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Bound states in a Yukawa potential: A Sturmian group-theoretical approach

J. P. Gazeau and A. Maquet

Laboratoire de Chimie Physique, Université Pierre et Marie Curie, 11, rue Pierre et Marie Curie, F-74231 Paris Cedex 05, France*

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The Schrödinger eigenvalue problem for a Yukawa potential is reexamined from a group-theoretical perspective. By using the Fock transformation, the Schrödinger operator is transformed into a compact or "inverse Sturmian" operator which is a linear superposition of local representation operators of SL(2,R). It may be approximated by finite-rank techniques, which provide a very useful method for obtaining accurate numerical results.

I. INTRODUCTION

The resolution of the Schrödinger equation for a particle bound in a Yukawa or static screened Coulomb potential has received considerable attention since the early days of quantum mechanics on account of its widespread range of applications.

The spherically symmetric Yukawa potential

$$V(r) = -ge^{-\mu r}/r \tag{1}$$

arises naturally as the position-space version of the solution of the Klein-Gordon equation for a static meson field.[1,2] The first attempts to solve the corresponding eigenvalue equation were inspired in particular by the deuteron problem.[1-5]

This potential is also of importance in plasma physics where it is known as the Debye-Hückel potential.[6-10] It accounts for the shielding by outer charges of the Coulomb field experienced by an atomic electron in a hydrogen plasma. The ensuing "drowning" of higher excited levels into the continuum corresponds to a limitation of the number of bound states, a fact of great importance in the calculation of electronic partition functions in plasmas.[6,11-13] In a similar way, as an approximate version of the Thomas-Fermi potential, it is also of interest in the calculation of the energy levels of impurity centers in doped semiconductors.[14,15]

In addition to these obvious physical applications, this potential, together with Hulthen's and the exponential potential, plays an important role as a good test case in potential scattering studies. In that respect abundant literature should be mentioned especially in relation with the use of functional analysis methods. For instance, the fact that the corresponding symmetrized kernels in the Lippmann-Schwinger equation are square-integrable gave rise to a number of important works. Some sources and general papers are quoted in Ref. 16. Also see Ref. 17 for papers dealing more specifically with the Yukawa potential.

Various approaches were proposed in order to approximately solve the eigenvalue problem associated with the corresponding Schrödinger equation

$$[-(\hbar^2/2m)\Delta - ge^{-\mu r}/r]\psi(\vec{r}) = E\psi(\vec{r}). \tag{2}$$

The more popular ones were as expected, the variational[5,7,8,14,15,18-20] and the perturbative[7-9,18] techniques. Very accurate results were also obtained by direct numerical integration of Eq. (2).[11,12,21-23] Regge trajectories were determined in that way[24] or by using continued-fraction expansions.[13,25]

For large values of the coupling constant g, the eigensolutions of Eq. (2) may be assumed to be expandable in a series of ascending powers of $1/g$.[26-29] An alternative method consists in expanding the screened potential itself in a power series in λr, where λ is a characteristic screening parameter.[30] A common feature of these methods is that they conveniently lend themselves to a perturbative analysis leading to accurate numerical determinations of the solutions.

We should also mention the quasiclassical approach[21,22] used in particular by Totsuji[10] in order to determine the (n,l) dependent critical screening radius $D_C(n,l) = 1/\mu_c(n,l)$ for which value the corresponding bound state (n,l) disappears.

Analytical methods for solving differential equation (2) has been investigated especially by Ecker and Weizel[6] who obtained approximate solutions valid for small values of the screening parameter μ. It is only recently that a general analytical solution of this equation has been given by expressing the standard solutions in terms of double contour integral representations.[31] It should be noted, however, that this latter result remains rather intricate and not so easy to use for practical purposes.

More global algebraic approaches based on the symmetry properties of Eq. (2) have been also investigated.[32,33] In particular, matrix elements of the Yukawa potential in an hydrogenic basis were evaluated in that way.[34,35]

Curiously enough the above-mentioned papers are quasiexclusively dedicated to the study of Eq. (2) as it stands in the position space, although the Yukawa potential accounts primarily for the static meson potential which is more naturally defined in momentum space. For instance, it should be noted that this latter representation makes clear the structure of the exchange propagator. The advantages encountered on using the momentum-space version of Eq. (2) have been clearly recognized in a celebrated paper by Levy,[36] but this recommendation did not receive much attention, at least for Yukawa-potential studies; see, however, the paper by Enflo[37] and references therein.

In some sense our work was inspired by these reflexions. Our feeling was reinforced by the well-known fact that it is by solving the integral Schrödinger equation in momentum space for the H atom, that Fock[38] removed the so-called "accidental degeneracy" of the energy levels, related to the $O(4)$ symmetry of the Coulomb potential. It should be emphasized, however, that this elegant demonstration was made possible because Fock implicitely solved the eigenvalue problem first for the dimensionless Coulomb "Sturmian" operator.[39-42] This "Sturmian" process consists of quantizing the coupling constant g for a given value of the energy E considered as a parameter.[39,40] More precisely, after introducing the momentum-like quantity $p_0=(-2mE)^{1/2}$ $(E<0)$ one quantizes the dimensionless ratio: $\nu=mg/(\hbar p_0)$.

In this paper we extend to the Yukawa potential the Fock method initially set up for the pure Coulomb case. By the way we show that this approach provides a more synthetic insight to the general determination of the spectrum and eigenfunctions in Eq. (2). It should be stressed that this method applies equally well to other types of potential of physical interest.[42]

In Sec. II the eigenvalue problem for the Schrödinger operator equation (2) is transformed by the means of a Fourier-Fock transformation,[41] in the eigenvalue problem for the associated "Inverse" Sturmian operator denoted Σ:

$$(I-\nu\Sigma)\phi=0\,. \tag{3}$$

It should be noted that Σ, which acts on the Hilbert space $L_c^2(S^3)$ of the square-integrable functions $\phi(\xi)$, $\xi\in S^3\approx \mathrm{SU}(2)$, corresponds merely to the usual operator $(E-H_0)^{-1}V$. In Sec. II we also make explicit the algebraic structure of Σ, by establishing that it may be considered as a linear superposition of representation operators of $SL(2,R)$.

Section III is devoted to a brief exposition of the properties of the operator Σ in a functional analysis perspective. These properties afford to approximate Σ by finite rank operators in an orthonormal basis on $L_c^2[\mathrm{SU}(2)]$.

