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Atomic orbitals of the nonrelativistic hydrogen atom in a four-dimensional Riemann space through the path integral formalism

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The Kustaanheimo–Stiefel transformation together with the well-known expansion of the kernel of an isotropic harmonic oscillator is used to generate the atomic orbitals of the nonrelativistic hydrogen atom in a four-dimensional Riemann space through the path integral formalism. Group theoretical implications of the present problem are briefly discussed.

I. INTRODUCTION

Feynman's path integrals[1-4] are known to play an important role in the solution of standard nontrivial quantum-mechanical problems. This procedure was used in the study of the bound states of an electron moving in a spherically symmetric potential, thus making it possible to obtain the phase jumps of $\pi/2$ which occur every time neighboring classical trajectories cross one another.[5] More recently, a straightforward analytical calculation of the s-like wave functions of the hydrogen atom was performed entirely within this formalism, in which the integral transform

$$W = \int d^3 r_b K(r_b, r_a) \tag{1}$$

is calculated by means of an exact summation of a "modified" perturbation expansion.[6] $K(r_b, r_a)$ is the density matrix of the hydrogen atom, written as a path integral ($\hbar = 1$ is used throughout this paper) i.e.,

$$K(r_b, r_a) = \int \mathfrak{D}[r] \exp\left\{ i \int [m\dot{r}^2/2 - V(r)] dt \right\}, \tag{2}$$

where $\mathfrak{D}[r]$ is the usual notation for Feynman's path integral.[3,7] To obtain an expansion for $K(r_b, r_a)$ the exponential function $\exp[-\int_{t_a}^{t_b} V(r) dt]$ has been developed as a power series in the argument.[8] Introducing the Fourier transform of the potential, each term of the series development in Eq. (2) gives a Gaussian path integral, which can be calculated using well-known techniques.[1,7]

Approximate analytic expressions for single electron wave functions of bound states in atoms or simple molecules are provided by the phase-integral approximation, sometimes called the WKB method. In particular, this approximation was applied to the Coulomb potential in momentum space, in which the location of the poles on the negative axis gives the Bohr formula for the bound-state energies, and the residues of the approximate Green's function were shown to yield all the exact wave functions for the bound states of the hydrogen atom.[5]

On the other hand, it is well known that only Gaussian path integrals can easily be computed. The hydrogen atom does not belong to this kind of problem and the calculation of the density matrix involving the Coulomb potential is a formidable task. Nevertheless, this has been carried out with success within Feynman's path integral formalism, in which the eigenvalues of the hydrogen atom are calculated in a closed form by transforming the Coulomb three-dimensional problem into one in four dimensions.[9,10] This procedure is justified as the degeneracy of bound states of the nonrelativistic hydrogen atom is known to be linked with its rotational invariance in four-dimensional Euclidean space. It was recognized that the momentum representation is most convenient for realizing this connection, an approach which has been used to obtain an explicit construction for the Green's function of this problem.[11] More recently, a semiclassical method of evaluating the path integral for the hydrogen atom was proposed,[12] in which the calculation is performed in configuration space with the Langer modification of the angular momentum.[13]

In the present paper, some analytical transformations introduced by Kleinert et al.[9,10] are used in order to transform the nonrelativistic hydrogen atom into a four-dimensional isotropic harmonic oscillator.

We begin, in Sec. II, by considering the details of such transformations, leading to a kernel, residues of which are the product of four one-dimensional harmonic oscillator wave functions. A brief discussion of the unified view of symmetry which emerges in such a treatment is also presented. In Sec. III, the well known expansion of the kernel of an isotropic harmonic oscillator is used to generate the hydrogenic wave functions Ψ_{nlm} as various combinations of the product of one-dimensional oscillator wave functions.

II. THEORY

Among the various procedures leading to an appropriate kernel for the hydrogen atom, that of Kleinert et al.,[9,10] in combination with the Kustaanheimo–Stiefel (KS) transformation,[14] seems to be the most useful one,

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since the algebraic manipulations involved in such a treatment lead to a Feynman's propagator in terms of only oscillator wave functions. We outline in some detail the various steps involved in such transformation.

