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On the spectrum of the hydrogen atom from the four-dimensional harmonic oscillator problem†

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Abstract. A direct derivation is given of the classic hydrogen atom spectrum (including the degeneracy of the levels) from the four-dimensional harmonic oscillator problem by performing a generalised trace operation to the latter where the initial states are related to the final states by a phase transformation.

1. Introduction

The purpose of this work is to derive the classic hydrogen-atom spectrum (including the degeneracy of the levels) directly from the four-dimensional (Duru and Kleinert 1982, Kustaanheimo and Steifel 1965) harmonic oscillator problem without solving the eigenvalue problem of the Schrödinger equation (or of the Green function) or without working out its equivalent functional path integral (Feynman and Hibbs 1965). Duru and Kleinert (1982) have recently reconsidered this problem from the path integral formulation in an intriguing but, unfortunately, quite complicated paper. Our approach is the following. First we relate (§ 2) the Green function of the hydrogen atom to the Green function of the four-dimensional harmonic oscillator by using, in the process, the four-dimensional variables introduced by Kustaanheimo and Steifel (1965) and Duru and Kleinert (1982). Finally we work out a generalised trace operation (§ 3) for the four-dimensional harmonic oscillator, where the final states are related to the initial states by a phase transformation. Using this expression in the Green function of § 2, we obtain in § 4 the energy levels and the degree of degeneracy of the hydrogen atom. The simplicity of this approach is that we do not have to solve for the Green function of the hydrogen-atom problem and we do not need any information on the eigenfunctions or their relations to the eigenfunctions of the harmonic oscillator.

2. Relation of the Green function to the harmonic oscillator one

We consider the four variables (Duru and Kleinert 1982, Kustaanheimo and Steifel 1965)

$$\begin{aligned} u_1 &= \sqrt{r}\sin(\tfrac{1}{2}\theta)\cos[\tfrac{1}{2}(\alpha+\varphi)] \qquad & u_2 &= \sqrt{r}\cos(\tfrac{1}{2}\theta)\sin[\tfrac{1}{2}(\alpha-\varphi)] \\ u_3 &= \sqrt{r}\cos(\tfrac{1}{2}\theta)\cos[\tfrac{1}{2}(\alpha-\varphi)] \qquad & u_4 &= \sqrt{r}\sin(\tfrac{1}{2}\theta)\sin[\tfrac{1}{2}(\alpha+\varphi)] \end{aligned} \tag{1}$$

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and the three-dimensional variables

$$x = r \sin\theta \cos\varphi \qquad y = r \sin\theta \sin\varphi \qquad z = r\cos\theta \tag{2}$$

and we note that

$$r = \sum_{i=1}^{4} u_i^2 \equiv u^2. \tag{3}$$

The Jacobian of the transformation $(r, \theta, \varphi, \alpha) \rightarrow (u_1, u_2, u_3, u_4)$ is given by $r \sin\theta/16$. The range of the fourth variable α is from 0 to 4π so that the volume of space associated with the following integrals is preserved:

$$\int_0^R \mathrm{d}r\, r^2 \int_{-1}^{1} \mathrm{d}(\cos\theta) \int_0^{2\pi} \mathrm{d}\varphi \int_0^{4\pi} \mathrm{d}\alpha = 16 \qquad 2\pi^2 \int_0^{\sqrt{R}} u^2 u^3\, \mathrm{d}u = \tfrac{16}{3}\pi^2 R^3 \tag{4}$$

where we have used (3) and the expression for the Jacobian. The Dirac delta functions are related through

$$\delta^3(\boldsymbol{r} - \boldsymbol{r}')\delta(\alpha - \alpha') = \frac{\delta^4(\boldsymbol{u} - \boldsymbol{u}')}{16u^2} \tag{5}$$

so that when we integrate over $\mathrm{d}^3\boldsymbol{r}\,\mathrm{d}\alpha \rightarrow 16u^2\,\mathrm{d}^4\boldsymbol{u}$ we get unity. From (5) we obtain upon integration over α, the expression for the three-dimensional delta function:

$$\delta^3(\boldsymbol{r} - \boldsymbol{r}') = \tfrac{1}{16}\int_0^{4\pi} \mathrm{d}\alpha \frac{\delta^4(\boldsymbol{u} - \boldsymbol{u}')}{u^2}. \tag{6}$$

The Laplacian operators are readily worked to be related by the equation

$$\nabla^2 + \frac{1}{r^2 \sin^2\theta} \frac{\partial^2}{\partial\alpha^2} = \frac{1}{4u^2} \nabla_u^2 \tag{7}$$

where

$$\nabla_u^2 = \sum_{i=1}^{4} \frac{\partial^2}{\partial u_i^2} \tag{8}$$

and ∇^2 is the three-dimensional Laplacian written in spherical coordinates.

