SOLUTION OF THE PATH INTEGRAL FOR THE H-ATOM

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The Green's function of the H-atom is calculated by a simple reduction of Feynman's path integral to gaussian form.

With increasing interest in path integral techniques both in field theory and many-body physics [1] it is worthwhile to study their application to the solution of standard non-trivial quantum-mechanical problems. Hopefully, this may help discovering new treatments of non-gaussian integrals.

In this note we present the execution of the path integral for the physically most important quantum-mechanical problem: the H-atom.

Feynman's [2] formula for the Green's function reads

$$K(\boldsymbol{x}_b, t_b; \boldsymbol{x}_a, t_a) = \int_{\boldsymbol{x}_a, t_a}^{\boldsymbol{x}_b, t_b} \mathcal{D}^3x \, \frac{\mathcal{D}^3 p}{[2\pi]^3} \exp\left\{ \mathrm{i} \int_{t_a}^{t_b} \mathrm{d}t (\boldsymbol{p}\cdot\dot{\boldsymbol{x}} - \boldsymbol{p}^2/2m + e^2/r)\right\}, \tag{1}$$

and is not readily integrable due to the $1/r$ potential. If we parametrize the paths in terms of a new auxiliary "time"

$$s(t) = \int^t \mathrm{d}\tau \, \frac{1}{r(\tau)}, \tag{2}$$

we arrive at ($' \equiv \mathrm{d}/\mathrm{d}s$)

$$K(\boldsymbol{x}_b, t_b; \boldsymbol{x}_a, t_a) = \int \mathcal{D}^3x \, \frac{\mathcal{D}^3 p}{[2\pi]^3} \exp\left[\mathrm{i} \int_{s(t_a)}^{s(t_b)} \mathrm{d}s \{\boldsymbol{p}(s)\cdot\boldsymbol{x}'(s) - r(s)\boldsymbol{p}^2(s)/2m + e^2\}\right]. \tag{3}$$

On the right-hand side s_b, s_a may be used as independent variables if the connection (2) is enforced via a δ-function as:

$$K(\boldsymbol{x}_b, t_b; \boldsymbol{x}_a, t_a) \equiv \int_{s_a}^{\infty} \mathrm{d}s_b \, \delta\left(t_b - t_a - \int_{s_a}^{s_b} \mathrm{d}s \, r(s)\right) \exp\{\mathrm{i}e^2(s_b - s_a)\}$$

$$\times\, r_b \int \mathcal{D}^3x \, \frac{\mathcal{D}^3 p}{[2\pi]^3} \exp\left\{ \mathrm{i} \int_{s_a}^{s_b} \mathrm{d}s (\boldsymbol{p}\cdot\boldsymbol{x}' - r\boldsymbol{p}^2/2m)\right\} \tag{4}$$

$$\equiv \int \frac{\mathrm{d}E}{2\pi} \exp\{-\mathrm{i}E(t_b - t_a)\} K(\boldsymbol{x}_b, \boldsymbol{x}_a; E) \tag{5}$$

$$= \int \frac{\mathrm{d}E}{2\pi} \exp\{-\mathrm{i}E(t_b - t_a)\} \int_{s_a}^{\infty} \mathrm{d}s_b \exp\{\mathrm{i}e^2(s_b - s_a)\}\, r_b \int \mathcal{D}^3x \, \frac{\mathcal{D}^3 p}{[2\pi]^3} \exp\left\{ \mathrm{i} \int_{s_a}^{s_b} \mathrm{d}s \left(\boldsymbol{p}\cdot\boldsymbol{x}' - \frac{r\boldsymbol{p}^2}{2m} + Er\right)\right\}. \tag{6}$$

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The last part of the equation arises, of course, from a Fourier decomposition of the δ-function. The expression may be multiplied, without changing it, by a dummy path integral involving a new, completely arbitrary pair of canonical coordinates x_4, p_4:

$$\int_{-\infty}^{\infty} \mathrm{d}(x_4)_b \left\{ \int_{(x_4)_a, s_a}^{(x_4)_b, s_b} \mathcal{D}x_4 \, \frac{\mathcal{D}p_4}{[2\pi]} \exp\left[\mathrm{i} \int_{s_a}^{s_b} \mathrm{d}s (p_4 x_4' - r(s) p_4^2/2m) \right] \right.$$

$$= \int \mathrm{d}p_4 \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}(x_4)_b \exp\{\mathrm{i}\,[(x_4)_b - (x_4)_a] p_4\} \exp\left\{ \frac{p_4}{2m} \int_{s_a}^{s_b} \mathrm{d}s\, r(s) \right\} = 1 \,. \tag{7}$$

