EXACT PATH INTEGRAL TREATMENT OF THE HYDROGEN ATOM

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Applying a space–time transformation discussed in a previous paper, the Feynman path integral for the Coulomb potential is calculated exactly by reducing it to gaussian form. The resulting Green function leads to a simple derivation of the energy spectrum and the complete (normalized) wavefunctions of the hydrogen atom.

In a previous paper [1] I derived a transformation formula for a class of non-linear space–time transformations in the radial path integral. The formula makes it possible to transform non-gaussian path integrals into gaussian ones. As a very simple illustration and consistency check we computed in ref. [1] the Feynman kernel of a free particle and (in imaginary time) the distribution function of a particle undergoing brownian motion (Bessel process).

In this note we shall apply the transformation formula to the Coulomb potential. To our knowledge, the following treatment represents the simplest path integral determination of the energy spectrum and the complete (normalized) wavefunctions of the hydrogen atom.

Earlier attempts to treat the Coulomb potential by means of path integrals can be found in the papers listed in ref. [2]. The first complete path integral treatment of the hydrogen atom was carried out by Kleinert and Duru [3] (see also ref. [4]).

In ref. [1] we considered three-dimensional quantum systems described by the hamiltonian $H = p^2/2 + V$ with spherically symmetric potentials $V = V(r)$ ($\hbar = m = 1$). In spherical coordinates the Feynman kernel K can be expanded into "partial waves" (see ref. [1], eq. (1)), where the radial kernel K_l (with fixed angular momentum l) is given by the radial path integral

$$K_l(T; r_b, r_a | V) = \int_{r(0)=r_a}^{r(T)=r_b} Dr(t) \exp\left(i \int_0^T dt \left[\tfrac{1}{2} \dot{r}^2 - l(l+1)/2r^2 - V(r) \right] \right). \tag{1}$$

K_l determines for a given angular momentum l the time evolution of the system from time t_a to the later time t_b ($T = t_b - t_a$) for fixed radii $r_a = |x(t_a)|$, $r_b = |x(t_b)|$. For the class of space–time transformations $t \to \tau$, $r(t) \to R(\tau)$ specified by

$$d\tau = \tfrac{1}{4}(2 - \nu)^2 r^{-\nu} dt, \quad R = r^{1-\nu/2}, \quad \nu < 2, \tag{2}$$

we derived in ref. [1] the transformation formula

$$k_l(E; r_b, r_a | V) = \frac{2i}{2 - \nu}(r_b r_a)^{\nu/4} \int_0^\infty d\tau\, K_{L_\nu}(\tau; r_b^{1-\nu/2}, r_a^{1-\nu/2} | W_\nu). \tag{3}$$

Here k_l denotes the time-independent radial kernel defined by

$$k_l(E; r_b, r_a | V) = i \int_0^\infty dT\, e^{iET}\, K_l(T; r_b, r_a | V) .\tag{4}$$

Eq. (3) connects the time-independent radial kernel k_l of the original quantum system with potential V to the radial kernel K_{L_ν} of a new quantum system with the new potential

$$W_\nu(R) = [4/(2 - \nu)^2] R^{2\nu/(2-\nu)} [V(R^{2/(2-\nu)}) - E] ,\tag{5}$$

and effective angular momentum

$$L_\nu = (4l + \nu)/2(2 - \nu) .\tag{6}$$

(The kernel K_{L_ν} in (3) is again defined by the corresponding path integral representation (1).)