The Green equation of the hydrogen atom may be written as ($\hbar = 1$):

$$\left(-\mathrm{i}\frac{\partial}{\partial t} - \frac{\nabla^2}{2m} + U(r)\right) G(x, x') = \delta^4(x - x') \qquad x^0 = t \tag{9}$$

with $U(r) = -Ze^2/r$, $x = (x^0, \boldsymbol{r})$, and we may write the Fourier integral

$$G(x, x') = \int \frac{\mathrm{d}k^0}{2\pi} \exp[\mathrm{i}k^0(x^0 - x'^0)]G(\boldsymbol{r}, \boldsymbol{r}'; k^0) \tag{10}$$

leading to the equation

$$\left(k^0 - \frac{\nabla^2}{2m} - \frac{Ze^2}{r}\right) G(\boldsymbol{r}, \boldsymbol{r}'; k^0) = \delta^3(\boldsymbol{r} - \boldsymbol{r}'). \tag{11}$$

In this equation $-k^0 \equiv E$ denotes the energy.

Similarly we define a Green function $H(u, u')$, where $u = (x^0, \boldsymbol{u})$,

$$H(u, u') = \int \frac{\mathrm{d}K^0}{2\pi} \exp[\mathrm{i}K^0(x^0 - x'^0)]H(\boldsymbol{u}, \boldsymbol{u}'; K^0). \tag{12}$$

The expression for the Laplacian operators in (7) and equation (11) suggests the following equation for $H(\boldsymbol{u}, \boldsymbol{u}'; K^0)$:

$$(-\nabla_u^2/2\mu + k^0u^2 - Ze^2)H(\boldsymbol{u}, \boldsymbol{u}'; -Ze^2) = \delta^4(\boldsymbol{u}-\boldsymbol{u}') \tag{13}$$

where we note that k^0 does not play the role of energy here but replaces the familiar expression $\mu\omega^2/2$ in the (four-dimensional) harmonic oscillator problem and $\mu = 4m$. To relate $G(\boldsymbol{r}, \boldsymbol{r}'; k^0)$ and $H(\boldsymbol{u}, \boldsymbol{u}'; -Ze^2)$, we carry out a Fourier transform for the latter, i.e. we write

$$H(\boldsymbol{u}, \boldsymbol{u}'; -Ze^2) = \frac{4}{\pi}\sum_{M=-\infty}^{\infty} \exp[\mathrm{i}M(\alpha-\alpha')/2]H_M(\boldsymbol{r}, \boldsymbol{r}') \tag{14}$$

where

$$H_M(\boldsymbol{r}, \boldsymbol{r}') = \tfrac{1}{16}\int_0^{4\pi} \mathrm{d}\alpha \exp(-\mathrm{i}M\alpha/2)H(\boldsymbol{u}, \boldsymbol{u}'; -Ze^2) \tag{15}$$

and the latter must satisfy the equation

$$\left(-\frac{2}{\mu}\nabla^2 + \frac{M^2}{r^2\sin^2\theta} + k^0 - \frac{Ze^2}{r}\right)H_M(\boldsymbol{r}, \boldsymbol{r}') = \delta^3(\boldsymbol{r}-\boldsymbol{r}') \tag{16}$$

so that (13) is verified, by using equation (5) and the property

$$\begin{aligned} 16r\delta^3(\boldsymbol{r}-\boldsymbol{r}')\sum_{M=-\infty}^{\infty}\frac{\exp[\mathrm{i}M(\alpha-\alpha')/2]}{4\pi} &= 16r\delta^3(\boldsymbol{r}-\boldsymbol{r}')\delta(\alpha-\alpha') \\ &= \delta^4(\boldsymbol{u}-\boldsymbol{u}'). \end{aligned} \tag{17}$$

