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Path integral for a relativistic spinless Coulomb system

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Abstract

The path integral for the relativistic spinless Coulomb system is solved, and the wave functions are extracted from the resulting amplitude.

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1. While the path integral of the nonrelativistic Coulomb system has been solved some 15 years ago [1] and further discussed by many authors [2–14], so that it has become conference [15] and textbook material [16], the relativistic problem has remained open – for particles of spin zero as well as spin-1/2 [2]. The purpose of this note is to fill this gap for spin-zero particles.

2. Consider first a free relativistic spinless particle of mass M. If $x^\mu(\lambda)$ describes its orbit in D spacetime dimensions in terms of some parameter λ, the classical action reads

$$\mathcal{A}_{\rm cl} = Mc \int_{\lambda_a}^{\lambda_b} d\lambda \sqrt{x'^2(\lambda)}, \tag{1}$$

where c is the velocity of light. This action cannot be used to set up a path integral for the time evolution amplitude since it would not yield the well-known Green function of a Klein–Gordon field. An action which serves this purpose can be constructed with the help of an auxiliary fluctuating variable $\rho(\lambda)$ and reads [3]

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[2] The problem of summing nonrelativistic fermion orbits in a Coulomb field has not even been satisfactorily *formulated.* There exists a paper entitled "Exact path integral solution of the path integral of the Dirac–Coulomb problem" by Kayed and Inomata [17], but contrary to what it suggested in its title, this paper does not address the above summation problem, circumventing it by using the Dirac equation for the Green function as an *input.* With well-known operator manipulations, this is decomposed into ordinary Schrödinger equations for the radial wave functions, for which equivalent path integral representations are derived by time-slicing. The final path integral involves good old boson orbits.

[3] For $\rho(\lambda) \equiv 1$, this was noted by Feynman and Hibbs [18].

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$$\mathcal{A} = \int_{\lambda_a}^{\lambda_b} \mathrm{d}\lambda \left(\frac{M}{2\rho(\lambda)} x'^2(\lambda) + \tfrac{1}{2} M c^2 \rho(\lambda) \right). \tag{2}$$

Classically, this action coincides with the original $\mathcal{A}_{\rm cl}$ since it is extremal for

$$\rho(\lambda) = \sqrt{x'^2(\lambda)}/c. \tag{3}$$

Inserting this back into (2) we see that $\mathcal{A}$ reduces to $\mathcal{A}_{\rm cl}$.

The action $\mathcal{A}_{\rm cl}$ is invariant under arbitrary reparametrizations

$$\lambda \to f(\lambda). \tag{4}$$

The action $\mathcal{A}$ shares this invariance, if $\rho(\lambda)$ is simultaneously transformed as

$$\rho \to \rho / f'. \tag{5}$$

The action $\mathcal{A}$ has the advantage of being quadratic in the orbital variable $x(\lambda)$. If the physical time is analytically continued to imaginary values so that the metric becomes Euclidean, the action looks like that of a nonrelativistic particle moving as a function of a pseudotime λ through a D-dimensional Euclidean spacetime, with a mass depending on λ.

3. To set up a path integral, the action has to be pseudotime-sliced, say at $\lambda_0 = \lambda_a, \lambda_1, \dots, \lambda_{N+1} = \lambda_b$. If $\epsilon_n = \lambda_n - \lambda_{n-1}$ denotes the thickness of the nth slice, the sliced action reads

$$\mathcal{A}^N = \sum_{n=1}^{N+1} \left(\frac{M}{2\rho_n \epsilon_n} (\Delta x_n)^2 + \tfrac{1}{2} M c^2 \epsilon_n \rho_n \right), \tag{6}$$

where $\rho_n \equiv \rho(\lambda_n)$, $\Delta x_n \equiv x_n - x_{n-1}$, and $x_n \equiv x(\lambda_n)$. A path integral $\int (\mathcal{D}^D x / \sqrt{\rho}^D)\, \mathrm{e}^{-\mathcal{A}/\hbar}$ may be defined as the limit $N \to \infty$ of the product of integrals

$$\frac{1}{(\sqrt{2\pi\hbar\epsilon_b \rho_b / M})^D} \prod_{n=1}^{N} \left(\int \frac{\mathrm{d}^D x_n}{(\sqrt{2\pi\hbar\epsilon_n \rho_n / M})^D} \right) \exp\left(-\frac{1}{\hbar} \mathcal{A}^N \right). \tag{7}$$

This can immediately be evaluated, yielding

$$\frac{1}{(\sqrt{2\pi\hbar L / Mc})^D} \exp\left(-\frac{Mc}{2\hbar} \frac{(x_b - x_a)^2}{L} - \frac{Mc}{2\hbar} L \right), \tag{8}$$

where the quantity

$$L \equiv c \sum_{n=1}^{N+1} \epsilon_n \rho_n \tag{9}$$

has the continuum limit

$$L = c \int_{\lambda_a}^{\lambda_b} \mathrm{d}\lambda\, \rho(\lambda). \tag{10}$$

Classically, this is the reparametrization invariant length of a path, as is obvious after inserting (3).

