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Exact Path-Integral Solution of the Dirac-Coulomb Problem

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An exact path-integral solution of the Dirac equation with a Coulomb potential is found. The energy-dependent Green's function of the second-order Dirac-Coulomb equation, expressed as a polar-coordinate path integral, is reduced to the exactly solvable path integral for an isotropic harmonic oscillator by a coordinate transformation combined with a local time rescaling. The Green's function of the linear Dirac equation is evaluated with the help of the Biedenharn transformation. The energy spectrum for the bound states is also obtained.

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That Feynman's path-integral approach to quantum mechanics[1] is severely limited in application has often been exemplified by the lack of path-integral solutions for the hydrogen atom and the spin problem. The Dirac-Coulomb problem, doubly burdened with the Coulomb potential and spin, appears to be another hopeless example. Very recently, however, exact path-integral treatments of the nonrelativistic Coulomb problem have become available.[2-4] A breakthrough has been made in the long-standing problem[5] with the help of a contact transformation combined with a rescaling of the local time interval. The hydrogen atom, insofar as the nonrelativistic case is concerned, is now kept under control. Furthermore, the kind of transformations used for the hydrogen atom has also been proven applicable to other nonrelativistic problems.[6] The fundamental issue of spin, on the other hand, still remains unsettled. The recent Grassmann-number formulation of a path integral for spin seems promising, but is far from being useful in handling interactions with external fields.[7] Feynman's formulation of an iterated Dirac equation,[8] involving spin matrices explicitly at the classical level, has been considered not only aesthetically unsatisfactory but also computationally complex. Nonetheless, the old idea still retains its unexpired practical value.[9]

In this paper, we report that the Dirac equation with a Coulomb potential can indeed be solved exactly by path integration. First, we reduce on the Biedenharn basis[10] the Green's function of the iterated Dirac-Coulomb equation into a radial path integral which has an effective action similar to that of the nonrelativistic hydrogen atom. Then, we convert the Coulomb radial path integral into the radial path integral for an isotropic harmonic oscillator by a coordinate transformation combined with a local time rescaling. In the nonrelativistic case,[2,3] the Kustaanheimo-Stiefel transformation has been used to reduce the Coulomb integral in R^3 into an oscillator integral in R^4. For evaluating our radial integral, such a bijective mapping is not appropriate. Instead, we adopt an alternative one-to-one mapping of the radial variable and the local timelike parameter. Obtaining the Green's function of the iterated Dirac equation, we find an explicit expression for the Green's function of the first-order Dirac equation with a Coulomb potential, and the exact bound-state energy spectrum for the Dirac-Coulomb system.

The Dirac equation with a Coulomb potential may be written as

$$(m-\hat{M})|\psi\rangle=0, \tag{1}$$

where $\hat{M}=-\beta\vec{\alpha}\cdot\vec{p}+\beta(E+Ze^2/r)$ in units $\hbar=c=1$. The form of the Dirac equation (1) is not unique. A similarity transformation, $\hat{M}_s=S\hat{M}S^{-1}$

and $|\psi_s\rangle = S|\psi\rangle$, converts (1) into $(m - \hat{M}_s)|\psi_s\rangle = 0$ without altering its physical content. Such a transformation sometimes simplifies the solution. What we shall specifically be concerned with is an equation which is related to the original Dirac equation (1) by the Biedenharn transformation.[10] The corresponding Green's function, $G = (m - \hat{M}_s + i0)^{-1}$, can be put in the form $G = (m + \hat{M}_s)g$, where $g = (m^2 - \hat{M}_s^2 + i0)^{-1}$. In the coordinate representation, this is

$$\langle \vec{r}''|G|\vec{r}'\rangle = [m + \hat{M}_s(\vec{r}'')]\langle \vec{r}''|g|\vec{r}'\rangle, \quad (2)$$

where

$$S^{-1}\hat{M}_s(\vec{r})S = i\beta\vec{\alpha}\cdot\nabla + \beta(E + Ze^2/r).$$

Here, we write the Green's function of the iterated Dirac equation in an integral form,

$$\langle \vec{r}''|g|\vec{r}'\rangle = (i/2m)\int_0^\infty \langle \vec{r}''|\exp[-iHu]|\vec{r}'\rangle\, du, \quad (3)$$

by introducing an operator $H = (m^2 - M_s^2)/(2m)$ and a parameter u. The integrand of (3) may be viewed from the structural similarity as the propagator of a system which, having an effective Hamiltonian H, evolves with the change of the timelike parameter u. As Feynman asserted,[1] the propagator can be put into a path integral. Thus, we attempt to evaluate (3) by path integration and to find an expression for the Green's function of the Dirac equation via (2).