Feynman's formula[1,3,7] for the Green's function, involving the Coulomb potential, reads

$$K(x_b, t_b; x_a, t_a) = \int_{x_a, t_a}^{x_b, t_b} \mathfrak{D}^3[x]\mathfrak{D}^3[p]/(2\pi)^3$$

$$\times \exp\left[i \int_{t_a}^{t_b} dt\,(p\dot{x} - p^2/2m + e^2/r)\right] , \qquad (3)$$

and is not readily integrable, due to the $1/r$ potential. Kleinert et al.[9] parametrize the paths in terms of a new

auxiliary "time"

$$s(t) = \int^t d\mathcal{T} 1/r(\mathcal{T}) . \qquad (4)$$

With this integral transformation, Eq. (3) can be written as ($' = d/ds$)

$$K(x_b, t_b; x_a, t_a) = \int \mathfrak{D}^3[x]\mathfrak{D}^3[p]/(2\pi)^3$$

$$\times \exp\left\{i \int_{s(t_a)}^{s(t_b)} ds[p(s) \cdot x'(s) - r(s)p^2(s)/2m + e^2]\right\} . \qquad (5)$$

If the connection (4) is enforced via a δ function, the propagator $K(x_b, t_b; x_a, t_a)$ can be cast in the form

$$K(x_b, t_b; x_a, t_a) = \int_{s_a}^{\infty} ds_b\,\delta\left[t_b - t_a - \int_{s_a}^{s_b} ds\,r(s)\right] \exp[ie^2(s_b - s_a)]r_b \int \mathfrak{D}^3[x]\mathfrak{D}^3[p]/(2\pi)^3 \exp\left[i \int_{s_a}^{s_b} ds\,(px' - rp^2/2m)\right] , \qquad (6)$$

$$= \int dE/2\pi \exp[-iE(t_b - t_a)]K(x_b, x_a; E) , \qquad (7)$$

where the energy propagator is given by

$$K(x_b, x_a; E) = \int_{s_a}^{\infty} ds_b \exp[ie^2(s_b - s_a)]r_b \int \mathfrak{D}^3[x]\mathfrak{D}^3[p]/(2\pi)^3 \exp\left[i \int_{s_a}^{s_b} ds\,(px' - rp^2/2m + Er)\right] \qquad (8)$$

and use has been made of the Fourier decomposition of the δ function.

Expression (7) may be multiplied, without changing it, by a dummy path integral involving a new, completely arbitrary pair of canonical coordinates x_4, p_4:

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

$$= \int dp_4/(2\pi) \int_{-\infty}^{\infty} d(x_4)_b \exp\{i[(x_4)_b - (x_4)_a]p_4\} \exp\left[-ip_4^2/2m \int_{s_a}^{s_b} ds\,r(s)\right] = 1 , \qquad (9)$$

where the last part of the equation arises, of course, from the integral properties of the δ function. This identity holds for any function $r(s)$, in particular for $r(s) = [x(s)^2]^{1/2}$. This choice brings the path integral in Eq. (8) to the four-dimensional form

$$\int_{-\infty}^{\infty} d(x_4)_b \int \mathfrak{D}^4[x]\mathfrak{D}^4[p]/(2\pi)^4$$

$$\times \exp\left[i \int_{s_a}^{s_b} ds\,(px' - rp^2/2m + Er)\right] . \qquad (10)$$

On introducing a fourth coordinate and momentum components, it is possible to get six generators of the angular momentum L_{ij} $(i, j = 1, 2, 3, 4)$. These six generators L_{ij} obey the same commutation relations as (L_x, L_y, L_z), and therefore constitute the generalization of the three generators L from three to four dimensions. The group that they generate can be shown to be the proper rotation group in four dimensions $O(4)$.[15] This evidently does not represent a geometrical symmetry[16] of the hydrogen atom, since the fourth components x_4 and p_4 are fictitious and cannot be identified with dynamical variables.[17,18] It turns out that the constants of the motion of the hydrogen atom in this space (a particular subspace of the Hilbert space) are the angular momentum L and M, where

$$M = (2\mu')^{-1}(p \times L - L \times p) - k\hat{r} \qquad (11)$$

is the Runge–Lenz–Pauli vector.[19] $\hat{r}$ stands for $r/|r|$; μ' is the reduced mass, and k denotes the strength of the potential. These operators satisfy the commutation relations of the Lie algebra that correspond to a symmetry transformation of the $O(4)$ group.