With $\mu = 4m$, we note from (11) that

$$G(\boldsymbol{r}, \boldsymbol{r}'; k^0) = H_0(\boldsymbol{r}, \boldsymbol{r}') \tag{18}$$

and from (15) we obtain for the Green function in question

$$G(\boldsymbol{r}, \boldsymbol{r}'; k^0) = \tfrac{1}{16}\int_0^{4\pi} \mathrm{d}\alpha\, H(\boldsymbol{u}(\boldsymbol{r}, \alpha), \boldsymbol{u}(\boldsymbol{r}', \alpha'); -Ze^2) \tag{19}$$

where we have used the notation $\boldsymbol{u} = \boldsymbol{u}(\boldsymbol{r}, \alpha)$, $\boldsymbol{u}' = \boldsymbol{u}(\boldsymbol{r}', \alpha')$.

We take the trace of (19) with respect to $\boldsymbol{r}'$ and we use the translational invariance of $H(\boldsymbol{u}, \boldsymbol{u}'; -Ze^2)$ in the transformation $\alpha \to \alpha+\delta$, $\alpha' \to \alpha'+\delta$ to obtain

$$\int_{R^3} \mathrm{d}^3\boldsymbol{r}'\, G(\boldsymbol{r}', \boldsymbol{r}'; k^0) = \frac{1}{4\pi}\int_0^{4\pi}\mathrm{d}\alpha \int_{R^4} u'^2\, \mathrm{d}^4\boldsymbol{u}'\, H(\boldsymbol{u}'_+, \boldsymbol{u}'; -Ze^2) \tag{20}$$

where $\boldsymbol{u}'_+$ denotes $\boldsymbol{u}'$ with α' in the latter displaced by α, i.e. $\alpha' \to \alpha'+\alpha$. Equation (20) will be used in § 4 to obtain the spectrum of the hydrogen atom.

3. Generalised trace operation for the harmonic oscillator

The eigenfunction of the one-dimensional harmonic oscillator may be written as

$$\phi_n(x) = (\mu\omega/\pi)^{1/4}\exp(-\mu\omega x^2/2)H_n((\mu\omega)^{1/2}x) \qquad n = 0, 1, 2, \ldots \tag{21}$$

with mass μ, where $H_n(x)$ are the Hermite polynomials having an integral representation (Gradshteyn and Ryzhik 1965, p 1033)

$$H_n(x)=\frac{(2)^n}{\sqrt{\pi}}\int_{-\infty}^{\infty}(x+\mathrm{i}t)^n\,\mathrm{e}^{-t^2}\,\mathrm{d}t. \tag{22}$$

The two-dimensional harmonic oscillator Green function may be written in the familiar form

$$\sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\exp[-\mathrm{i}\omega T(n_1+n_2+1)]\phi_{n_1}(x_1)\phi_{n_2}(x_2)\phi_{n_1}(y_1)\phi_{n_2}(y_2) \tag{23}$$

with $T=t_1-t_2$, and with $\omega(n_1+n_2+1)$ denoting its energy levels. Upon using the integral representation (22), one readily obtains the well known expression for the Green function (23):

$$\begin{aligned}(\mu\omega/\pi)\exp(-\mathrm{i}\omega T)&\exp[-\mu\omega(x_1^2+x_2^2+y_1^2+y_2^2)/2]\\ &\times\exp\left(-\frac{\mu\omega(x_1^2+x_2^2+y_1^2+y_2^2)\exp(-2\mathrm{i}\omega T)}{[1-\exp(-2\mathrm{i}\omega T)]}\right)\\ &\times\exp\left(\frac{2\mu\omega(x_1y_1+x_2y_2)\exp(-2\mathrm{i}\omega T)}{[1-\exp(-2\mathrm{i}\omega T)]}\right).\end{aligned} \tag{24}$$