As usual,[10,11] we employ the radial momentum operator $p_r = (\vec{r}\cdot\vec{p} - i)/r$, the Dirac operator $K = \beta(\vec{\sigma}\cdot\vec{L} + 1)$, and the Martin-Glauber operator $\mathscr{L} = -(\beta K + iZe^2\alpha_r)$ with $\alpha_r = \vec{\alpha}\cdot\vec{r}/r$ to express the effective Hamiltonian in (3). Namely,

$$S^{-1}HS = \frac{p_r^2}{2m} + \frac{\mathscr{L}(\mathscr{L}+1)}{2mr^2} - \frac{a}{r} - \frac{k^2}{2m},$$

where $a = Ze^2E/m$ and $k^2 = E^2 - m^2$. If $\mathscr{L}(\mathscr{L}+1)$ is diagonalized by S commuting with p_r and r so that $S\mathscr{L}(\mathscr{L}+1)S^{-1}|\lambda\rangle = \lambda(\lambda+1)|\lambda\rangle$, then the Green's function (3) can be given in polar coordinates as follows:

$$\langle \vec{r}''|g|\vec{r}'\rangle = \sum_\lambda \langle\theta''\phi''|\lambda\rangle\langle r''|g_\lambda|r'\rangle\langle\lambda|\theta'\phi'\rangle, \quad (4)$$

with the radial Green's function

$$\langle r''|g_\lambda|r'\rangle = (i/2m)\int\langle r''|\exp(-iH_\lambda u)|r'\rangle\, du, \quad (5)$$

where

$$H_\lambda = \frac{p_r^2}{2m} + \frac{\lambda(\lambda+1)}{2mr^2} - \frac{a}{r} - \frac{k^2}{2m}. \quad (6)$$

The propagator in u evolution of (5), having the effective radial Hamiltonian (6), is identical in form, except for the contribution from the last constant term of (6), with the radial propagator of the nonrelativistic hydrogen atom.[4]

Before getting into the path-integral calculation of the radial Green's function (5), we have to specify the value of λ in (6). Customarily, the solutions of the Dirac-Coulomb problem are classified by the respective eigenvalues, $j(j+1)$, μ, κ, and $\tilde{\beta}$ of the mutually commuting operators J^2, J_3, K, and β. As is well known, $j = \frac{1}{2}, \frac{3}{2}, \ldots$; $\mu = -j, -j+1, \ldots, j-1, j$; $\kappa = \pm(j+\frac{1}{2})$; $\tilde{\beta} = \pm 1$. The Martin-Glauber operator $\mathscr{L}$ can be simultaneously diagonalized by the Biedenharn transformation[10]; that is, $\mathscr{L}_s = S\mathscr{L}S^{-1} = -\beta K[1 - (Ze^2/K^2)]^{1/2}$, where $S = \exp[\frac{1}{2}i\beta\alpha_r \tanh^{-1}(Ze^2/K)]$. Hence, the eigenvalues of $\mathscr{L}_s$ are given by $\gamma = \pm[\kappa^2 - Z^2e^4]^{1/2}$. Since $\lambda(\lambda+1) = \gamma(\gamma+1)$, we have

$$\lambda(\gamma) = |\gamma| + \tfrac{1}{2}(\mathrm{sgn}\gamma - 1). \quad (7)$$

Therefore, we identify the angular functions $\langle\theta\phi|\lambda\rangle$ with the simultaneous eigenstates $\langle\theta\phi|j, \mu, \kappa, \tilde{\beta}\rangle$. More explicitly, we write the angular states as

$$\langle\theta\phi|j,\mu,\kappa,-1\rangle = \begin{pmatrix} 0 \\ \chi_\kappa^\mu \end{pmatrix}, \qquad \langle\theta\phi|j,\mu,\kappa,1\rangle = \begin{pmatrix} \chi_{-\kappa}^\mu \\ 0 \end{pmatrix}, \quad (8)$$

χ_κ^μ being the two-component spinors

$$\chi_\kappa^\mu(\theta,\phi) = \sum_\nu (l\tfrac{1}{2}\mu - \nu\nu|j\mu)\, Y_l^{\mu-\nu}(\theta,\phi)\chi_{1/2}^\nu. \quad (9)$$

Apparently, we are dealing with the Dirac equation (1) in the Biedenharn representation.[10,11] Using (6) in (5) and noticing that $\mathrm{sgn}\kappa = \pm\mathrm{sgn}\gamma$ for $\tilde{\beta} = \mp 1$, we obtain the Green's function for the second-order Dirac equation,

$$\langle \vec{r}''|g|\vec{r}'\rangle = \sum_{j,\kappa}\langle r''|g_{\lambda(\gamma)}|r'\rangle\, \Omega^j_{\kappa,\kappa}(\theta''\phi''|\theta'\phi')\beta^2, \quad (10)$$

where

$$\Omega^j_{\kappa,\kappa'}(\theta''\phi''|\theta'\phi') = \sum_\mu \chi_\kappa^\mu(\theta'',\phi'')\chi_{\kappa'}^{\mu\dagger}(\theta',\phi'). \quad (11)$$

