) is done at each pseudo-time s_n , then due to the quadratic nature of (7) one has

$$(\mathbf{x}_n - \mathbf{x}_{n-1})^2 = (\mathbf{u}_n - \mathbf{u}_{n-1})^2 (\mathbf{u}_n + \mathbf{u}_{n-1})^2, \tag{11}$$

such that the kinetic terms become

$$\sum_{n=1}^{N+1} \frac{(\mathbf{x}_n - \mathbf{x}_{n-1})^2}{2\epsilon r_{n-1}} = \sum_{n=1}^{N+1} \frac{(\mathbf{u}_n + \mathbf{u}_{n-1})^2}{2\epsilon \mathbf{u}_{n-1}^2} (\mathbf{u}_n - \mathbf{u}_{n-1})^2, \tag{12a}$$

$$\sum_{n=1}^{N+1} \frac{(\mathbf{x}_n - \mathbf{x}_{n-1})^2}{2\epsilon r_n^{1/2} r_{n-1}^{1/2}} = \sum_{n=1}^{N+1} \frac{(\mathbf{u}_n + \mathbf{u}_{n-1})^2}{2\epsilon (\mathbf{u}_n^2 \mathbf{u}_{n-1}^2)^{1/2}} (\mathbf{u}_n - \mathbf{u}_{n-1})^2. \tag{12b}$$

The further steps in ref. [3] (and ref. [4]) however, are mistaken. The measure of integration transforms into

$$\frac{1}{2\pi i \epsilon} \frac{u_{N+1}^2}{u_0^2} \prod_{n=1}^N \int \frac{d^2 u_n 4u_n^2}{2\pi i \epsilon r_n} = \frac{1}{2} \frac{4}{2\pi i \epsilon \times 2} \prod_{n=1}^N \left(\int \frac{d^2 u_n 4}{2\pi i \epsilon \times 2} \right) \prod_{n=1}^{N+1} \frac{u_n^2}{u_{n-1}^2}, \quad (13a)$$

$$\frac{1}{2\pi i \epsilon} \prod_{n=1}^N \int \frac{d^2 u_n 4u_n^2}{2\pi i \epsilon r_n} = \frac{1}{2} \frac{4}{2\pi i \epsilon \times 2} \prod_{n=1}^N \left(\int \frac{d^2 u_n 4}{2\pi i \epsilon \times 2} \right). \quad (13b)$$

The extra factors 1/2 in the integrals of $d^2 u_n$ correct for the fact that if u runs through the two-dimensional space, x does so twice. The jacobian is $\partial(x_{1n}, x_{2n})/\partial(u_{1n}, u_{2n}) = 4u_n^2$, not $(u_n + u_{n-1})^2$ as stated in eq. (18) of ref. [5] (and two lines before eq. (13) of ref. [5]). Moreover, there is no freedom in choosing $\bar{r}_n \equiv \frac{1}{4}[(u_n + u_{n-1})^2]$ instead of r_{n-1} , as claimed in the last sentence of p. 388 of ref. [4] (and before eq. (13) of ref. [5]). Once it is decided which of the formulas (2a)–(2c) should be used, the time sliced form of the factor $f(r)$ is uniquely prescribed to be $f(r_n)$, $f(r_{n-1})$ or $f^{1/2}(r_n)f^{1/2}(r_{n-1})$, respectively. According to eq. (17) in ref. [4] and eq. (5) in ref. [5]) those authors decided to use the form (2b) (their prefactor r_N shows this). Hence, to be consistent, they should have proceeded with the factors r_{n-1} . It was the impermissible “choice” of \bar{r}_n which compensated the mistake in the measure of integration and led to the correct result.

Let us see how to do things properly. The grated form, the path integral in u_n space reads

$$\frac{1}{2} \int_0^\infty ds e^{ie^2 s} \frac{4}{2\pi i \epsilon \times 2} \prod_{n=1}^N \left(\int \frac{d^2 u_n 4}{2\pi i \epsilon \times 2} \right) \prod_{n=1}^{N+1} \left(\frac{u_n^2}{u_{n-1}^2} \right) \times \exp \left[i \sum_{n=1}^{N+1} \left(\frac{(u_n + u_{n-1})^2 (u_n - u_{n-1})^2}{u_{n-1}^2 2\epsilon} + \epsilon E u_{n-1}^2 \right) \right], \quad (14a)$$

$$\int_0^\infty ds e^{ie^2 s} \prod_{n=1}^N \left(\int \frac{d^2 u_n 4}{2\pi i \epsilon \times 2} \right) \exp \left[i \prod_{n=1}^{N+1} \left(\frac{(u_n + u_{n-1})^2 (u_n - u_{n-1})^2}{\sqrt{u_n^2 u_{n-1}^2} 2\epsilon} + \epsilon E \sqrt{u_n^2 u_{n-1}^2} \right) \right]. \quad (14b)$$