We now turn to the energy propagator, introducing a canonical change of variables through the K–S transformation[14] from (x, p) to (u, p_u), such that

$$r = u^2 = [x^2(s)]^{1/2} , \qquad (12)$$

and construct a map from R^4 into physical space R^3. Let $u_1, \ldots, u_n \in R^n$ be Cartesian coordinates. Then, one can generate an $n \times n$ linear orthonormal matrix A with the norm of each row $\| \cdot \| = u_1^2 + \cdots + u_n^2$ for $n = 1, 2, 4, 8$.[20] Particularly, in R^4

$$A(u) = \begin{pmatrix} u_3 & u_4 & u_1 & u_2 \\ -u_2 & -u_1 & u_4 & u_3 \\ -u_1 & u_2 & u_3 & -u_4 \\ u_4 & -u_3 & u_2 & -u_1 \end{pmatrix} . \qquad (13)$$

The space R^4 is mapped onto $R^3 \ni (x_1, x_2, x_3)$ by A with the annihilation condition

$$dx_4 = 2(u_4\,du_1 - u_3\,du_2 + u_2\,du_3 - u_1\,du_4) = 0 \ , \qquad (14)$$

thus showing explicitly that x_4 is a cyclic coordinate of the system.

The matrix transformation $x - A(u)\ u = 0$ becomes

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = A(u) \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} = \begin{pmatrix} 2(u_1 u_3 + u_2 u_4) \\ 2(-u_1 u_2 + u_3 u_4) \\ -u_1^2 + u_2^2 + u_3^2 - u_4^2 \\ 0 \end{pmatrix} \ . \qquad (15)$$

In momentum space, $p = (p_1, p_2, p_3) \in R^3$ and $p_u \in R^4$

$$\begin{pmatrix} p_1 \\ p_2 \\ p_3 \\ p_4 \end{pmatrix} = (2|r|)^{-1} A(u) \begin{pmatrix} (p_u)_1 \\ (p_u)_2 \\ (p_u)_3 \\ (p_u)_4 \end{pmatrix}$$

$$= (2|r|)^{-1} \begin{pmatrix} u_3(p_u)_1 + u_4(p_u)_2 + u_1(p_u)_3 + u_2(p_u)_4 \\ -u_2(p_u)_1 - u_1(p_u)_2 + u_4(p_u)_3 + u_3(p_u)_4 \\ -u_1(p_u)_1 + u_2(p_u)_2 + u_3(p_u)_3 - u_4(p_u)_4 \\ 0 \end{pmatrix} \ . \qquad (16)$$

That is, p_4 is a constant of the motion. From Eqs. (12) and (16), the Laplacian operator in this particular four-dimensional Riemann subspace becomes

$$4rp^2 = p_u^2 \equiv -\nabla_4^2 \ , \qquad (17)$$

an equation which will be useful to express the energy propagator $K(x_b, x_a ; E)$ in the (u, p_u) space. To this end, we first apply the definition of Feynman integral to the four-dimensional form of the path integral (10):

$$\int \mathfrak{D}^4[x] \mathfrak{D}^4[p]/(2\pi)^4 \exp\left[i \int_{s_a}^{s_b} ds\,(px' - rp^2/2m + Er)\right]$$

$$= \lim_{\substack{n \to \infty \\ \epsilon \to 0}} \int \cdots \int \prod_{j=1}^{4}\left[\prod_{i=1}^{n} dx_i^j \prod_{i=1}^{n+1} dp_i^j/(2\pi)^4\right] \exp\left\{i \sum_{i=1}^{n+1}[p_i(x_i - x_{i-1}) - \epsilon rp_i^2/2m + \epsilon Er]\right\} \ , \qquad (18)$$

where

$$\epsilon = s_i - s_{i-1}\ , \qquad x_0 = x_a\ ;\ x_{n+1} = x_b\ , \qquad s_0 = s_a\ ;\ s_{n+1} = s_b\ . \qquad (19)$$