Now let us turn to the path integration of the radial Green's function (5). Following the time-

slicing procedure, we express the radial propagator in the integrand of (5) as

$$\langle r''|\exp(-iH_\lambda u)|r'\rangle = (r'r'')^{-1}\lim_{N\to\infty}\int\exp[i\sum_{j=1}^{N}S(\tau_j)]\prod_{j=1}^{N}\left(\frac{m}{2\pi i\tau_j}\right)^{1/2}\prod_{j=1}^{N-1}dr_j, \tag{12}$$

where $r_j = r(u_j)$, $r_0 = r'$, $r_N = r''$, $\tau_j = u_j - u_{j-1}$, and $u = \sum\tau_j$. In (12), $S(\tau_j)$ is an effective short "time" radial action given by

$$S(\tau_j) = m(\Delta r_j)^2/2\tau_j - \lambda(\lambda+1)\tau_j/2mr_jr_{j-1} + a\tau_j/r_j + k^2\tau_j/2m. \tag{13}$$

In the absence of the Coulomb term in (13), the path integral (12) can easily be calculated. However, the Coulomb potential complicates the problem.

To carry out the integration of (12), we change the radial variable r_j into a new variable ρ_j and the local interval τ_j into a new interval σ_j by

$$\rho_j = r_j^{1/2}; \quad \sigma_j = \tau_j/4\bar{r}_j, \tag{14}$$

where $\bar{r}_j = (r_jr_{j-1})^{1/2} = \rho_j\rho_{j-1} = \bar{\rho}_j^2$. With (14), the action (13) becomes

$$S(\sigma_j) = \frac{m(\Delta\rho_j)^2}{2\sigma_j} + \frac{m(\Delta\rho_j)^4}{8\sigma_j\bar{\rho}_j^2} - \frac{2\lambda(\lambda+1)\sigma_j}{m\bar{\rho}_j^2} + 4a\sigma_j - \tfrac{1}{2}m\omega^2\bar{\rho}_j^2\sigma_j, \tag{15}$$

where $\omega = 2ik/m$. At the same time, the measure of (12) changes as

$$\prod_{j=1}^{N}\left(\frac{m}{2\pi i\sigma_j}\right)^{1/2}\prod_{j=1}^{N-1}dr_j = (4\rho'\rho'')^{-1/2}\prod_{j=1}^{N}\left(\frac{m}{2\pi i\sigma_j}\right)^{1/2}\prod_{j=1}^{N-1}d\rho_j. \tag{16}$$

These alterations do not make (12) integrable. The second term of (15) involves $(\Delta\rho_j)^4$, which hinders the path integration from being completed. As can be easily shown, however, the following formula is valid for n integer and $|A|$ large ($\mathrm{Re}A > 0$):

$$\int x^{2n}\exp[-Ax^2 + Bx^4 + O(x^6)]\,dx = \int x^{2n}\exp[-Ax^2 + \tfrac{3}{4}BA^{-2} + O(A^{-3})]\,dx, \tag{17}$$

so that the second term of (15) may be replaced by an equivalent term, $-3\sigma_j/(8m\bar{\rho}_j)$. As a result, the radial propagator (12) can be put into the form

$$\langle r''|\exp(-iH_\lambda u)|r'\rangle = \tfrac{1}{2}(\rho'\rho'')^{-3/2}\exp(4ia\sigma)\tilde{K}_\lambda(\rho'',\rho';\sigma) \tag{18}$$

with the propagator in σ evolution,

$$\tilde{K}_\lambda(\rho'',\rho';\sigma) = (\rho'\rho'')^{-1}\lim_{N\to\infty}\int\exp[i\sum_{j=1}^{N}\tilde{S}(\sigma_j)]\prod_{j=1}^{N}\left(\frac{m}{2\pi i\sigma_j}\right)^{1/2}\prod_{j=1}^{N-1}d\rho_j, \tag{19}$$

where

$$\tilde{S}(\sigma_j) = m(\Delta\rho_j)^2/2\sigma_j - \lambda'(\lambda'+1)\sigma_j/2m\bar{\rho}_j^2 - \tfrac{1}{2}m\omega^2\bar{\rho}_j^2 \tag{20}$$