It differs from that of the two-dimensional harmonic oscillator in several ways due to the time slicing:

The kinetic term contains *two* very sharp nearly gaussian peaks, one around $u_n = u_{n-1}$ and one around $u_n = -u_{n-1}$. Near the first, we expand the exponent

$$\frac{(u_n + u_{n-1})^2 (u_n - u_{n-1})^2}{u_{n-1}^2 2\epsilon} = 4\Delta u_n^2 \left(1 + \frac{u_{n-1} \cdot \Delta u_n}{u_{n-1}^2} + \frac{\Delta u_n^2}{4u_{n-1}^2} \right),$$

$$\frac{(u_n + u_{n-1})^2 (u_n - u_{n-1})^2}{\sqrt{u_n^2 u_{n-1}^2} 2\epsilon} = 4\Delta u_n^2 \left(1 - \frac{1}{4} \frac{\Delta u_n^2}{u_{n-1}^2} + \frac{1}{2} \frac{(u_{n-1} \cdot \Delta u_n)^2}{(u_{n-1}^2)^2} - \dots \right), \quad (15)$$

where

$$\Delta u_n \equiv u_n - u_{n-1}. \quad (16)$$

Near the second, we expand in the same way except that

$$\Delta u_n = -u_n - u_{n-1}. \quad (17)$$

The product in the measure (13a) is expanded accordingly, near each peak, as

$$\frac{u_n^2}{u_{n-1}^2} = 1 + 2 \frac{u_{n-1} \cdot \Delta u_n}{u_{n-1}^2} + \frac{\Delta u_n^2}{u_{n-1}^2}. \quad (18)$$

So, the product of all $\mathbf{u}_n^2/\mathbf{u}_{n-1}^2$ ratios in (14a) can be written as

$$\exp\left(\sum_{n=1}^{N+1} \log(\mathbf{u}_n^2/\mathbf{u}_{n-1}^2)\right) = \exp\left[\sum_{n=1}^{N+1} \left(2 \frac{\mathbf{u}_{n-1} \cdot \Delta \mathbf{u}_n}{\mathbf{u}_{n-1}^2} + \frac{\Delta \mathbf{u}_n^2}{\mathbf{u}_{n-1}^2} - 2 \frac{(\mathbf{u}_{n-1} \cdot \Delta \mathbf{u}_n)^2}{(\mathbf{u}_{n-1}^2)^2} + \dots\right)\right]. \tag{19}$$

We now integrate out successively $d^2u_1, d^2u_2, \dots, d^2u_N$ or $d^2\Delta u_1, d^2\Delta u_2, \dots, d^2\Delta u_N$, each integral over $d^2\Delta u_n$ being performed at fixed \mathbf{u}_{n-1} . The harmonic part of the energy gives the product of symmetrized harmonic oscillator amplitudes of mass 4, for infinitesimal pseudo-times ϵ ,

$$\frac{1}{2} \int_0^\infty ds e^{ie^2s} \prod_{n=1}^N \left(\int d^2u_n\right) \prod_{n=1}^{N+1} \frac{1}{2} [\langle \mathbf{u}_n \epsilon | \mathbf{u}_{n-1} 0 \rangle + \langle -\mathbf{u}_n \epsilon | \mathbf{u}_{n-1} 0 \rangle]. \tag{20}$$

If there were no further point splitting terms, this product would result in the total symmetrized amplitude

$$\frac{1}{2} \int_0^\infty ds e^{ie^2s} \frac{1}{2} (\langle \mathbf{u}_b s_b | \mathbf{u}_a 0 \rangle + \langle -\mathbf{u}_b s_b | \mathbf{u}_a 0 \rangle), \tag{21}$$

which is the desired final result (recall eqs. (23)–(26) in ref. [7]).

What remains to do is to convince ourselves that the additional

$$\exp\left\{\sum_{n=1}^{N+1} \left[\frac{2\mathbf{u}_{n-1} \cdot \Delta \mathbf{u}_n}{\mathbf{u}_{n-1}^2} + \frac{\Delta \mathbf{u}_n^2}{\mathbf{u}_{n-1}^2} - 2 \frac{(\mathbf{u}_{n-1} \cdot \Delta \mathbf{u}_n)^2}{(\mathbf{u}_{n-1}^2)^2} + i \frac{\Delta \mathbf{u}_n^2}{2\epsilon} 4 \left(\frac{\mathbf{u}_{n-1} \cdot \Delta \mathbf{u}_n}{\mathbf{u}_{n-1}^2} + \frac{1}{4} \frac{\Delta \mathbf{u}_n^2}{\mathbf{u}_{n-1}^2}\right)\right]\right\}, \tag{22a}$$