A numerical exploitation of the preceding results is presented in Sec. IV. As a natural basis we choose the Coulomb Sturmian, the corresponding matrix elements being already known. The computation of the eigenvalues of Σ, Eq. (3), and consequently of the Schrödinger operator, Eq. (2), is then reduced to standard matrix calculus. As we shall show the method compares very favorably to more-sophisticated and time-consuming numerical techniques. For instance, even for the simplest two-state Sturmian basis one may obtain eigenenergy values accurate to within a few parts in one thousand for typical magnitudes of the strength and screening of the potential.

II. APPROACH TO THE SCHRÖDINGER PROBLEM VIA THE FOCK METHOD

A. Fock transformation and Sturmian operator

The Fourier transform of the Schrödinger equation, Eq. (2), is written

$$(p^2/2m-E)\psi(\vec{p})=\hat{V}\Psi(\vec{p})\,, \tag{4}$$

with

$$\hat{V}\Psi(\vec{p})=\frac{g}{2\pi^2\hbar}\int d\vec{p}\,'\,\Psi(\vec{p}\,')[|\vec{p}-\vec{p}\,'|^2+\mu^2\hbar^2]^{-1}\,. \tag{4$'$}$$

For a fixed value of $p_0=(-2mE)^{1/2}$; $E<0$, the Fock transformation $\mathfrak{F}_{p_0}$ may be considered as a two-step operation, i.e., a change of variable and the introduction of a multiplicative weight.

1. Change of variable (p_0 fixed)

The change of variable[38]

$$\vec{\xi}=2p_0\vec{p}/(p_0^2+p^2)\,,\quad \xi_0=(p_0^2-p^2)/(p_0^2+p^2)\,, \tag{5}$$

establishes a one-to-one correspondance between a point $\xi=(\xi_0,\vec{\xi})$ of the unit hypersphere S^3 in R^4,

$$\xi^2+\xi_0^2=1\,,$$

and its stereographic projection onto the hyper-

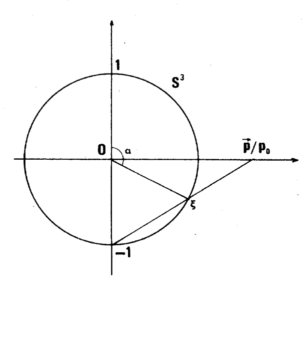

FIG. 1. South-pole Fock-stereographic projection of the hypersphere S^3 onto the hyperplane $\vec{p}/p_0$; $\xi=(\xi_0,\vec{\xi})$; $\xi_0=\cos\alpha$; $\vec{\xi}=(\xi_1,\xi_2,\xi_3)$.

plane $\vec{p}/p_0$; see Fig. 1.

The surface element $d\mu(\xi)$ on the hypersphere S^3 is related to the volume element $d\vec{p}$ in momentum space by

$$d\mu(\xi) = (|1+\xi|^2/2p_0)^3 d\vec{p}\,, \quad 1 \equiv (1, \vec{0})\,, \tag{6}$$

where $|\ |$ denotes the modulus of a quadrivector.

The distance $(|\vec{p}-\vec{p}'|^2 + \mu^2\hbar^2)$ may be transformed accordingly and after some lengthy calculations one would obtain

$$(|\vec{p}-\vec{p}'|^2+\mu^2\hbar^2) = [(p_0^2+p^2)(p_0+p'^2)/4p_0^2] \times (\beta^2|1+\xi|^2|1+\xi'|^2 + |\xi-\xi'|^2)\,, \tag{7}$$

where the dimensionless quantity β is $\beta = \mu\hbar/(2p_0)$. It should be noted that the structure of this expression is somewhat intricated: for instance, we cannot in this way get a separable form of the Yukawaian kernel. We shall give additional insights into that problem by reexamining it in a group-theoretical perspective in Sec. II B. In the pure Coulomb case ($\beta = 0$) expression (7) contains merely the Euclidean distance $|\xi - \xi'|$ between two points on S^3. As a consequence, the Coulomb Schrödinger equation, obtained from Eq. (4) by replacing $\mu = 0$, may be transformed in the $O(4)$ invariant integral equation for the four-dimensional spherical harmonics. This goal is achieved by introducing a multiplicative weight. The same procedure will be used in the Yukawa case as detailed in the following.

2. *Introduction of a multiplicative weight*

$$\phi = \mathfrak{F}_{p_0}\Psi\,, \quad \phi(\xi) = 4p_0^{3/2}|1+\xi|^{-4}\Psi(\vec{p})\,, \tag{8}$$

where $\Psi \in L_C^2(R^3)$ and $\phi \in L_C^2(S^3)$. This relation establishes the Fock correspondence between the Hilbert spaces $L_C^2(R^3)$ and $L_C^2(S^3)$. Reciprocally one has

$$\Psi = \mathfrak{F}_{p_0}^{-1}\phi\,, \quad \Psi(\vec{p}) = 4p_0^{5/2}(p_0^2+p^2)^{-2}\phi(\xi)\,. \tag{8$'$}$$

Accordingly the respective scalar products are related by

$$(\Psi_1, \Psi_2)_{L_C^2(R^3)} = \int_{R^3} d\vec{p}\, \Psi_1(\vec{p})\Psi_2^*(\vec{p}) = \tfrac{1}{2}(|1+\xi|^2\phi_1, \phi_2)\,, \tag{9}$$

and conversely by

$$(\phi_1, \phi_2)_{L_C^2(S^3)} = \int_{S^3} d\mu(\xi)\phi_1(\xi)\phi_2^*(\xi) = \tfrac{1}{2}p_0^{-2}((p_0^2+p^2)\Psi_1, \Psi_2)\,. \tag{9$'$}$$

It should be pointed out that the multiplicative weights appearing in Eqs. (8) and (9) are usually justified, in the pure Coulomb potential case, by using the virial theorem which may be formulated as follows[38]:

$$E(\Psi, \Psi) = -(p^2/2m\Psi, \Psi)\,. \tag{10}$$

However, the higher-symmetry properties of the Coulomb problem should not hide the fact that formulas (8) and (9) imply a more-general statement according to which the Fock transformation $\mathfrak{F}_{p_0}$ is meaningful only if one has

$$\|(p_0^2+p^2)^{1/2}\Psi\|^2_{L_C^2(R^3)} \equiv ((p_0^2+p^2)\Psi, \Psi)_{L_C^2(R^3)} < \infty\,, \tag{10$'$}$$

i.e., if Ψ belongs to the domain of the quadratic form defined by the operator $(p_0^2+p^2)$. This condition is closely connected to the fact that, in position space, the Fourier transform of Ψ *must* belong to the domain of the Laplace operator p^2. Since this domain represents the natural framework of quantum mechanics for interacting particles, these properties certainly deserve a deeper investigation resorting to the powerful techniques of functional analysis. In that more-sophisticated way one can define a new Hilbert subspace $L_{+1}^2(R^3) \subset L_C^2(R^3)$ called the "first Sobolev" subspace,[16] provided with the scalar product

$$(\Psi_1, \Psi_2)_{L_{+1}^2(R^3)} \equiv \tfrac{1}{2}p_0^{-2}((p_0^2+p^2)\Psi_1, \Psi_2)_{L_C^2(R^3)}\,. \tag{11}$$