If we put $\nu = 1$, $V(r) = -e^2/r$, we obtain from (3) the following relation for the kernel k_l^H of the H-atom

$$k_l^H(E; r_b, r_a) = 2i(r_b r_a)^{1/4} \int_0^\infty d\tau\, K_{2l+1/2}(\tau; \sqrt{r_b}, \sqrt{r_a} | W_1) .\tag{7}$$

Eq. (5) gives for the new potential

$$W_1(R) = -4e^2 - 4ER^2 \equiv -4e^2 + \tfrac{1}{2}\Omega^2 R^2 ,\tag{8}$$

which leads to a complete factorization of the dependence on the coupling constant e^2

$$K_{2l+1/2}(\tau; \sqrt{r_b}, \sqrt{r_a} | W_1) = \exp(i4e^2\tau) K_{2l+1/2}^{osc}(\tau; \sqrt{r_b}, \sqrt{r_a}) .\tag{9}$$

Here K^{osc} is the kernel of a harmonic oscillator with frequency $\Omega = 2\sqrt{-2E}$. Inserting (9) in (7) we obtain

$$k_l^H(E; r_b, r_a) = 2i(r_b r_a)^{1/4} \int_0^\infty d\tau\, \exp(i4e^2\tau) K_{2l+1/2}^{osc}(\tau; \sqrt{r_b}, \sqrt{r_a}) ,\tag{10a}$$

or

$$k_l^H(E; r_b, r_a) = 2(r_b r_a)^{1/4} k_{2l+1/2}^{osc}(4e^2; \sqrt{r_b}, \sqrt{r_a}) .\tag{10b}$$

Since the path integration for the harmonic oscillator can be carried out, eqs. (10) represent the complete path integral solution of the hydrogen atom. It only remains to extract the energy spectrum and the wavefunctions from (10). There are several ways to achieve this.

Inserting the path integral result for the kernel K_l^{osc} (see ref. [1], eq. (27)) in (10a) we arrive at the following integral representation for the kernel of the hydrogen atom

$$k_l^H(E; r_b, r_a) = 2i(-1)^{l+1} \sqrt{r_b r_a} \int_0^\infty \frac{dx}{\sinh x} \exp[2i\mu x + ik(r_b + r_a) \coth x]\, J_{2l+1}(2k\sqrt{r_b r_a}/\sinh x) ,\tag{11}$$

with $k = \sqrt{2E}$, $\mu = e^2/k$ (J_{2l+1} is the Bessel function). In order to determine the energy values and the wavefunctions, we make the variable transformation $y = e^{-2x}$ in (11)

$$k_l^H(E; r_b, r_a) = 2\sqrt{r_b r_a} \int_0^1 dy\, y^{l-i\mu} Q_{2l+1}(A, B; y) .\tag{12}$$

Here we have introduced the function

$$Q_\lambda(A, B; y) = \frac{y^{-\lambda/2}}{1-y} \exp\left(-\frac{A+B}{2} \frac{1+y}{1-y}\right) I_\lambda\left(\frac{2\sqrt{ABy}}{1-y}\right), \quad A = -2ikr_a, \quad B = -2ikr_b. \tag{13}$$

$(I_\lambda$ is the modified Bessel function). Q_λ can be expanded in a power series in y (ref. [5], p. 1038; for a proof see ref. [6])[+1]

$$Q_\lambda(A, B; y) = \sum_{n_r = 0}^{\infty} y^{n_r} \frac{n_r!}{\Gamma(n_r + \lambda + 1)} (AB)^{\lambda/2} e^{-(A+B)/2} L_{n_r}^\lambda(A) L_{n_r}^\lambda(B), \tag{14}$$

where $L_{n_r}^\lambda$ denote the Laguerre polynomials defined by

$$L_{n_r}^\lambda(x) = \binom{n_r + \lambda}{n_r} F(-n_r, 1 + \lambda; x), \tag{15}$$

$(F(a, b; x)$ is the confluent hypergeometric function). With (14) the y-integration in (12) generates poles in the energy plane (the dots indicate a contribution which is regular for $E < 0$)

$$\int_0^1 dy\, y^{l - i\mu + n_r} = \frac{1}{(n_r + l + 1) - i\mu} = \frac{e^4(n_r + l + 1)^{-3}}{[-e^4/2(n_r + l + 1)^2] - E} + \dots, \tag{16}$$

which by means of eq. (23b) of ref. [1] determine the discrete energy spectrum of the hydrogen atom

$$E_{ln_r}^H = -e^4/2(n_r + l + 1)^2 = -e^4/2n^2. \tag{17}$$

Obviously, n is the principal quantum number (defined by $n = n_r + l + 1$), and n_r has the meaning of the radial quantum number.