The usual trace operation in (24) is defined by setting $x_1=y_1$, $x_2=y_2$ and integrating over x_1 and x_2 ($-\infty<x_1<\infty$, $-\infty<x_2<\infty$). We define a *generalised* trace operation through the following. We set

$$x_1=(1/\sqrt{2})(U+U^*)\qquad x_2=(-\mathrm{i}/\sqrt{2})(U-U^*) \tag{25}$$

and

$$y_1=\frac{\exp(\mathrm{i}\alpha/2)}{\sqrt{2}}U+\frac{\exp(-\mathrm{i}\alpha/2)}{\sqrt{2}}U^*\qquad y_2=-\mathrm{i}\frac{\exp(\mathrm{i}\alpha/2)}{\sqrt{2}}U+\mathrm{i}\frac{\exp(-\mathrm{i}\alpha/2)U^*}{\sqrt{2}} \tag{26}$$

where α is an arbitrary real number. We note that

$$\begin{aligned}&x_1^2+x_2^2+y_1^2+y_2^2=2(x_1^2+x_2^2)\\ &x_1y_1+x_2y_2=(x_1^2+x_2^2)\cos(\tfrac{1}{2}\alpha).\end{aligned} \tag{27}$$

Upon using (27) in (24) and carrying out the elementary Gaussian integrals over x_1 and x_2 ($-\infty<x_1<\infty$, $-\infty<x_2<\infty$), we obtain for the integral of (24) the expression

$$\begin{aligned}\exp(-\mathrm{i}\omega T)[1+\exp(-2\mathrm{i}\omega T)-2\exp(-\mathrm{i}\omega T)\cos(\tfrac{1}{2}\alpha)]^{-1}&=\tfrac{1}{2}[\cos(\omega T)-\cos(\tfrac{1}{2}\alpha)]^{-1}\\ =-\tfrac{1}{4}[\sin(\tfrac{1}{2}\omega T+\tfrac{1}{4}\alpha)\sin(\tfrac{1}{2}\omega T-\tfrac{1}{4}\alpha)]^{-1}&\\ =\frac{\exp[-\mathrm{i}(\tfrac{1}{2}\omega T+\tfrac{1}{4}\alpha)]\exp[-\mathrm{i}(\tfrac{1}{2}\omega T-\tfrac{1}{4}\alpha)]}{\{1-\exp[-\mathrm{i}(\omega T+\tfrac{1}{2}\alpha)]\}\{1-\exp[-\mathrm{i}(\omega T-\tfrac{1}{2}\alpha)]\}}.&\end{aligned} \tag{28}$$

We may rewrite (28) in the form of a double series to obtain for the *generalised* trace of the two-dimensional Green function in (24):

$$\sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\exp[-\mathrm{i}\omega T(n_1+n_2+1)]\exp[-\mathrm{i}\tfrac{1}{2}\alpha(n_1-n_2)] \tag{29}$$

where α is an arbitrary real number.

We note that the four variables u_1, u_2, u_3, u_4 defined in (1) may be rewritten as

$$\begin{aligned} u_1 &= \frac{\exp(\mathrm{i}\alpha/2)}{\sqrt{2}} U_1 + \frac{\exp(-\mathrm{i}\alpha/2)}{\sqrt{2}} U_1^* \\ u_2 &= -\frac{\mathrm{i}}{\sqrt{2}} \exp(\mathrm{i}\alpha/2) U_2 + \frac{\mathrm{i}}{\sqrt{2}} \exp(-\mathrm{i}\alpha/2) U_2^* \\ u_3 &= \frac{\exp(\mathrm{i}\alpha/2)}{\sqrt{2}} U_2 + \frac{\exp(-\mathrm{i}\alpha/2)}{\sqrt{2}} U_2^* \\ U_4 &= -\frac{\mathrm{i}}{\sqrt{2}} \exp(\mathrm{i}\alpha/2) U_1 + \frac{\mathrm{i}}{\sqrt{2}} \exp(-\mathrm{i}\alpha/2) U_1^* \end{aligned} \tag{30}$$

in terms of variables U_1, U_1^*, U_2, U_2^*, with the latter independent of α. Upon comparison of (30) with (26), we conclude upon squaring (29) that the generalised trace of the four-dimensional harmonic oscillator is given by

$$\begin{aligned} \int_{R^4} \mathrm{d}^4\boldsymbol{u}'\, H(\boldsymbol{u}'_+, \boldsymbol{u}') &= \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \sum_{n_3=0}^{\infty} \sum_{n_4=0}^{\infty} \exp[-\mathrm{i}\omega T(n_1+n_2+n_3+n_4+2)] \\ &\quad \times \exp[-\mathrm{i}\tfrac{1}{2}\alpha(n_1-n_2+n_3-n_4)] \end{aligned} \tag{31}$$