Notice that this identity holds for any function $r(s)$, in particular for $r(s) \equiv (\boldsymbol{x}^2(s))^{1/2}$. This choice brings the path integral in eq. (6) to the four-dimensional form

$$\int_{-\infty}^{\infty} \mathrm{d}(x_4)_b \int \mathcal{D}^4 x \, \frac{\mathcal{D}^4 p}{[2\pi]^4} \exp\left\{ \mathrm{i} \int_{s_a}^{s_b} \mathrm{d}s (p \cdot x' - r p^2/2m + E r) \right\} . \tag{8}$$

We now introduce a canonical change of variables[‡1] from (x, p) to (u, p_u) such that $r = u^2$

$$x_a = \sum_{b=1}^{4} A_{ab}(u) u_b \quad (a = 1, 2, 3), \quad dx_4 = 2 \sum_{b=1}^{4} A_{4b}(u)\, \mathrm{d}u_b, \quad p_a = \frac{1}{2r} \sum_{b=1}^{4} A_{ab}(u) (p_u)_b \quad (a = 1, 2, 3, 4), \tag{9}$$

with a matrix

$$A(u) = \begin{pmatrix} u_3 & u_4 & u_1 & u_2 \\ -u_2 & -u_1 & u_4 & u_3 \\ -u_1 & u_2 & u_3 & -u_4 \\ u_4 & -u_3 & u_2 & -u_1 \end{pmatrix} . \tag{10}$$

Then the expression (8) becomes

$$\frac{1}{16 r_b} \int_{-\infty}^{\infty} \frac{\mathrm{d}(x_4)_b}{r_b} \int_{x_a, (x_4)_a}^{x_b, (x_4)_b} \mathcal{D}^4 u \, \frac{\mathcal{D}^4 p_u}{[2\pi]^4} \exp\left\{ \mathrm{i} \int_{s_a}^{s_b} \mathrm{d}s (p_u \cdot u' - p_u^2/2\mu - \tfrac{1}{2}\mu\omega^2 u^2) \right\} , \tag{11}$$

where $\mu = 4m$ and $\omega^2 = -E/2m$. Apart from the integral over $\mathrm{d}(x_4)_b / r_b$, this is the Green's function of a harmonic oscillator in four dimensions. In order to do this integral we express u in terms of

$$\boldsymbol{x} = r \begin{pmatrix} \sin\theta \cos\varphi \\ \sin\theta \sin\varphi \\ \cos\theta \end{pmatrix} , \tag{12}$$

and an auxiliary angle α in the form

$$u = \sqrt{r} \begin{pmatrix} \sin\frac{1}{2}\theta \cos\frac{1}{2}(\alpha + \varphi) \\ \sin\frac{1}{2}\theta \sin\frac{1}{2}(\alpha + \varphi) \\ \cos\frac{1}{2}\theta \cos\frac{1}{2}(\alpha - \varphi) \\ \cos\frac{1}{2}\theta \sin\frac{1}{2}(\alpha - \varphi) \end{pmatrix} . \tag{13}$$

‡1 Applied a long time ago in astronomy [3].

Then $\int_{-\infty}^{\infty} \mathrm{d}(x_4)_b/r_b$ can be rewritten as

$$\int_{-\infty}^{\infty} \frac{\mathrm{d}(x_4)_b}{r_b} = \int_0^{4\pi} \mathrm{d}\alpha_b \sum_{\alpha_b \to \alpha_b + 4\pi n} , \quad n = \pm 1, \pm 2, \pm 3, \ldots, \tag{14}$$

thereby decomposing it into a sum over periodically shifted end point values of the angle α_b and an integral over one period. Since the paths going to a certain final u_b can arrive at any $\alpha_b + 4\pi n$, the sum is part of the Green's function of the harmonic oscillator (as always if cyclic variables are used [1]). Thus (11) can be rewritten as