If the amplitude (8) is multiplied by $\frac{1}{2}\lambda_C$, where $\lambda_C = \hbar/Mc$ is the Compton wavelength of the particle, an integral over all positive L yields the correct Klein–Gordon amplitude

$$(x_b|x_a) = \frac{1}{(2\pi)^{D/2}}\left(\frac{Mc}{\hbar\sqrt{x^2}}\right)^{D/2-1} K_{D/2-1}(Mc\sqrt{x^2}/\hbar), \tag{11}$$

where $K_\nu(z)$ is the modified Bessel function.

The result does not depend on the choice of $\rho(\lambda)$, this being a manifestation of the reparametrization invariance. We may therefore write the continuum version of the path integral for the relativistic free particle as

$$(x_b|x_a) = \frac{1}{2}\lambda_C \int_0^\infty \mathrm{d}L \int \mathcal{D}\rho\,\Phi[\rho] \int \frac{\mathcal{D}^D x}{(\sqrt{\rho})^D}\,\mathrm{e}^{-\mathcal{A}}, \tag{12}$$

where $\Phi[\rho]$ denotes a convenient gauge-fixing functional, for instance $\Phi[\rho] = \delta[\rho - 1]$ which fixes $\rho(\lambda)$ to unity everywhere.

To understand the factor $1/(\sqrt{\rho})^D$ in the measure of (12), we make use of the canonical form of the action (2),

$$\mathcal{A}[p,x] = \int_{\lambda_a}^{\lambda_b} \mathrm{d}\lambda\left(-\mathrm{i}px' + \frac{\rho(\lambda)p^2}{2M} + \frac{1}{2}Mc^2\rho(\lambda)\right). \tag{13}$$

After pseudotime slicing, it reads

$$\mathcal{A}^N[p,x] = \sum_{n=1}^{N+1}\left(-\mathrm{i}p_n(x_n - x_{n-1}) + \rho_n\epsilon_n\frac{p_n^2}{2M} + \frac{1}{2}Mc^2\epsilon_n\rho_n\right). \tag{14}$$

At a fixed $\rho(\lambda)$, the path integral then has the usual canonical measure

$$\int \mathcal{D}^D x \int \frac{\mathcal{D}^D p}{(2\pi\hbar)^D}\,\mathrm{e}^{-\mathcal{A}[p,x]/\hbar} \approx \prod_{n=1}^{N}\left(\int \mathrm{d}^D x_n\right)\prod_{n=1}^{N+1}\left(\int \frac{\mathrm{d}^D p_n}{(2\pi\hbar)^D}\right)\mathrm{e}^{-\mathcal{A}^N[p,x]/\hbar}. \tag{15}$$

By integrating out the momenta, we obtain (7) with the action (6).

4. The fixed-energy amplitude is related to (12) by a Laplace transformation,

$$(\boldsymbol{x}_b|\boldsymbol{x}_a)_E \equiv -\mathrm{i}\int_{x_a^0}^\infty \mathrm{d}x_b^0\,\mathrm{e}^{E(x_b^0 - x_a^0)/\hbar}(x_b|x_a), \tag{16}$$

where x^0 denotes the temporal component and $\boldsymbol{x}$ the purely spatial part of the D-dimensional vector x. The poles and cut of $(\boldsymbol{x}_b|\boldsymbol{x}_a)_E$ along the energy axis contain all information on the bound and continuous eigenstates of the system. The fixed-energy amplitude has the path integral representation

$$(\boldsymbol{x}_b|\boldsymbol{x}_a)_E = \int_0^\infty \mathrm{d}L \int \mathcal{D}\rho\,\Phi[\rho] \int \frac{\mathcal{D}^{D-1}\boldsymbol{x}}{(\sqrt{\rho})^{D-1}}\,\mathrm{e}^{-\mathcal{A}_E/\hbar}, \tag{17}$$

with the action

$$\mathcal{A}_E = \int_{\lambda_a}^{\lambda_b} d\lambda \left(\frac{M}{2\rho(\lambda)} x'^2(\lambda) - \rho(\lambda) \frac{E^2}{2Mc^2} + \tfrac{1}{2} Mc^2 \rho(\lambda) \right). \tag{18}$$

This is seen by writing the temporal part of the sliced D-dimensional action (6) in the canonical form (14). By integrating out the temporal coordinates x_n^0 in (15), we obtain N δ-functions. These remove N integrals over the momentum variables p_n^0, leaving only a single integral over a common p^0. The Laplace transform (16), finally, eliminates also this integral, making p^4 equal to $-iE/c$. In the continuum limit, we thus obtain the action (18).