where $\boldsymbol{u}'_+$ is defined below equation (20). What is needed in (20) is the expression for $\int u'^2\, \mathrm{d}^4\boldsymbol{u}'\, H(\boldsymbol{u}'_+, \boldsymbol{u}')$. But this is easy to obtain as we may modify the harmonic oscillator potential $\mu\omega^2 u^2/2$ to $\mu\omega_0^2 u^2/2$ where $\omega_0 = (\omega^2 + 2\lambda/\mu)^{1/2}$, take the partial derivative $(\mathrm{i}/T)\partial/\partial\lambda$ of (31) and then set $\lambda = 0$. This leads to

$$\begin{aligned} \int_{R^4} \mathrm{d}^4\boldsymbol{u}'\, u'^2 H(\boldsymbol{u}'_+, \boldsymbol{u}') &= \sum_{n_1,\ldots,n_4=0}^{\infty} \frac{(n_1+n_2+n_3+n_4+2)}{\mu\omega} \exp[-\mathrm{i}\omega T(n_1+n_2+n_3+n_4+2)] \\ &\quad \times \exp[-\mathrm{i}\tfrac{1}{2}\alpha(n_1-n_2+n_3-n_4)]. \end{aligned} \tag{32}$$

From the definition of the integral in (12), we then obtain

$$\begin{aligned} \int_{R^4} \mathrm{d}^4\boldsymbol{u}'\, u'^2 H(\boldsymbol{u}'_+, \boldsymbol{u}'; K^0) &= \frac{1}{\mathrm{i}\mu\omega} \sum_{n_1,\ldots,n_4=0}^{\infty} \frac{(n_1+n_2+n_3+n_4+2)\exp[-\mathrm{i}\tfrac{1}{2}\alpha(n_1-n_2+n_3-n_4)]}{[K^0+\omega(n_1+n_2+n_3+n_4+2)-\mathrm{i}\varepsilon]} \end{aligned} \tag{33}$$

with $T = x^0 - x'^0$.

4. The hydrogen atom

According to (20), we have to integrate (33) over α thus leading to

$$\begin{aligned} \frac{1}{4\pi}\int_0^{4\pi} \mathrm{d}\alpha \int_{R^4} \mathrm{d}^4\boldsymbol{u}'\, u'^2 H(\boldsymbol{u}'_+, \boldsymbol{u}'; K^0) &= \frac{1}{\mathrm{i}\mu\omega} \sum_{n_1,\ldots,n_4}^{*} \frac{(n_1+n_2+n_3+n_4+2)}{[K^0+\omega(n_1+n_2+n_3+n_4+2)-\mathrm{i}\varepsilon]} \end{aligned} \tag{34}$$

where Σ^* stands for a sum over all non-negative integers n_1, n_2, n_3, n_4 such that $n_1 - n_2 + n_3 - n_4 = 0$. By setting $n_1 + n_3 = n_2 + n_4 = n - 1$, we obtain for (34):

$$\frac{1}{\mathrm{i}} \sum_{n=1}^{\infty} \frac{2n^3}{\mu\omega(K^0 + 2n\omega - \mathrm{i}\varepsilon)}. \tag{35}$$

Upon making the identification $K^0 = -Ze^2$, $\mu = 4m$, $\frac{1}{2}\mu\omega^2 = k^0$, we obtain, from (20) and (35),

$$\int_{R^3} \mathrm{d}^3 r' \, G(\boldsymbol{r}', \boldsymbol{r}'; k^0) = \frac{1}{\mathrm{i}} \sum_{n=1}^{\infty} \frac{n^2}{2\sqrt{k^0}} \frac{1}{(\sqrt{k^0} - \sqrt{2m} Ze^2/2n - \mathrm{i}\varepsilon)}. \tag{36}$$

Near the poles this is given by the formal expression

$$\frac{1}{\mathrm{i}} \sum_{n=1}^{\infty} \frac{n^2}{(k^0 - Z^2 e^4 m/2n^2 - \mathrm{i}\varepsilon)} \tag{37}$$

leading to the classic hydrogen-atom energy levels

$$-k^0 = E_n = -\frac{Z^2 e^4 m}{2n^2} \qquad n = 1, 2, \ldots$$

with a degree of degeneracy n^2.

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