With (14), (16) and (17) we obtain for (12)

$$k_l^H(E; r_b, r_a) = \sum_{n_r = 0}^{\infty} \frac{e^2}{(n_r + l + 1)^2} \frac{n_r!}{(n_r + 2l + 1)!} \frac{(AB)^{l+1} e^{-(A+B)/2} L_{n_r}^{2l+1}(A) L_{n_r}^{2l+1}(B)}{E_{ln_r}^H - E} + \dots. \tag{18}$$

It is now a simple matter to determine the residues of the energy poles and to obtain thereby the reduced (normalized) radial wavefunctions (see ref. [1], eq. (23b)) of the hydrogen atom

$$\chi_{ln}^H(r) = (e/n)[(n - l - 1)!/(n + l)!]^{1/2} \rho^{l+1} e^{-\rho/2} L_{n-l-1}^{2l+1}(\rho), \tag{19}$$

expressed in terms of the principal quantum number n and the angular momentum l ($l = 0, 1, \dots, n - 1, \rho = 2e^2 r/n$). This completes our path integral treatment of the hydrogen atom.

Another way to solve the problem [which avoids the integrations involved in (10a), (11) and (12)] starts with relation (10b) and replaces both kernels by their respective spectral decompositions

$$\sum_{n_r = 0}^{\infty} \frac{\chi_{ln_r}^H(r_b) \chi_{ln_r}^H(r_a)}{E_{ln_r}^H - E} + k_l^H(E; r_b, r_a)_{cont} = 2(r_b r_a)^{1/4} \sum_{n_r = 0}^{\infty} \frac{\chi_{2l+1/2\, n_r}^{osc}(\sqrt{r_b}) \chi_{2l+1/2\, n_r}^{osc}(\sqrt{r_b})}{E_{2l+1/2\, n_r}^{osc} - 4e^2}, \tag{20}$$

("cont" denotes the contribution from the continuous spectrum, $E > 0$). From the well-known eigenvalues of the three-dimensional harmonic oscillator (which can be determined from eq. (27) of ref. [1] by using again the series (14)), $E_{ln_r}^{osc} = \Omega(2n_r + l + 3/2)$, one obtains ($\Omega = 2\sqrt{-2E}$)

$$E_{2l+1/2\, n_r}^{osc} = 4\sqrt{-2E}(n_r + l + 1) = 4\sqrt{-2E}\, n, \tag{21}$$

[+1] The series (14) is absolutely convergent for arbitrary real or complex values of A and B as long as $|y| < 1$.

and

$$\frac{1}{E^{osc}_{2l+1/2\,n_r} - 4e^2} = \frac{(e^2 + \sqrt{-2En})/8n^2}{[-e^4/2n^2] - E} . \tag{22}$$

A comparison of the poles in the energy plane on both sides of eq. (20) leads for $E < 0$ immediately to the H-atom spectrum (17). It is amusing to see how the hydrogen spectrum is generated by the completely different oscillator spectrum via eq. (22)! Comparing the residues of the poles on both sides of (20) one is led to the wavefunctions of the hydrogen atom expressed in terms of the well-known wavefunctions of the harmonic oscillator. The result agrees, of course, with eq. (19).

If one is only interested in the determination of the energy spectrum, there is still another way. One simply notices that the integral (11) can be carried out [2] with the result $(r_b \geqslant r_a)$

$$k_l^H(E; r_b, r_a) = ik^{-1} [\Gamma(l + 1 - i\mu)/(2l + 1)!] W_{i\mu, l+1/2}(B) M_{i\mu, l+1/2}(A) , \tag{23}$$

where W and M are the Whittaker functions as defined in ref. [5], p. 1059. The gamma function in (23) has simple poles at $l + 1 - i\mu = -n_r$, $n_r = 0, 1, 2, ...,$ which yield again the hydrogen spectrum (17).