Introducing the K–S transformation [Eqs. (12), (15), and (16)], the "measure"[21] of the Feynman integral in the (u, p_u) space becomes

$$\prod_{j=1}^{4}\left[\prod_{i=1}^{n} dx_i^j \prod_{i=1}^{n+1} dp_i^j/(2\pi)^4\right] = \prod_{j=1}^{4}\left[\prod_{i=1}^{n} du_i^j\,d(p_u)_i^j/(2\pi)^4 J(x/u)J(p/p_u)\right] 1/16r_b^2 \ , \qquad (20)$$

where $J(x/u)$ and $J(p/p_u)$ are the Jacobians in coordinate and momentum space, respectively, of the linear transformations (15) and (16),

$$J(x/u) = 16r^2 \ , \quad \text{in } r \text{ space} \ , \qquad (21)$$

$$J(p/p_u) = (16r^2)^{-1} \ , \quad \text{in } p \text{ space} \ . \qquad (22)$$

In Eq. (20), the occurrence of the multiplicative factor $1/16r_b^2$ is due to the fact that there exists one more momentum integration (i.e., dp_{n+1}^j), i.e., the measure is not invariant under the point canonical transformations.

Using these results, together with Eqs. (12) and (17), the path integral (10) is transformed in

$$1/16r_b \int_{-\infty}^{\infty} d(x_4)_b/r_b \int_{x_a,(x_4)_a}^{x_b,(x_4)_b} \mathfrak{D}^4[u]\mathfrak{D}^4[p_u]/(2\pi)^4 \exp\left[i \int_{s_a}^{s_b} ds\,(p_u u' - p_u^2/2\mu - 1/2\,\mu\omega^2 u^2)\right] \ , \qquad (23)$$

where $\mu = 4m$ and $\omega^2 = -E/2m$ and is recognized, apart from the integral over $d(x_4)_b/r_b$, to be the Green's function of an isotropic harmonic oscillator in four dimensions.

We now express the K–S transformation [Eq. (12)] in polar coordinates through an auxiliary angle α in the form

$$u = r^{1/2} \begin{pmatrix} \sin 1/2\,\theta \cos 1/2\,(\alpha + \varphi) \\ \sin 1/2\,\theta \sin 1/2\,(\alpha + \varphi) \\ \cos 1/2\,\theta \cos 1/2\,(\alpha - \varphi) \\ \cos 1/2\,\theta \sin 1/2\,(\alpha - \varphi) \end{pmatrix} \ , \qquad (24)$$

where α is the cyclic variable in polar coordinates.

The first integral in the expression (23) is an average over r_b with respect to the continuous variable x_4. On performing the transformation (24), we discretize integrating over a cycle $(0-4\pi)$, and increase the upper limit of the integration path in $\pm 4n\pi$. Since the end points are homotopically equivalent, the integral can be decomposed into a sum over periodically shifted end point values of the angle α_b and an integral over one period. That is

$$\int_{-\infty}^{\infty} d(x_4)_b/r_b = \int_0^{4\pi} d\alpha_b \sum_{\alpha_b - \alpha_b + 4n\pi} \quad (n = \pm 1, \pm 2, \pm 3, \dots)$$

$$= \int_0^{-4\pi} d\alpha_b + \int_0^{-8\pi} d\alpha_b + \cdots + \int_0^{-4j\pi} d\alpha_b + \cdots + \int_0^{4\pi} d\alpha_b + \int_0^{8\pi} d\alpha_b + \cdots + \int_0^{4j\pi} d\alpha_b + \cdots \, . \tag{25}$$

Each of the integrals (25) indicate the different paths contributing to the propagator from a fixed point in R^4. The sum is part of the Green's function of the harmonic oscillator (as always if cyclic variables are used).[22] Thus, Eq. (23) can be written as

$$1/16r_b \int_0^{4\pi} d\alpha_b [\mu\omega/(2\pi i \sin \omega T)]^2 \exp\{-\pi[\mu\omega/(2\pi i \sin \omega T)][(u_a^2 + u_b^2)\cos \omega T - 2u_a u_b]\} \, , \tag{26}$$

where $s_b - s_a = T$, and

$$[\mu\omega/(2\pi i \sin \omega T)]^{1/2} \exp\{i\mu\omega/(2 \sin \omega T)[(u_a^2 + u_b^2)\cos \omega T - 2u_a u_b]\} \tag{27}$$

is the kernel of an isotropic harmonic oscillator in R^4.