As a consequence we have the following remarkable result according to which $L_{+1}^2(R^3)$ *and* $L_C^2(S^3)$ *are* $\mathfrak{F}_{p_0}$ *isomorphic.* Such a statement strongly suggests that $L_C^2(S^3)$ is the most natural Hilbert space for describing nonrelativistic one-particle bound states.

With the help of these transformation formulas the eigenvalue problem for the Schrödinger operator acting on $L_{+1}^2(R^3)$, Eq. (4), is Fock transformed into the following eigenvalue equation for the so-called Sturmian (or more properly inverse Sturmian) operator Σ acting on $L_C^2(S^3)$:

$$(I - \nu\Sigma)\phi(\xi) = 0\,, \quad \phi \in L_C^2(S^3)\,, \tag{12}$$

with the fundamental subsidiary "quantization condition"

$$\nu \times (\text{eigenvalue of } \Sigma) = 1 \tag{13}$$

where

$$\nu = mg/(p_0\hbar) \quad \text{and} \quad \Sigma = 2p_0\hbar\mathfrak{F}_{p_0}(p_0^2+p^2)^{-1}\hat{V}\mathfrak{F}_{p_0}^{-1}\,. \tag{14}$$

Note that the Yukawa potential $V(r) = -ge^{-\mu r}/r$ is $L^2 \cap L^1$ in the position space [i.e., one has, respectively, $\int d\vec{r}|V(r)| < \infty$ and $\int |V(r)|^2 d\vec{r} < \infty$]. This property ensures that its Fourier transform is consequently defined everywhere on $L_{+1}^2(R^3)$ in momentum space (see for instance, Simon[16]).

More explicitly, on account of Eqs. (4), (4′), (6), and (7) one has

$$\Sigma\phi(\xi)=\int_{S^3} d\mu(\xi')\Sigma(\xi,\xi')\phi(\xi') , \qquad (14')$$

where

$$\Sigma(\xi,\xi')=(2\pi^2)^{-1}(\beta^2|1+\xi|^2|1+\xi'|^2+|\xi-\xi'|^2)^{-1} . \qquad (14'')$$

These results will be reconsidered from a group-theoretical standpoint in Sec. II B. Such an approach will permit us to show that Σ is a linear superposition of representation operators on $SL(2,R)$. Then, functional analysis theorems will allow us to demonstrate that Σ is a compact operator, result ensuring that the eigenequation (12) may be solved (at least approximately!) by finite-rank techniques.

B. Group-theoretical approach to the Fock transformation

We shall give first an another geometric interpretation of the Fock transformation: let x be $x=(p_0,\vec{p})\in R^4$. Again the Fock transformation may be described as a stereographic projection of the unit hypersphere S^3 onto the hyperplane H_{p_0} defined by the quadrivectors x with the same scalar part p_0 (see Fig. 2):

$$H_{p_0}=s(p_0)\cdot S^3 , \quad S^3=s^{-1}(p_0)\cdot H_{p_0} . \qquad (15)$$

The correspondence between the unit four vector $(\xi_0,\vec{\xi})\in S^3$ and its projection $x=(p_0,\vec{p})\in H_{p_0}$ is merely given by formulas (5): $\xi=s^{-1}(p_0)\cdot x$.

A group-theoretical interpretation of this latter projection may be given by identifying first the x space $\simeq R^4$ to the quaternion field $H=R_+\times SU(2)$

$$x=(p_0,\vec{p})=\begin{bmatrix} p_0+ip_1 & -p_3+ip_2 \\ p_3+ip_2 & p_0-ip_1\end{bmatrix} , \quad \vec{p}=(p_1,p_2,p_3) ,$$

$$xx'=(p_0p_0'-\vec{p}\cdot\vec{p}', p_0\vec{p}'+p_0'\vec{p}+\vec{p}\times\vec{p}') ,$$

$$|x|^2=\det x=p_0^2+\vec{p}^2 \text{ (Euclidean norm on } H) .$$

In the following, for notational convenience, any real number will be identified with a quaternion, the vectorial part of which being $\equiv\vec{0}$: $\alpha\in R$, $(\alpha,\vec{0})\equiv\alpha$. Then, one defines the SL(2, R) conformal action on H as

$$g=\begin{bmatrix} a & b \\ c & d\end{bmatrix}\in SL(2,R) , \quad g\cdot x\equiv(ax+b)(cx+d)^{-1}\in H . \qquad (16)$$

The change of variable equations (5) associated to the Fock transformation may be considered as a particular conformal action. As a matter of fact we remark that by introducing $\bar{x}$, the quaternionic conjugate of x: $\bar{x}=(p_0,-\vec{p})=(2p_0-x)$, the unit four vector ξ may be written

$$\xi=x^2|x|^{-2}=x\bar{x}^{-1}=x(2p_0-x)^{-1}=\begin{bmatrix} 1 & 0 \\ -1 & 2p_0\end{bmatrix}\cdot x .$$

The action of this latter matrix is equivalent to that of the following element of SL(2, R) which may be identified with $s^{-1}(p_0)$:

$$s^{-1}(p_0)=\begin{bmatrix} (2p_0)^{-1/2} & 0 \\ -(2p_0)^{-1/2} & (2p_0)^{1/2}\end{bmatrix}$$

and (17)

$$s(p_0)=\begin{bmatrix} (2p_0)^{1/2} & 0 \\ (2p_0)^{-1/2} & (2p_0)^{-1/2}\end{bmatrix} .$$

$s(p_0)$ induces a one-to-one correspondence between the subgroup [isomorphic to and briefly denoted as SU(2)] of unit modulus quaternions, homeomorphic to S^3, and the hyperplane H_{p_0} of quaternions with the same scalar part p_0.