5. The path integral (17) forms the basis for studying relativistic particles in an external time-independent potential $V(\boldsymbol{x})$. This is introduced into the path integral (17) by simply substituting the energy E by $E - V(\boldsymbol{x})$.

For an attractive Coulomb potential in $D - 1 = 3$ spatial dimensions, the above substitution changes the second term in the action (18) to

$$\mathcal{A}_{\rm int} = -\int_{\lambda_a}^{\lambda_b} d\lambda\, \rho(\lambda) \frac{(E + e^2/|\boldsymbol{x}|)^2}{2Mc^2}. \tag{19}$$

The associated path integral is calculated with the help of a Duru–Kleinert transformation [1] as follows.

First, we increase the three-dimensional configuration space in a trivial way by a dummy fourth component x^4 (as in the nonrelativistic case). The additional variable x^4 is eliminated at the end by an integral $\int dx_a^4/|\boldsymbol{x}_a| = \int d\gamma_a$ (see Eqs. (13.114) and (13.121) in Ref. [16]). Then we perform a Kustaanheimo–Stiefel transformation $dx^\mu = 2A(u)^\mu_\nu du^\nu$ (Eq. (13.101) in Ref. [16]). This changes $x'^{\mu 2}$ into $4\vec{u}^2\vec{u}'^2$, with the arrow indicating the four-vector nature of $\vec{u}$. The transformed action reads

$$\mathcal{A}_E = \int_{\lambda_a}^{\lambda_b} d\lambda \left[\frac{4M\vec{u}^2}{2\rho(\lambda)} \vec{u}'^2(\lambda) + \frac{\rho(\lambda)}{2Mc^2\vec{u}^2} \left((M^2c^4 - E^2)\vec{u}^2 - 2Ee^2 - \frac{e^4}{\vec{u}^2} \right) \right]. \tag{20}$$

We now choose the gauge $\rho(\lambda) = 1$, and go from λ to a new parameter s via the time transformation $d\lambda = f\,ds$ with $f = \vec{u}^2$. This leads to the Duru-Kleinert-transformed action

$$\mathcal{A}_E^{\rm DK} = \int_{s_a}^{s_b} ds \left[\frac{4M}{2} \vec{u}'^2(s) + \frac{1}{2Mc^2} \left((M^2c^4 - E^2)\vec{u}^2 - 2Ee^2 - \frac{e^4}{\vec{u}^2} \right) \right]. \tag{21}$$

It describes a particle of mass $\mu = 4M$ moving as a function of the "pseudotime" s in a harmonic oscillator potential of frequency

$$\omega = \frac{1}{2Mc} \sqrt{M^2c^4 - E^2}. \tag{22}$$

The oscillator possesses an additional attractive potential $-e^4/2Mc^2\vec{u}^2$ which is conveniently parametrized in the form of a centrifugal barrier

$$V_{\rm extra} = \hbar^2 \frac{l_{\rm extra}^2}{2\mu\vec{u}^2}, \tag{23}$$

whose squared angular momentum has the negative value

$$l^2_{\rm extra} \equiv -4\alpha^2, \tag{24}$$

where α denotes the fine-structure constant $\alpha \equiv e^2/\hbar c \approx 1/137$. In addition, there is also a trivial constant potential

$$V_{\rm const} = -\frac{E}{Mc^2}e^2. \tag{25}$$

If we ignore, for a moment, the centrifugal barrier $V_{\rm extra}$, the solution of the path integral can immediately be written down (compare Eq. (13.121) in Ref. [16]),

$$(\boldsymbol{x}_b|\boldsymbol{x}_a)_E = -\mathrm{i}\frac{\hbar}{2Mc}\frac{1}{16}\int_0^\infty \mathrm{d}L\, \mathrm{e}^{e^2EL/Mc^2\hbar}\int_0^{4\pi}\mathrm{d}\gamma_a\,(\vec{u}_bL|\vec{u}_a0), \tag{26}$$

where $(\vec{u}_bL|\vec{u}_a0)$ is the time evolution amplitude of the four-dimensional harmonic oscillator.