In order to relate the propagator $K(x_b, x_a; E)$ [Eq. (8)] with the harmonic oscillator wave functions, we perform the spectral decomposition of the integrand of Eq. (26) and symmetrize it in u_b (since $\alpha_b - \alpha_b + 2\pi$ corresponds to $u_b - -u_b$) and expand, for $E < 0$, as

$$[\mu\omega/(2\pi i \sin \omega T)]^2 \exp\{-\pi[\mu\omega/(2\pi i \sin \omega T)][(u_a^2 + u_b^2)\cos \omega T - 2u_a u_b]\} = \sum_{n_i = 0}^{\infty} \exp\left[-i\omega\left(\sum_{i=1}^4 n_i + 2\right)T\right] \Phi_{n_1 n_2 n_3 n_4}(u_b)\Phi^*_{n_1 n_2 n_3 n_4}(u_a) \, , \tag{28}$$

where

$$\Phi_{n_1 n_2 n_3 n_4}(u) = \prod_{i=1}^4 \phi_{n_i}(u_i) \tag{29}$$

being the $\phi_{n_i}(u_i)$ $(i = 1, 2, 3, 4)$, the one-dimensional harmonic oscillator wave functions, i.e., they constitute the basis functions in a four-dimensional Riemann space. The n_i are subjected to the constraint

$$\sum_{i=1}^4 n_i = 2(n-1) = 0, 2, 4, \dots \, . \tag{30}$$

Finally, inserting Eq. (28) in the propagator (8), after a straightforward algebra, we are led to

$$K(x_b, x_a; E) = -m/p_0^2 \sum_{n=0}^{\infty} i(1 - \nu/n)^{-1} \int_0^{2\pi} d\alpha_b$$
$$\times [(p_0/8n)^{1/2}\Phi_{n_1 n_2 n_3 n_4}(u_b)][(p_0/8n)^{1/2}\Phi^*_{n_1 n_2 n_3 n_4}(u_a)], \tag{31}$$

where the variables ν and p_0 stand short for $\nu = e^2/2\omega = (-me^4/2E)^{1/2}$ and $p_0 = (-2mE)^{1/2}$. The sum in Eq. (31) displays explicitly the bound states poles at

$$E_n = -me^4/2n^2 \, , \quad n = 1, 2, 3, \dots \, , \tag{32}$$

with the residues being the wave functions in unconventional quantum numbers. In this connection, it should be pointed out that it is rather remarkable that almost all quantum numbers can be interpreted as invariants of certain groups. In fact, the K–S transformation is closely connected to the $SU(2) \otimes SU(2)$ symmetry of the Kepler motion which exhibits the dynamical symmetry $SO(4)$. Clearly, there is a nice isomorphism between the two groups.[23]

In the three-dimensional space, the Schrödinger equation for the hydrogen atom is separable in spherical polar and parabolic coordinates. While its separability in the former is related to the spherical symmetry of the central Coulomb potential, its separability in the latter is attributed to the "hidden" symmetry which is responsible for the degeneracy peculiar to the potential. In what follows, we show that the expansion of the kernel (27) makes it possible to express the hydrogen atom wave functions in the above mentioned four-dimensional Riemann space.

III. ATOMIC ORBITALS OF THE HYDROGENIC OSCILLATOR

We will use the four-dimensional results of Sec. II to evaluate the atomic orbitals of the nonrelativistic hydrogen atom. This will be performed through the residues of the first order poles of the propagator (31). To this end, use of the K–S transformation will be made. In particular, this transformation with u given by Eq. (24) makes it possible to reduce the dynamical symmetry of the hydrogen atom described by the $O(4)$ generators to the geometrical symmetry of $O(3)$.[18,20,24-26] In order to proceed, the kernel describing the motion of an isotropic harmonic oscillator is expanded in exponential functions of time multiplied by products of energy eigenfunctions:[3]

$$[\mu\omega/(2\pi i \sin \omega T)]^{1/2} \exp\{i\mu\omega/(2 \sin \omega T)[(u_a^2 + u_b^2)\cos \omega T$$

$$- 2u_a u_b]\} = \sum_{j=0}^{\infty} \exp(-iE_j T)\phi_j(u_b)\phi_j^*(u_a) \, . \tag{33}$$