Within this framework the Yukawa propagator $(|\vec{p}-\vec{p}'|^2+\mu^2\hbar^2)^{-1}$ entering the Schrödinger equation in momentum space, Eq. (4), is transformed by using a so-called "scalar boost":

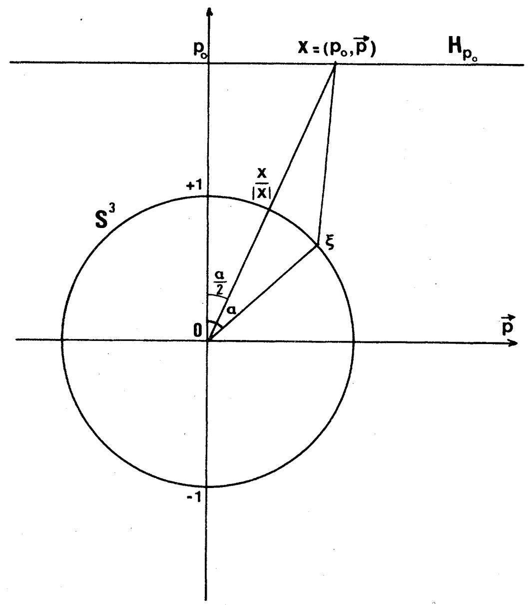

FIG. 2. Fock-stereographic projection may be equivalently considered as a two-step transformation: first the four-vector $x=(p_0,\vec{p})\in H_{p_0}$ is reduced to its unit part $x/|x|\in S^3$; second ξ is obtained from the latter by doubling the polar angle. Such a rotation permits to fold the hyperplane H_{p_0} onto S^3.

$$x=(p_0,\vec{p})\,;\; t_{-\mu\hbar}\cdot x=(p_0-\mu\hbar,\vec{p})\,, \tag{18}$$

where

$$t_{-\mu\hbar}=\begin{bmatrix}1 & -\mu\hbar\\ 0 & 1\end{bmatrix}\in SL(2,R)\,,$$

thus

$$(|\vec{p}-\vec{p}'|^2+\mu^2\hbar^2)^{-1}=|x'-t_{-\mu\hbar}\cdot x|^{-2}\,, \tag{19}$$

with $x'=(p_0,\vec{p}')$.

Now the SL(2,R) conformal action on the H Euclidean distance is

$$x,y\in H\,,\quad g=\begin{bmatrix}a & b\\ c & d\end{bmatrix}\in SL(2,R)\,,$$
$$|cx+d|\;|g\cdot x-g\cdot y|\;|cy+d|=|x-y|\,. \tag{20}$$

By introducing the above defined dimensionless parameter β, see Eq. (7), and

$$g(\beta)\equiv s^{-1}(p_0)t_{\mu\hbar}s(p_0)=\begin{bmatrix}1+\beta & \beta\\ -\beta & 1-\beta\end{bmatrix}\,, \tag{21}$$

the Fock-transformed distance is

$$|x'-t_{-\mu\hbar}\cdot x|$$
$$=(2p_0)^{-1}|x|\;|x'|\;|\beta\xi+1+\beta|\;|\xi'-g^{-1}(\beta)\cdot\xi|\,. \tag{22}$$

Note that $g^{-1}(\beta)=g(-\beta)$. Accordingly, the inverse Sturmian kernel $\Sigma(\xi,\xi')$ [see Eq. (14″)] becomes

$$\Sigma(\xi,\xi')=(2\pi^2)^{-1}|\beta\xi+1+\beta|^{-2}\;|\xi'-g^{-1}(\beta)\cdot\xi|^{-2}\,. \tag{23}$$

The advantage encountered using such an approach is that, by rendering apparent a SL(2,R) group action on H, one makes easiest a separation of the variables ξ and ξ' via finite rank approximations.

C. Algebraic structure of the Sturmian operator

Let us display the algebraic structure of the operator Σ in connection with a (local) reducible representation of SL(2,R).[43]

We define that representation via the "harmonic extension"[44] of an element ϕ of $L^2_C(S^3)$:

$$\Phi(x)=\int_{S^3}d\mu(\xi')\frac{1-|x|^2}{|\xi'-x|^4}\,\phi(\xi') \tag{24}$$

for all x such that $|x|<1$, and

$$\Phi(x)=\phi(x)\quad\text{for all } x\equiv S^3\,.$$

Φ is harmonic for $|x|<1$. Note, in Eq. (24), the use of the four-dimensional Poisson kernel.[38]

We now introduce the following action $\mathcal{T}$ of SL(2,R):

$$g^{-1}=\begin{bmatrix}a & b\\ c & d\end{bmatrix}\in \mathrm{SL}(2,R)\,,\quad \phi\in L^2_C(S^3)\,,$$

$$\mathcal{T}(g)\phi(\xi)=|c\xi+d|^{-2}\Phi(g^{-1}\cdot\xi)$$

where Φ is the "harmonic extension" of ϕ. Clearly, this action is only defined if $|g^{-1}\cdot\xi|\leq 1$.

Let Γ be the subset of SL(2,R), leaving invariant the unit ball in H under the conformal action:

$$\Gamma=[g\in\mathrm{SL}(2,R)\,,|g^{-1}\cdot x|\leq 1$$
$$\text{for all } x \text{ such that } |x|\leq 1] \tag{25}$$

One may verify that Γ is a semigroup, i.e., (i) the identify matrix $I\in\Gamma$; (ii) if $g_1\in\Gamma$ and $g_2\in\Gamma$, then $g_1g_2\in\Gamma$; in particular, $g(\beta)\in\Gamma$ (see Fig. 3). Similary one may also verify that action $\mathcal{T}$ is a representation of the semigroup Γ, i.e., the following fundamental property takes place:

$$\mathcal{T}(g_1g_2)=\mathcal{T}(g_1)\mathcal{T}(g_2)\,, \tag{26}$$

for all $g_1,g_2\in\Gamma$. The most important tool we shall use in that work is furnished by the following proposition:

Proposition 1: The Sturmian operator Σ is a "linear superposition" of representation operators $\mathcal{T}(g)$ for g varying into Γ. Explicitly,

$$\Sigma=\int_0^{+\infty}dt\,\mathcal{T}(g(\beta)d(t))\,, \tag{27}$$

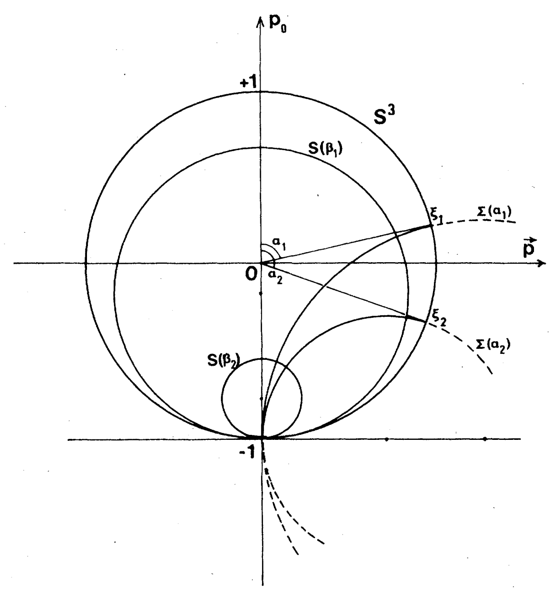

FIG. 3. Geometrical interpretation of the conformal transformation $g(-\beta)\cdot\xi=((1-\beta)\xi-\beta)\,(\beta\xi+(1+\beta))^{-1}$, where $\xi\in S^3$ has a polar angle α. For α (respectively, $\beta>0$) fixed, the trajectories are located on hyperspheres denoted $\Sigma(\alpha)$ [respectively, $S(\beta)$]. Here $\beta_2>\beta_1$. One may verify that $S(0)=S^3$ and $S(+\infty)=-1$.

where

$$d(t)=\begin{bmatrix} e^{t/2} & 0 \\ 0 & e^{-t/2}\end{bmatrix}\in\Gamma$$

is a "conformal dilatation."

Here the identity between operators is viewed as

$$(\Sigma\phi_1,\phi_2)=\int_0^{+\infty} dt\,(\mathcal{T}(g(\beta)d(t))\,\phi_1,\phi_2)\,, \qquad (27')$$

for all $\phi_1,\phi_2\in L^2_C(S^3)$, such that the right-hand of Eq. (27′) makes sense and is continuous in ϕ_1 and ϕ_2.

Indeed, on the one hand we have (see Fig. 3)

$$|d(-t)g(-\beta)\cdot\xi|\leq 1 \quad \text{for all } \xi\in S^3$$

and for all $t,\beta\in[0,+\infty[$. Explicitly the matrix:

$$(g(\beta)d(t))^{-1}=d(-t)g(-\beta)=\begin{bmatrix} e^{-t/2}(1-\beta) & -e^{-t/2}\beta \\ e^{t/2}\beta & e^{t/2}(1+\beta)\end{bmatrix}$$

is an element of Γ^{-1} for $\beta,t\geq 0$, i.e., its conformal action contracts the unit ball in H for all $t>0$ and $\beta>0$. On the other hand, we can check, by resorting to a trick similar to that used by Schwinger[38]:

$$\int_0^\infty dt\,e^{-t}\,|\xi-e^{-t}x|^{-4}(1-e^{-2t}|x|^2)$$

$$=\int_0^1 dz\,|\xi-zx|^{-4}(1-z^2|x|^2)=|\xi-x|^{-2}\,,$$

and it is sufficient to apply the above identity to formula (23) with $x=g^{-1}(\beta)\cdot\xi$.

In Sec. III we shall make an extensive use of the proposition 1, in order to state some important properties of the operator Σ.

III. FUNCTIONAL ANALYSIS OF OPERATOR Σ AND PARTIAL WAVE ANALYSIS

A. Quantization condition

Let us enumerate the essential properties of operator Σ.

Proposition 2. Operator Σ is an Hilbert-Schmidt self-adjoint integral operator on $L^2_C(S^3)$. The Hermiticity of Σ is a straightforward consequence of the following important relation:

$$(\Sigma\phi_1,\phi_2)_{L^2_C(S^3)}=(h/p_0)(\hat{V}\Psi_1,\Psi_2)_{L^2_C(R^3)} \qquad (28)$$

The Hilbert-Schmidt property, as well as the self-adjointness, are direct consequence of well-known theorems: see, for instance, Byron and Fuller,[45] Simon,[16] or Weinberg, Scadron, and Wright.[17]

In particular, the Hilbert-Schmidt norm of Σ can be calculated by using the superposition relation Eq. (27).

$$\|\Sigma\|^2_{L^2}\equiv\mathrm{Tr}(\Sigma)^2=\int_0^\infty dt\int_0^\infty dt'\,\chi(g(\beta)d(t)g(\beta)d(t'))\,, \qquad (29)$$

where $\chi(g)=\mathrm{Tr}\mathcal{T}(g)$, which is the "character" of the representation $\mathcal{T}$, is given by (see Appendix B)

$$\chi(g)=\frac{\mathrm{Tr}g^{-1}}{[(\mathrm{Tr}g^{-1})^2-4]^{1/2}}\,,\quad g\in\mathrm{SL}(2,R)\,. \qquad (30)$$

The double integration in Eq. (29) is easily carried out and one obtains

$$\|\Sigma\|^2_{L^2}=\frac{1}{2\beta(1+\beta)}=\frac{2p_0^2}{\mu\hbar(\mu\hbar+2p_0)}\,. \qquad (31)$$

In Eq. (31), the Coulomb singularity $\mu=0$, i.e., $\beta=0$ is well displayed. The spectrum of Σ, as in the case of any compact self-adjoint operator, consists of a decreasing bound sequence of real eigenvalues (of finite multiplicity) σ_q,[45] with $\sigma_q\to 0$ as $q\to+\infty$ and

$$\sigma_1=\|\Sigma\|\equiv\sup_{\|\phi\|=1}\|\Sigma\phi\|$$

$$\leq\|\Sigma\|_{L^2}=[2\beta(1+\beta)]^{-1/2}\,. \qquad (32)$$

The "quantization condition" [Eq. (13)]

$$\nu^{-1}=\sigma\Leftrightarrow\sigma^{-1}=\nu$$

may be considered as an algebraic equation where the unknown can be taken as $\beta=\mu\hbar/2p_0$.

The real positive solutions of this equation provide the bound states energy values, whereas the other solutions correspond to resonances and virtual states. More precisely the following proposition (see Simon[16] and Gazeau[42]) ensures the validity of the Fock Sturmian approach to the Schrödinger bound states problem for a Yukawa potential.

Proposition 3: Let V be a potential such that the corresponding inverse Sturmian operator $\Sigma=2p_0\hbar\mathfrak{F}_{p_0}|x|^{-2}\hat{V}\mathfrak{F}^{-1}_{p_0}$ is self-adjoint *on* $L^2_C(S^3)$ for at least one real positive value of p_0.