Inserting the integral representation (11) in the partial wave expansion $(\cos \theta = x_b \cdot x_a / r_b r_a)$

$$k^H(E; x_b, x_a) = \sum_{l=0}^{\infty} \frac{2l + 1}{4\pi r_b r_a} k_l^H(E; r_b, r_a) P_l(\cos \theta) , \tag{24}$$

and using

$$\sum_{l=0}^{\infty} (2l + 1)(-1)^l J_{2l+1}(x) P_l(\cos \theta) = \tfrac{1}{2} x J_0(x \cos(\theta/2)) , \tag{25}$$

we obtain the following integral representation for the time-independent Feynman kernel of the hydrogen atom

$$k^H(E; x_b, x_a) = \frac{k}{2\pi i} \int_0^{\infty} \frac{dx}{\sinh^2 x} \exp[2i\mu x + ik(r_b + r_a) \coth x] J_0\left(\frac{2k\sqrt{r_b r_a} \cos(\theta/2)}{\sinh x}\right) . \tag{26}$$

Relations (26) and (23) have been first derived by Hostler [7], and (in momentum space) by Schwinger [8].

We conclude with the remark that the results of this note can be extended to the more general potential $(g, e^2$ and V_0 are real constants)

$$\bar{V}(r) = g/r^2 - e^2/r + V_0 , \tag{27}$$

which (for $\nu = 1$) leads according to (5) to the new potential $(\bar{\Omega} = 2\sqrt{2(V_0 - E)})$

$$\bar{W}_1(R) = 4g/R^2 - 4e^2 + \tfrac{1}{2} \bar{\Omega}^2 R^2 . \tag{28}$$

The kernel $\bar{k}_l$ (belonging to the potential $\bar{V}$) satisfies again relation (7), but with $K_{2l+1/2}$ replaced by

$$K_{2l+1/2}(\tau; \sqrt{r_b}, \sqrt{r_a} | \bar{W}_1) = \exp(i4e^2\tau) K_{\bar{l}}^{\overline{osc}}(\tau; \sqrt{r_b}, \sqrt{r_a}) . \tag{29}$$

Here $\bar{l}$ is defined by $\bar{l}(\bar{l} + 1) = (2l + 1/2)(2l + 3/2) + 8g$ and $\overline{osc}$ refers to a harmonic oscillator with frequency $\bar{\Omega}$. We thus obtain (in analogy to (10b)) the relation

$$\bar{k}_l(E; r_b, r_a) = 2(r_b r_a)^{1/4} k_{\bar{l}}^{\overline{osc}}(4e^2; \sqrt{r_b}, \sqrt{r_a}) . \tag{30}$$

Looking for the energy poles and their residues in (30), we get for the discrete spectrum of the potential (27)

[2] The calculation proceeds as in ref. [1], eq. (28), where we already performed the integration for the special case $\mu = 0$.

$(\kappa = [(l + 1/2)^2 + 2g]^{1/2}, g > -1/8)$

$$\bar{E}_{ln_r} = V_0 - e^4/2[n_r + 1/2 + \kappa]^2 , \tag{31}$$

and for the reduced radial wavefunctions $(\rho = 2e^2r/(n_r + 1/2 + \kappa))$

$$\bar{\chi}_{ln_r}(r) = N_{ln_r}\rho^{\kappa+1/2}e^{-\rho/2}F(-n_r, 1 + 2\kappa;\rho) , \quad N_{ln_r} = \frac{e}{n_r + 1/2 + \kappa}\frac{1}{\Gamma(1 + 2\kappa)}[\Gamma(n_r + 1 + 2\kappa)/n_r!]^{1/2} . \tag{32}$$

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