On expanding the left-hand side of this equation in successive powers of $\exp(i\omega T)$, the different one-dimensional oscillators eigenfunctions can be obtained. Since the residues of Eq. (31) contain the basic functions in a four-dimensional Riemann space, we cite some of them. On going as far as $j = 2$, the following is obtained (see the Appendix):

$$\phi_0(u_i) = (\mu\omega/\pi)^{1/4} \exp[-(\mu\omega/2)u_i^2] \, , \tag{34.1}$$

$$\phi_1(u_i) = (2\mu\omega)^{1/2}u_i\,\phi_0(u_i) \, , \tag{34.2}$$

$$\phi_2(u_i) = 2^{-1/2}(1 - 2\mu\omega u_i^2)\phi_0(u_i) \, . \tag{34.3}$$

Taking into account Eq. (30), it can easily be seen that when $n=1$, the only combination of the n_i is $n_i = 0$. Taking the residue of the propagator (31), the wave function of the lowest energy level of the hydrogen atom is

$$\Psi_{100} = (2\pi)^{1/2}(p_0/8)^{1/2}\Phi_{0000} . \tag{35.1}$$

When $n=2$, there exist different combinations of the n_i obeying constraint (30), so that the hydrogenic wave functions Ψ_{nlm} can be expressed as various combinations of the functions $\Phi_{n_1n_2n_3n_4}(u)$ given in Eq. (29). The first few cases are given below:

$$\Psi_{200} = (2\pi)^{1/2}(p_0/16)^{1/2}(\Phi_{2000} + \Phi_{0200} + \Phi_{0020} + \Phi_{0002}) , \tag{35.2}$$

$$\Psi_{211} = (2\pi)^{1/2}(p_0/16)^{1/2}(\Phi_{1010} + \Phi_{0101}) , \tag{35.3}$$

$$\Psi_{210} = (2\pi)^{1/2}(p_0/16)^{1/2}(\Phi_{0110} - \Phi_{1001}) , \tag{35.4}$$

$$\Psi_{21-1} = (2\pi)^{1/2}(p_0/16)^{1/2}(\Phi_{2000} + \Phi_{0200} - \Phi_{0020} - \Phi_{0002}) . \tag{35.5}$$

Similar results have been obtained by Chen[24] in the study of the Stark effect of the hydrogen atom. On using Eqs. (34) together with the K–S transformation as given by Eq. (24), the different hydrogenic atomic orbitals are easily generated.

It should be pointed out that on using the $SO(2,1)$ algebra generators and through the study of the N-dimensional Schrödinger equation, the equivalence between the hydrogen atom and the isotropic harmonic oscillator was established.[27] Finally, it was recently reported that the realization of a stereographic projection of the coordinates of an isotropic four-dimensional harmonic oscillator on two orthogonal unit hyperboloids in a six-dimensional space is a new form of geometrizing the Coulomb field, that is, the homomorphism between $SO(4,2)$ and $SU(4,2)$ was explicitly demonstrated.[28]

IV. CONCLUSIONS

The K–S transformation [Eqs. (12), (15), and (16)], together with the expansion of the kernel of an isotropic harmonic oscillator, has been used to get the atomic orbitals of the nonrelativistic hydrogen atom in a four-dimensional Riemann space through the path integral formalism. From an analytical expression for the propagator of the hydrogen atom, not only the energy spectrum was recovered, but, also, the hydrogenic wave functions as a linear combination of the isotropic harmonic oscillator wave functions were obtained. The

transformation (12) has also been used to solve the hydrogen atom confined into a sphere,[29] and in fact, this seems to be particularly suitable to algebraically generalize the equivalence between this system and the isotropic harmonic oscillator to any N.[27,30,31] The present approach, clearly connected with the calculation of non-Gaussian path integrals, seems to be mathematically more elegant and shows the necessary ductility to undertake the study of simple (but not trivial) confined standard quantum systems.[26,32-35] It could probably provide more insight in connection with astrophysics and hot plasmas.

APPENDIX

In this Appendix, we show that an appropriate expansion of the kernel (27) leads to the different harmonic oscillator eigenfunctions.