There are no time-slicing corrections for the same reason as in the three-dimensional case. This is ensured by the affine connection of the Kustaanheimo–Stiefel transformation satisfying

$$\Gamma_\mu{}^{\mu\lambda} = g^{\mu\nu}e_i{}^\lambda\partial_\mu e^i{}_\nu = 0 \tag{27}$$

(see the discussion in Section 13.6 of Ref. [16]).

A γ_a-integration leads to

$$(\boldsymbol{x}_b|\boldsymbol{x}_a)_E = -\mathrm{i}\frac{\hbar}{2Mc}\frac{M\kappa}{\pi\hbar}\int_0^1 \mathrm{d}\varrho\frac{\varrho^{-\nu}}{(1-\varrho)^2}I_0\left(2\kappa\frac{2\sqrt{\varrho}}{1-\varrho}\sqrt{\tfrac{1}{2}(r_br_a+\boldsymbol{x}_b\boldsymbol{x}_a)}\right)\exp\left(-\kappa\frac{1+\varrho}{1-\varrho}(r_b+r_a)\right), \tag{28}$$

with the variable

$$\rho \equiv \mathrm{e}^{-2\omega L} \tag{29}$$

and the parameters

$$\nu = \frac{e^2}{2\omega\hbar}\frac{E}{Mc^2} = \frac{\alpha}{\sqrt{M^2c^4/E^2-1}}, \qquad \kappa = \frac{\mu\omega}{2\hbar} = \frac{1}{\hbar c}\sqrt{M^2c^4-E^2} = \frac{E}{\hbar c}\frac{\alpha}{\nu}. \tag{30}$$

We now use the well-known expansion

$$I_0(z\cos(\tfrac{1}{2}\theta)) = \frac{2}{z}\sum_{l=0}^{\infty}(2l+1)P_l(\cos\theta)I_{2l+1}(z) \tag{31}$$

and obtain the partial wave decomposition

$$(\boldsymbol{x}_b|\boldsymbol{x}_a)_E = \frac{1}{r_br_a}\sum_{l=0}^{\infty}(r_b|r_a)_{E,l}\frac{2l+1}{4\pi}P_l(\cos\theta) = \frac{1}{r_br_a}\sum_{l=0}^{\infty}(r_b|r_a)_{E,l}\sum_{m=-l}^{l}Y_{lm}(\hat{\boldsymbol{x}}_b)Y^*_{lm}(\hat{\boldsymbol{x}}_a), \tag{32}$$

with the usual notation for Legendre polynomials and spherical harmonics. The radial amplitude is, therefore,

$$(r_b|r_a)_{E,l} = -\mathrm{i}\frac{\hbar}{2Mc}\sqrt{r_br_a}\frac{2M}{\hbar}\int_0^\infty \mathrm{d}y\frac{1}{\sinh y}\,\mathrm{e}^{2\nu y}\exp[-\kappa\coth y(r_b+r_a)]\,I_{2l+1}\left(2\kappa\sqrt{r_br_a}\frac{1}{\sinh y}\right). \tag{33}$$

At this place, the additional centrifugal barrier (23) is incorporated via the replacement

$$2l+1 \rightarrow 2\tilde{l}+1 \equiv \sqrt{(2l+1)^2 + l_{\rm extra}^2} \tag{34}$$

(as in Eqs. (8.146) and (14.237) in Ref. [16]). The integration over y yields

$$(r_b|r_a)_{E,l} = -\mathrm{i}\frac{\hbar}{2Mc}\frac{M}{\hbar\kappa}\frac{\Gamma(-\nu+\tilde{l}+1)}{(2\tilde{l}+1)!}W_{\nu,\tilde{l}+1/2}(2\kappa r_b)M_{\nu,\tilde{l}+1/2}(2\kappa r_a) \tag{35}$$

(compare Eq. (9.64) in Ref. [16]; see also p. 139 in Ref. [15]).

This fixed-energy amplitude has poles in the gamma function whenever $\nu-\tilde{l}-1 = 0,1,2,\dots$. They determine the bound-state energies of the Coulomb system. Subsequent formulas can be simplified by introducing the small positive l-dependent parameter

$$\delta_l \equiv l - \tilde{l} = l + \tfrac{1}{2} - \sqrt{(l+\tfrac{1}{2})^2 - \alpha^2} \approx \frac{\alpha^2}{2l+1} + \mathrm{O}(\alpha^4). \tag{36}$$

With this, the pole positions are given by $\nu = \tilde{n}_l \equiv n - \delta_l$, with $n = l+1, l+2, l+3, \dots$, and the bound state energies become

$$E_{nl} = \pm Mc^2\left(1 + \frac{\alpha^2}{(n-\delta_l)^2}\right)^{-1/2} \approx \pm Mc^2\left[1 - \frac{\alpha^2}{2n^2} - \frac{\alpha^4}{n^3}\left(\frac{1}{2l+1} - \frac{3}{8n}\right) + \mathrm{O}(\alpha^6)\right]. \tag{37}$$

Note the appearance of the plus-minus sign as a characteristic property of energies in relativistic quantum mechanics. A correct interpretation of the negative energies as positive energies of antiparticles is straightforward within quantum field theory; it will not be discussed here.