$$\exp\left\{\prod_{n=1}^{N+1} \left[i \frac{\Delta \mathbf{u}_n^2}{2\epsilon} 4 \left(-\frac{1}{4} \frac{\Delta \mathbf{u}_n^2}{\mathbf{u}_{n-1}^2} + \frac{1}{2} \frac{(\mathbf{u}_{n-1} \cdot \Delta \mathbf{u}_n)^2}{(\mathbf{u}_{n-1}^2)^2} + \dots\right)\right]\right\}, \tag{22b}$$

do not produce any further contributions. The principal danger is that of additional centrifugal barrier type of terms of the form $\sum_{n=1}^{N+1} \epsilon/\mathbf{u}_{n-1}^2 \rightarrow \int_0^\infty ds'/\mathbf{u}^2(s')$. In order to see that these are absent we use the fact that $\Delta \mathbf{u}_n^2$ is small of order ϵ such that we can proceed perturbatively. The correlation functions of $\Delta \mathbf{u}_n$ at fixed \mathbf{u}_{n-1} are

$$\langle \Delta u_n^i \Delta u_n^j \rangle = \frac{1}{4} i \epsilon \delta_{nn'} \delta^{ij}. \tag{23}$$

To lowest order in perturbation theory, the first and fourth terms in (22a) disappear, since they are odd in $\Delta \mathbf{u}_n$. The other terms give

$$i \left(\frac{1}{2\mathbf{u}_{n-1}^2} - \frac{1}{2\mathbf{u}_{n-1}^2} - \frac{1}{4\mathbf{u}_{n-1}^2}\right) \epsilon = -\frac{i\epsilon}{4\mathbf{u}_{n-1}^2}, \quad i \left(\frac{1}{4\mathbf{u}_{n-1}^2} - \frac{1}{4\mathbf{u}_{n-1}^2}\right) \epsilon = 0. \tag{24a, b}$$

To second order in perturbation theory we have to add to (24a) the expectation

$$\left\langle \frac{1}{2!} \left[\sum_{n=1}^{N+1} 2 \frac{\mathbf{u}_{n-1} \cdot \Delta \mathbf{u}_n}{\mathbf{u}_{n-1}^2} + i \frac{\Delta \mathbf{u}_n^2}{2\epsilon} 4 \frac{\mathbf{u}_{n-1} \cdot \Delta \mathbf{u}_n}{\mathbf{u}_{n-1}^2} \right]^2 \right\rangle, \tag{25}$$

which gives an additional $i\epsilon/4\mathbf{u}_{n-1}^2$ thereby cancelling (24a). Hence there are no centrifugal barrier types of terms.

To complete the argument we have to show that when doing an intermediate integral over d^2u_n at fixed \mathbf{u}_{n-1}

$$A(\mathbf{u}_n) \int d^2u_n \exp(-4\Delta \mathbf{u}_n^2/2\epsilon) (1 + \dots) B(\mathbf{u}_{n-1}), \tag{26}$$

where $A(\mathbf{u}_n)$ is the product of integrals *after* \mathbf{u}_n , $B(\mathbf{u}_{n-1})$ collects those before \mathbf{u}_n , and the dots stand for the expansion terms of (22a, b), that these terms do not produce any first derivative terms of $A(\mathbf{u}_{n-1})$, $(\partial/\partial \mathbf{u}_{n-1})A(\mathbf{u}_{n-1})\epsilon$, and that the second derivative term has the usual Schrödinger form $(\epsilon/2M)(\partial^2/\partial \mathbf{u}_{n-1}^2)A(\mathbf{u}_{n-1})$ (with $M=4$ in the present case). Thus we expand

$$A(\mathbf{u}_n) = A(\mathbf{u}_{n-1}) + \partial_i A(\mathbf{u}_{n-1}) \Delta u_n^i + \frac{1}{2} \partial_i \partial_j A(\mathbf{u}_{n-1}) \Delta u_n^i \Delta u_n^j + \dots, \quad (27)$$

and form the averages. It is obvious that the second derivative terms are not modified by the dotted terms in (27) since these would be of order ϵ^2 . As far as the first derivative terms are concerned we calculate in the case (22a)

$$\partial_i A(\mathbf{u}_{n-1}) \left\langle \Delta u_n^i \left(2 \frac{\mathbf{u}_{n-1} \cdot \Delta \mathbf{u}_n}{u_{n-1}^2} + i \frac{\Delta u_n^2}{2\epsilon} 4 \frac{\mathbf{u}_{n-1} \cdot \Delta \mathbf{u}_n}{u_{n-1}^2} \right) \right\rangle,$$

and see that the two contributions cancel each other, as they should. In the case (22b) there are no such terms at all.

Thus we have proved that the non-trivial factors appearing when doing the Duru–Kleinert transformation in the time sliced form all cancel each other and the path integral of the H atom reduces to the product of purely gaussian factors whose result is the symmetrized amplitude of the two-dimensional harmonic oscillator.

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