$$\frac{1}{16 r_b} \int_0^{4\pi} \mathrm{d}\alpha_b \, F^4(s_b - s_a) \exp\{-\pi F^2(s_b - s_a)[(r_a + r_b)\cos\omega(s_b - s_a) - 2u_a \cdot u_b]\}, \tag{15}$$

where $F(s_b - s_a)$ is the usual fluctuation factor of the one-dimensional oscillator

$$F(s_b - s_a) = [\mu\omega/2\pi \mathrm{i} \sin\omega(s_b - s_a)]^{1/2} . \tag{16}$$

Performing the integral over $\mathrm{d}\alpha_b$ one obtains

$$(\pi/4r_b) F^4(s_b - s_a) I_0(2\pi F^2(s_b - s_a)\, 2^{-1/2}(r_a r_b + \boldsymbol{x}_a \cdot \boldsymbol{x}_b)^{1/2}) \exp\{-\pi F^2(s_b - s_a)(r_a + r_b)\cos\omega(s_b - s_a)\}, \tag{17}$$

which may be inserted into eq. (6) to yield the closed expression for the H-atom Green's function:

$$K(\boldsymbol{x}_b, \boldsymbol{x}_a; E) = -\mathrm{i}\frac{m p_0}{\pi} \int_0^1 \mathrm{d}\rho \frac{\bar{\rho}^{\nu}}{(1-\rho)^2} I_0\left(2p_0 \frac{(2\rho)^{1/2}}{1-\rho}(r_a r_b + \boldsymbol{x}_a \cdot \boldsymbol{x}_b)^{1/2}\right) \exp\left\{-p_0 \frac{1+\rho}{1-\rho}(r_a + r_b)\right\}. \tag{18}$$

Here we have deformed the contour into the complex plane by setting $s = -\mathrm{i}\tilde{s}$ with $\tilde{s}$ real and substituted $\rho = \exp\{-2\omega(\tilde{s}_b - \tilde{s}_a)\}$. The variables ν and p_0 stand short for $\nu \equiv e^2/2\omega = (-me^4/2E)^{1/2}$ and $p_0 = (-2mE)^{1/2}$.

The representation is, of course, the Fourier transform of Schwinger's [4] formula and has the same region of convergence ν.

As far as wave functions are concerned, we may symmetrize the integrand of (15) in u_b (since $\alpha_b \to \alpha_b + 2\pi$ corresponds to $u_b \to -u_b$) and expand, for $E < 0$ as

$$\sum_{n_i=0}^{\infty} \exp\left\{-\mathrm{i}\omega\left(\sum_{i=1}^{4} n_i + 2\right)(s_b - s_a)\right\} \psi_{n_1 n_2 n_3 n_4}(u_b)\psi^*_{n_1 n_2 n_3 n_4}(u_a), \tag{19}$$

where $\Sigma_{i=1}^4 n_i = 2(n-1) = 0, 2, 4, \ldots$ and $\psi_{n_1 n_2 n_3 n_4}(u)$ denotes the product of four usual oscillator wave functions. Inserting this into (4) gives

$$K(\boldsymbol{x}_b, \boldsymbol{x}_a; E) = -\frac{m}{p_0^2} \sum_{n=0}^{\infty} \frac{\mathrm{i}}{1 - \nu/n} \int_0^{2\pi} \mathrm{d}\alpha_b \left(\sqrt{\frac{p_0}{8n}}\, \psi_{n_1 n_2 n_3 n_4}(u_b)\right)\left(\sqrt{\frac{p_0}{8n}}\, \psi^*_{n_1 n_2 n_3 n_4}(u_a)\right). \tag{20}$$

The sum displays explicitly the bound state poles at

$$E_n = -me^4/2n^2, \quad n = 1, 2, 3, \ldots, \tag{21}$$

with the residues being the wave functions in unconventional quantum numbers. For $E > 0$ the eq. (20) requires analytical continuation via Sommerfeld–Watson transformation. This provides for the continuum wave functions. The details of this will be discussed elsewhere.

For previous attempts to calculate the Coulomb path integral see refs. [5,6].

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