and $\lambda' = 2\lambda + \frac{1}{2}$. The effective action (20) is now identical in form with the radial action of an isotropic harmonic oscillator in three dimensions. Thus, the propagator in u evolution of (5), reduced to the radial path integral for an oscillator, can be calculated, the result of this calculation being[12]

$$\tilde{K}_\lambda(\rho'',\rho';\sigma) = (\rho'\rho'')^{-1/2}(-im\omega)\csc(\omega\sigma) \times\exp[\tfrac{1}{2}im\omega(\rho'^2+\rho''^2)\cot(\omega\sigma)]I_{\lambda'+1/2}[-im\omega\rho'\rho''\csc(\omega\sigma)], \tag{21}$$

where $I_\nu(z)$ is the modified Bessel function. Using this in (18) and setting $\rho'^2 = r'$, $\rho''^2 = r''$, $m\omega = 2ik$, $\lambda' = 2\lambda + \frac{1}{2}$, $\sigma = \tau/(4\rho'\rho'')$, $p = -imak$, and $q = k\tau(4r'r''m^2)^{-1/2}$, we can write the radial Green's function (5) as

$$\langle r''|g_\lambda|r'\rangle = (r'r'')^{-1/2}\int\exp(-2pq)\exp[ik(r'+r'')\coth q] \times I_{2\lambda+1}[-2ik(r'r'')^{1/2}\operatorname{csch}q]\operatorname{csch}q\,dq. \tag{22}$$

The integration of this type has often appeared in previous calculations.[3,4,6] Now we simply use the result to obtain the radial Green's function ($r' > r''$) in a closed form,

$$\langle r''|g_\lambda|r'\rangle = \frac{\Gamma(p+\lambda+1)}{2ikr'r''\Gamma(2\lambda+2)} M_{-p,\lambda+1/2}(-2ikr'')\, W_{-p,\lambda+1/2}(-2ikr'), \tag{23}$$

where $M_{p,\nu}(z)$ and $W_{p,\nu}(z)$ are the Whittaker functions. This coincides with the result obtained earlier by a different method.[13] The full Green's function for the second-order Dirac equation is given by (10) with (23).

The Green's function of the first-order Dirac equation (1) can be derived from (2). Since we have applied the Biedenharn transformation in order to diagonalize $\mathscr{L}$, the operator $\hat{M}_s(\vec{r}'')$ in (2), when acting on the κ state, takes the form

$$\hat{M}_s(\vec{r}) = i\beta\alpha_r[\partial/\partial r + (1-\gamma\beta)/r + (Ze^2E/\gamma)\beta] + (\kappa E/\gamma)\beta. \tag{24}$$

Furthermore, the Whittaker function $M_{\lambda(\gamma)}$ in (23) satisfies the recurrence relations

$$D_\pm[r^{-1}M_{\lambda(\pm\gamma)}] = \pm i\,\mathrm{sgn}\gamma[m^2-(\kappa E/\gamma)^2]^{1/2}[r^{-1}M_{\lambda(\mp\gamma)}], \tag{25}$$

where $D_\pm = d/dr + (1\pm\gamma)/r \mp Ze^2E/\gamma$. Applying (24) and (25) to (2), we arrive at the Green's function for the Dirac-Coulomb problem,

$$\begin{aligned}\langle \vec{r}''|G|\vec{r}'\rangle = \sum\nolimits_{j,\kappa}[\Gamma(p+\lambda+1)/2ikr'r''\Gamma(2\lambda+2)]\, W_{-p,\lambda+1/2}(-2ikr') \\ \times\{[m-(\kappa E/\gamma)]M_{-p,\lambda+1/2}(-2ikr'')\,\Omega^j_{\kappa,\kappa}(\theta''\phi''|\theta'\phi')\beta^2 \\ - ik\,\mathrm{sgn}\gamma M_{-p,\bar{\lambda}+1/2}(-2ikr'')\,\Omega^j_{\kappa,-\kappa}(\theta''\phi''|\theta'\phi')\alpha_1\alpha_2\alpha_3\},\end{aligned} \tag{26}$$

where $\lambda=\lambda(\gamma)$ and $\bar{\lambda}=\lambda(-\gamma)$.

The bound-state energy spectrum can be found from the poles of the spectral function, $G(E)=\int\langle\vec{r}|G|\vec{r}\rangle\, d^3r$. Indeed, the poles arise from the Γ function in (26) when $p+\lambda+1=-n$ ($n=0,1,2,\ldots$). Note that here $p=-iZe^2E(E^2-m^2)^{-1/2}$. Apparently these poles yield the standard formula

$$E_{nj\kappa} = m[1+Z^2e^4(n+\lambda)^{-2}]^{-1/2}, \tag{27}$$

where λ has been given by (7).

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