Then $\psi\in L^2_C(R^3)$ satisfies to the Schrödinger eigenvalue equation

$$(p^2/2m-gV-E)\psi=0\,,$$

if, and only if, $\phi=\mathfrak{F}_{p_0}\psi$, $p_0=(-2mE)^{1/2}$, satisfies to the Sturmian eigenvalue equation

$$(I-\nu\Sigma)\phi=0\,.$$

Now let σ_q be an eigenvalue of Σ and ϕ_q a corresponding eigenvector. Then it exists one and only one real positive solution p_{0q}, in the p_0 variable, of the equation

$$\nu=\sigma_q^{-1}\,,$$

and a normalized state vector Ψ_q corresponding to ϕ_q may be obtained from Eq. (8′):

$$\Psi_q(\vec{p}) = \frac{4p_{0q}^{5/2}}{(p_{0q}^2+p^2)^2} \frac{\phi_q(\xi_q)}{[\int d\mu(\xi')(1+\xi_0')|\phi_q(\xi')|^2]^{1/2}}, \quad (33)$$

where $\xi_q = s^{-1}(p_{0q})\cdot(p_{0q}, \vec{p})$.

On the other hand, inequality (32) provides an useful estimate on the conditions of existence of bound states. For that purpose it is convenient to introduce the fundamental dimensionless parameter K characterizing the strength and the range of the Yukawa potential:

$$K = mg/\mu\hbar^2. \quad (34)$$

We have

$$\nu^{-1} = (2K\beta)^{-1} \leq [(2\beta(1+\beta)]^{-1/2}$$

or, equivalently,

$$0 < 2p_0/\mu\hbar \leq 2K^2 - 1. \quad (35)$$

Thus, there exists a bound state only if $K \geq 1/\sqrt{2} = 0.707$. This condition, although less severe, is very close of that given by Totsuji,[10] $K \geq \frac{1}{4}\pi = 0.7854$ and by Rogers *et al.*,[12] $K \geq 0.8399$. Consequently, the energy of the ground state is roughly bounded from below by

$$E \geq -(\mu^2\hbar^2/8m)(2K^2-1)^2. \quad (35')$$

In the following, we shall adopt the Rydberg unit system:

$$E = \nu^{-2} \Longleftrightarrow mg^2/2\hbar^2 = -1;$$

Eq. (35′) is now written

$$E \leq (1/4K^2)(2K^2-1)^2. \quad (35'')$$

B. Finite rank techniques for eigenvalue problems

The essence of a compact operator lies in the fact that it is the norm limit of a sequence of operators of finite rank. Thus, the operator Σ can be approximated in norm by a sequence of hermitian matrices of increasing rank f: $((\Sigma)_{\mu\mu'})$, $0 \leq \mu, \mu' \leq f$, defined by

$$\Sigma = \sum_{\mu,\mu'} \phi_\mu(\Sigma)_{\mu\mu'}(\ \ ,\phi_{\mu'}), \quad (36)$$

where $\{\phi_\mu\}$ is some orthonormal basis of $L_C^2(S^3)$.

A natural good choice for this basis is the set of S^3 spherical harmonics, or "Coulomb Sturmian basis":

$$\{\phi_\sigma\} = \{y_N\}; \quad N = n,l,m; \quad n \geq 1, 0 \leq l \leq n-1, |m| \leq l; \quad (37)$$

l is recognized as the orbital quantum number.

The proposition 1 gives the related matrix elements of Σ via those of the operator $\mathcal{T}(g)$:

$$(\Sigma)_{NN'} \equiv (\Sigma y_{N'}, y_N) = \int_0^\infty dt\, \mathcal{T}_{NN'}(g(\beta)\,d(t)). \quad (38)$$

The matrix elements $\mathcal{T}_{NN'}(g)$ have been explicited in other works[35,41,42] (see also Ref. 34 where they are implicitely given):

$$(\Sigma)_{NN'} = (nn')^{-1/2}\delta_{ll'}\delta_{mm'}\tau^{-(l+1)}_{n-l-1,n'-l-1}(g(\beta)), \quad (39)$$

where $\tau^u_{kk'}(g)$ is the matrix element of a "local" multiplier representation of SL(2,R) (see Miller, Ref. 43). The exact expressions of $\tau^u_{kk'}(g)$ is given in Appendix A.

Let us now separate the variable on the S^3 sphere in the following form:

$$\phi(\xi) = a_l(\alpha)\sin^l\alpha\, y_{lm}(\theta,\varphi), \quad (40)$$

where α, θ, φ are the spherical coordinates of $\xi \in S^3$, and $\{y_{lm}\}$ are the usual spherical harmonics.

The initial eigenvalue problem becomes

$$(I - \nu\Sigma_l)a_l = 0. \quad (41)$$

The operator Σ_l now acts on the Hilbert space of functions a_l satisfying to

$$\int_0^\pi d\alpha\,(\sin\alpha)^{2l+1}|a_l(\alpha)|^2 < \infty. \quad (42)$$

From Eq. (39), this projected operator is also a linear superposition of representation operators $\tau^{-(l+1)}(g)$. Moreover Σ_l is a trace class operator. The value of its trace is given in Appendix B.

IV. RESULTS

The theoretical analysis performed in Sec. I–III leads to a very simple efficient finite-rank method for computing the eigenvalues of the Sturmian operator Σ and consequently of the Schrödinger equation (1). For each value of the angular momentum number l, the matrix elements of Σ_l in the Coulomb Sturmian basis are:

$$(\Sigma_l)_{k,k'} = [(k+l+1)(k'+l+1)]^{-1/2} \times \tau^{-(l+1)}_{kk'}(g(\beta)); \quad k,k' \geq 0, \quad (43)$$

where $\tau^{-(l+1)}_{kk'}(g(\beta))$ are given in Appendix A.

The nth-order finite-rank-approximated eigenvalue of Σ_l are simply the roots of the secular equation:

$$\det[[(k+l+1)(k'+l+1)]^{-1/2} \times \tau^{-(l+1)}_{kk'}(g(\beta)) - \delta_{kk'}/\nu] = 0, \quad (44)$$

with $0 \leq k,k' \leq n-1$. In fact Eq. (44) should be considered where β is the unknown and the "eigenvalue" $1/\nu$ is written $1/\nu = (E)^{-1/2} = (2K\beta)^{-1}$ for $\beta > 0$. The finite-rank approximation of order n consists on retaining the nth order leading minor within the infinite determinant which elements are given by Eq. (A2) (with the additive factor $-\delta_{kk'}/2K\beta$ for the diagonal ones).