To find the wave functions, we approximate near the poles $\nu \approx \tilde{n}_l$,

$$\Gamma(-\nu+\tilde{l}+1) \approx -\frac{(-1)^{n_r}}{n_r!}\frac{1}{\nu-\tilde{n}_l},$$
$$\frac{1}{\nu-\tilde{n}_l} \approx \frac{2}{\tilde{n}_l}\frac{\hbar^2\kappa^2}{2M}\left(\frac{E}{Mc^2}\right)^2\frac{2Mc^2}{E^2-E_{nl}^2}, \qquad \kappa \approx \frac{E}{Mc^2}\frac{1}{a_H}\frac{1}{\tilde{n}_l}, \tag{38}$$

with the radial quantum number $n_r = n - l - 1$. In analogy with a corresponding nonrelativistic equation (Eq. (13.203) in Ref. [16]), the latter equation can be rewritten as

$$\kappa = \frac{1}{\tilde{a}_H}\frac{1}{\nu}, \tag{39}$$

where

$$\tilde{a}_H \equiv a_H\frac{Mc^2}{E} \tag{40}$$

denotes a modified energy-dependent Bohr radius. Instead of being $1/\alpha \approx 137$ times the Compton wave length of the electron $\hbar/Mc$, the modified Bohr radius which sets the length scale of relativistic bound states involves the energy E instead of the rest energy Mc^2.

With the above parameters, the positive-energy poles in the gamma function can be written as

$$-\mathrm{i}\Gamma(-\nu+\tilde{l}+1)\frac{M}{\hbar\kappa} \approx \frac{(-1)^{n_r}}{\tilde{n}_l^2 n_r!}\frac{1}{\tilde{a}_H}\left(\frac{E}{Mc^2}\right)^2\frac{2Mc^2\mathrm{i}\hbar}{E^2-E_{nl}^2}. \tag{41}$$

Using this behavior and a property of the Whittaker functions (see Eq. (9.80) in Ref. [16]), we write the contribution of the bound states to the spectral representation of the fixed-energy amplitude as

$$(r_b|r_a)_{E,l} = \frac{\hbar}{Mc} \sum_{n=l+1}^{\infty} \left(\frac{E}{Mc^2}\right)^2 \frac{2Mc^2 \mathrm{i}\hbar}{E^2 - E_{nl}^2} R_{nl}(r_b) R_{nl}(r_a) + \dots . \tag{42}$$

A comparison between the pole terms in (35) and (42) renders the radial wave functions

$$R_{nl}(r) = \frac{1}{\tilde{a}_H^{1/2} \tilde{n}_l} \frac{1}{(2\tilde{l}+1)!} \sqrt{\frac{(\tilde{n}_l + \tilde{l})!}{(n-l-1)!}} (2r/\tilde{n}_l \tilde{a}_H)^{\tilde{l}+1} \mathrm{e}^{-r/\tilde{n}_l \tilde{a}_H} M(-n+l+1, 2\tilde{l}+2, 2r/\tilde{n}_l \tilde{a}_H)$$

$$= \frac{1}{\tilde{a}_H^{1/2} \tilde{n}_l} \sqrt{\frac{(n-l-1)!}{(\tilde{n}+\tilde{l})!}} \mathrm{e}^{-r/\tilde{n}\tilde{a}_H} (2r/\tilde{n}_l \tilde{a}_H)^{\tilde{l}+1} L_{\tilde{n}_l - l - 1}^{2\tilde{l}+1} (2r/\tilde{n}_l \tilde{a}_H).$$

The properly normalized total wave functions are

$$\psi_{nlm}(x) = \frac{1}{r} R_{nl}(r) Y_{lm}(\hat{x}). \tag{43}$$

The continuous wave functions are obtained in the same way as in the nonrelativistic case (see Eqs. (13.211)–(13.219) in Ref. [16]).

This concludes the solution of the path integral of the relativistic spinless Coulomb system.

More details on this subject can be found in Chapter 19 of the 2nd edition (1995) of the textbook [16].

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