Using the relations

$$i \sin \omega T = \tfrac{1}{2} \exp(i\omega T)[1 - \exp(-2i\omega T)] ,$$
$$\cos \omega T = \tfrac{1}{2} \exp(i\omega T)[1 + \exp(-2i\omega T)] , \tag{A1}$$

we can write the left-hand side of Eq. (33) as

$$(\mu\omega/\pi)^{1/2} \exp(-i\omega T/2)[1 - \exp(-2i\omega T)]^{-1/2} \exp\left\{-\mu\omega/2\right.$$

$$\times \left[(u_a^2 + u_b^2)\left(\frac{1+\exp(-2i\omega T)}{1-\exp(-2i\omega T)}\right) - \frac{4u_a u_b \exp(-i\omega T)}{1 - \exp(-2i\omega T)}\right]\right\} . \tag{A2}$$

Following Feynman,[3] we can obtain a series having the form of the right-hand side of Eq. (33) if we expand Eq. (A2) in successive powers of $\exp(-i\omega T)$. We shall illustrate the method by going only as far as $j=2$ in Eq. (33). Expanding the left-hand side of Eq. (33) to this order, we have

$$(\mu\omega/\pi)^{1/2} \exp(-i\omega T/2)(1 + \tfrac{1}{2}\exp(-2i\omega T) + \cdots) \exp(-\mu\omega/2\{(u_a^2 + u_b^2)[1 + 2\exp(-2i\omega T) + \cdots] - 4u_a u_b \exp(-i\omega T) + \cdots\}), \tag{A3}$$

which, upon rearrangement, leads to

$$(\mu\omega/\pi)^{1/2} \exp[-\mu\omega/2(u_a^2 + u_b^2)] \exp(-i\omega T/2)[1 + \tfrac{1}{2}\exp(-2i\omega T) + \cdots]$$

$$\times \exp\{-\mu\omega/2[2(u_a^2 + u_b^2)\exp(-2i\omega T) - 4u_a u_b \exp(-i\omega T) + \cdots]\} , \tag{A4}$$

or

$$(\mu\omega/\pi)^{1/2} \exp[-\mu\omega/2(u_a^2 + u_b^2)] \exp(-i\omega T/2)[1 + \tfrac{1}{2}\exp(-2i\omega T)]$$

$$\times [1 + 2\mu\omega\, u_a u_b \exp(-i\omega T) + 2\mu^2\omega^2\, u_a^2 u_b^2 \exp(-2i\omega T) - \mu\omega(u_a^2 + u_b^2)\exp(-2i\omega T) + \cdots] . \tag{A5}$$

From this, we can pick out the coefficient of the lowest term. It is

$$(\mu\omega/\pi)^{1/2}\exp[-\mu\omega/2(u_a^2 + u_b^2)]\exp(-i\omega T/2)$$

$$= \exp(-iE_0 T)\phi_0(u_a)\phi_0^*(u_b) \ . \tag{A6}$$

That is, $E_0 = \omega/2$ and

$$\phi_0(u_i) = (\mu\omega/\pi)^{1/4}\exp(-\mu\omega u_i^2/2) \ . \tag{A7}$$

The next-order term in the expansion is

$$(\mu\omega/\pi)^{1/2}\exp(-i\omega T/2)\exp(-i\omega T)\exp[-\mu\omega/2(u_a^2 + u_b^2)]$$

$$\times 2\mu\omega\, u_a u_b = \exp(-iE_1 T)\phi_1(u_b)\phi_1^*(u_a) \ , \tag{A8}$$

which implies that $E_1 = 3/2\,\omega$, and

$$\phi_1(u_i) = (2\mu\omega)^{1/2}u_i\,\phi_0(u_i) \ . \tag{A9}$$

The next term corresponds to $E_2 = 5/2\,\omega$. The part of the term depending on u_a and u_b is

$$(\mu\omega/\pi)^{1/2}\exp[-\mu\omega/2(u_a^2 + u_b^2)]$$

$$\times[\tfrac{1}{2} + 2\mu^2\omega^2 u_a^2 u_b^2 - \mu\omega(u_a^2 + u_b^2)] \ . \tag{A10}$$

This must be the same as $\phi_2(u_b)\phi_2^*(u_a)$. Since the expression in the brackets can be written as

$$\tfrac{1}{2}(2\mu\omega u_a^2 - 1)(2\mu\omega u_b^2 - 1) \ , \tag{A11}$$

we find

$$\phi_2(u_i) = 2^{-1/2}(2\mu\omega u_i^2 - 1)\phi_0(u_i) \ . \tag{A12}$$

All of the wave functions may be obtained in this manner. However, it is a difficult algebraic problem to get the general form for ϕ_n directly from this expansion. Further details can be found in Feynman's book.[3]

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