The actual computation is performed by using a standard "regula falsi" routine for finding the real E zeroes of the characteristic equation (44). On account of their polynomial character, see Eq. (A3), the elements of the characteristic determinant and consequently the determinant itself, may be evaluated to any desired accuracy. More precisely at each step of the calculation the determinant was computed with the help of an usual double-precision Gauss-Jordan routine.

The main result of our numerical investigations is the constated excellent convergence of the finite-rank approximation with respect to its order. For instance with $n=20$ one recovers exactly the most accurate results previously published by Rogers *et al.*[12] and Roussel *et al.*[19] (see Table II.) It should be stressed, however, that even the lowest-order approximations lead to surprisingly accurate results. For instance, in the first approximation, i.e., $k=k'=0$ in Eq. (43), one has (see also Table I)

$$(\Sigma_l)_{0,0}=(l+1)^{-1}(1+\beta)^{-(2l+2)}, \tag{45}$$

and the characteristic equation reduces to

$$2K\beta-(l+1)(1+\beta)^{2l+2}=0. \tag{46}$$

For a given l, this equation in β has, at most, two real positive roots for

$$K\geq(l+1)^2[(2l+2)/(2l+1)]^{2l+1}. \tag{47}$$

When specialized further to the case of S states it becomes

$$2K\beta-(1+\beta)^2=0. \tag{48}$$

The roots, which are real for $K>2$, are, respectively,

$$\beta=K-1\pm[(k-1)^2-1]^{1/2}. \tag{49}$$

The approximated eigenenergy of the ground state is given by one of these roots: $\beta_{1s}=K-1-[(K-1)^2-1]^{1/2}$; thus, $E_{1s}=(2K\beta_{1s})^{-2}$. It is remarkable that the ground-state energy obtained in a so simple way is accurate to within a few parts in 10^5 at least for realistic values of the screening parameter $K\geq 50$; see Table II.

The corresponding normalized first-order approximated eigenfunction reads

$$\Psi_{1s}(\vec{p})=4p_0^{5/2}(p_0^2+\vec{p}^2)^{-2}. \tag{50}$$

It should be noted that the other root in Eq. (48) does not have any direct physical meaning. In order to get a better understanding of the significance of this particularity it is worthy to note that the first approximation consists on replacing the Yukawaian symetric kernel

$$[|\vec{p}-\vec{p}'|^2+\mu^2\hbar^2]^{-1} \tag{51}$$

by the following separable one:

$$(2p_0)^4(p_0^2+\vec{p}^2)^{-1}(2p_0+\mu\hbar)^{-2}(p_0^2+\vec{p}'^2)^{-1}. \tag{51$'$}$$

This approximated potential kernel is now *energy dependent* on account of the presence of parameter p_0. This property impedes obtaining orthogonalized eigenvectors of the Schrödinger operator. The existence of the "pirate" root in Eq. (48) is thus only a consequence of the kind of approximation used.

With the help of expression (A2) the matrix elements $(\Sigma_l)_{k,k'}$, are easily computed and the char-

TABLE I. Matrix elements and characteristic polynomials up to third order for the finite-rank approximation to the Yukawa "inverse Sturmian" operator in a Coulomb Sturmian basis; $\beta=\mu\hbar/2(-2mE)^{1/2}$; $K=mg/\mu\hbar^2$.

$$\begin{bmatrix} \dfrac{(1+\beta)^{-(2l+2)}}{(l+1)} & -[2/(l+2)]^{1/2}\beta(1+\beta)^{-(2l+3)} & [(2l+3)/(l+3)]^{1/2}\beta^2(1+\beta)^{-(2l+4)} \\ & \dfrac{[1+2(l+1)\beta^2]}{l+2}(1+\beta)^{-(2l+4)} & -[2(2l+3)/(l+2)(l+3)]^{1/2}[1+(l+1)\beta^2]\beta(1+\beta)^{-(2l+5)} \\ \text{Sym.} & & \dfrac{1+2(2l+3)\beta^2+(l+1)(2l+3)\beta^4}{l+3}(1+\beta)^{-(2l+6)} \end{bmatrix}$$

Characteristic Polynomials:

I: $2K\beta-(1+\beta)^{(2l+2)}(l+1)$

II: $4K^2\beta^2-2K\beta(1+\beta)^{(2l+2)}[(1+\beta)^2(l+2)+(1+2(l+1)\beta^2)(l+1)]+(l+1)(l+2)(1+\beta)^{4l+6}$

III: $(l+1)(l+2)(l+3)(1+\beta)^{(6l+12)}+8K^3\beta^3$

$-4K^2\beta^2(1+\beta)^{(2l+2)}[(l+3)(1+\beta)^4+(l+1)(1+2(l+1)\beta^2+(l+1)(2l+3)\beta^4)+(l+2)(1+\beta)^2(1+2(2l+3)\beta^2)]$

$+2K\beta(1+\beta)^{(4l+6)}[(l+2)(l+3)(1+\beta)^4+(l+1)(l+3)(1+\beta)^2(1+2(l+1)\beta^2)+(l+1)(l+2)(1+2(2l+3)\beta^2+(l+1)(2l+3)\beta^4)]$

TABLE II. Eigenenergies of the low-lying states as a function of the screening length for various orders of the finite-rank approximation. Energies are in Rydberg units. It should be noted that the 20th-order approximation permits to recover all the exact results previously obtained in particular by Rogers, Graboske, and Harwood (RGH) (Ref. 12).

K		$1s$	$2s$	$2p$	$3s$	$3p$	$3d$	$4s$	$4p$	$4d$	$4f$	$5d$	$5f$	$6f$
∞	(Coulomb)	1.000	0.2500	0.2500	0.1111	0.1111	0.1111	0.0625	0.0625	0.0625	0.0625	0.0400	0.0400	0.0278
200	first	0.9900		0.2400										
	second	0.9900	0.2400	0.2401		0.1010	0.1014							
	third	0.9900	0.2401	0.2401	0.1010	0.1014	0.1014		0.05217	0.05299	0.05294	0.02934	0.03068	0.01668
	.													
	.													
	.													
	20th	0.9900	0.2401	0.2401	0.1014	0.1014	0.1014	0.05307	0.05305	0.05301	0.05294	0.03081	0.03075	0.01889
	RGH	0.9900	0.2401	0.2401	0.1014	0.1014	0.1014	0.05307	0.05305	0.05301	0.05294	0.03081	0.03075	0.01889
50	first	0.9602		0.2104			0.0715							
	second	0.9606	0.2100	0.2119		0.06987	0.07481							
	third	0.9606	0.2123	0.2119	0.06905	0.07526	0.07502			0.02737	0.02878			
	.													
	.													
	.													
	20th	0.9606	0.2123	0.2119	0.07604	0.07570	0.07503	0.03076	0.03047	0.02988	0.02898	0.01134	0.01060	0.0039
	RGH	0.9606	0.2123	0.2119	0.07604	0.07570	0.07503	0.03076	0.03047	0.02988	0.02898	0.01134	0.01060	0.0039
20	first	0.9012		0.1521										
	second	0.9036	0.1495	0.1609										
	third	0.9036	0.1626	0.1615			0.03218							
	.													
	.													
	.													
	20th	0.9036	0.1635	0.1615	0.03870	0.03712	0.03383	0.00618						
	RGH	0.9036	0.1635	0.1615	0.03870	0.03712	0.03383	0.00618						
5	first	0.6198												
	second	0.6520												
	third	0.6535												
	.													
	.													
	.													
	20th	0.6536	0.02421	0.00820										
	RGH	0.6536	0.02421	0.00820										
2	first													
	second	0.2624												
	third	0.2890												
	.													
	.													
	.													
	20th	0.2962												
	RGH	0.2962												

acteristic equations [Eq. (44)] may be explicitly written at least for the lowest orders of approximation: see Table I. As it may be seen in Table II the second- and third-order approximations lead to numerical results very accurate since the deviation from the "exact" results of Rogers *et al.*[12] and Roussel *et al.*[19] does not exceed a few percent for the lowest-lying states. The only limitation of our method lies in the fact that, for a given l, the maximum number of eigenvalues we can obtain is equal to the order of the approximation.

As we already mentioned higher-order approximations may be carried out by resorting to standard numerical methods for computing the characteristic determinant. For instance the extensive tables given in Refs. 12 and 19 are recovered with the help of a finite rank approximation of order 20. In the meantime one may compute also the expansion coefficient $C_{nl}(p_{0q})$ of the eigenvector on the corresponding reduced Coulomb Sturmian basis, see Eqs. (37) and (40):

$$\phi_{q;lm}(\xi)=\sum_{n=l+1}^{k_{\max}+l+1} C_{n,l}(p_{0q})y_{nlm}(\xi)\,, \tag{52}$$

where $n=k+l+1$; $k_{\max}+1$ is the order of the finite-rank approximation and the index q labels the eigenvalue considered: $p_{0q}=(-2mE_q)^{1/2}$.

The corresponding expression of the approximated normalized eigenfunction in momentum space is then obtained from Eq. (33):

$$\psi_{q,lm}(\vec{p})=\frac{4p_{0q}^{5/2}\phi_{q,lm}(\xi)}{(p_{0q}^2+\vec{p}^{\,2})^2\mathcal{G}_{k_{\max},l}(p_{0q})}\,, \tag{53}$$

where $\mathcal{G}_{k_{\max},l}(p_{0q})$ is the "normalization" integral

$$\mathcal{G}_{k_{\max},l}(p_{0q})=\sum_{n,n'\geq l+1}^{k_{\max}+l+1}\int d\mu(\xi')(1+\xi_0')C_{nl}(p_{0q})C_{n'l}(p_{0q})\times y_{nlm}(\xi')y^*_{n'lm}(\xi')\,, \tag{54}$$

which, on using the orthogonality properties of the four-dimensional spherical harmonics, is readily transformed as

$$\mathcal{G}_{k_{\max},l}(p_{0q})=\sum_{n=l+1}^{k_{\max}+l+1}C_{nl}^2(p_{0q})+\sum_{n,n'\geq l+1}^{k_{\max}+l+1}\int d\mu(\xi')\times C_{nl}(p_{0q})C_{n'l}(p_{0q})\xi_0'y_{nlm}(\xi')y^*_{n'lm}(\xi')\,. \tag{55}$$

The latter integral may be transformed further with the help of the following "ladder" formula:

$$\begin{aligned}\xi_0'y_{nlm}(\xi')&=\cos\alpha' y_{nlm}(\xi')\\&=\frac{1}{2}\left(\frac{(n-l)(n+l+1)}{n(n+1)}\right)^{1/2}y_{n+1,lm}(\xi')\\&\quad+\frac{1}{2}\left(\frac{(n-l-1)(n+l)}{n(n-1)}\right)^{1/2}y_{n-1,lm}(\xi')\,,\end{aligned} \tag{56}$$

which represents a four-dimensional generalization of the well-known properties of usual surface spherical harmonics $y_{lm}(\theta\varphi)$.[47]

One has eventually:

$$\begin{aligned}\mathcal{G}_{k_{\max},l}(p_{0q})=\sum_{n=l+1}^{k_{\max}+l+1}\Bigg[C_{nl}^2(p_{0q})&+\frac{1}{2}\left(\frac{(n-l)(n+l+1)}{n(n+1)}\right)^{1/2}C_{nl}(p_{0q})C_{n+1,l}(p_{0q})\\&+\frac{1}{2}\left(\frac{(n+l)(n-l-1)}{n(n-1)}\right)^{1/2}C_{nl}(p_{0q})C_{n-1,l}(p_{0q})\Bigg]\,.\end{aligned} \tag{57}$$

From the set of functions $\psi_{q;lm}(\vec{p})$ it would be an easy matter to determine transition amplitudes between bound states along the lines developed in Ref. 19. Although the set of functions $\psi_{q;lm}(\vec{p})$ ($q\leq k_{\max}+1$, order of the finite-rank approximation is not an orthogonal set, it should be pointed out that these functions are "almost" orthogonal

$$\lim_{k_{\max}\to\infty}(\Psi_{q;lm},\Psi_{q';lm})=\delta_{q,q'}\quad(q,q'\leq k_{\max}+1)\,.$$

V. CONCLUSION

In that paper we have presented a SL$(2,R)$ group-theoretical approach to the Schrödinger eigenvalue problem for a Yukawa potential. The Sturmian technique we used leads naturally to very accurate finite-rank approximated eigenvalues even in the lowest orders of approximation. It should be added that our method may be used successfully for other types of potentials, spherically symmetric or not.[42]

As a matter of fact the calculation of matrix elements for the corresponding Sturmian operator is reduced once and for all, to those of matrix elements of representation operators of SL$(2,R)$ in the symmetric potential case, or a larger group otherwise.[41]

For instance, out formalism may be extended to the case of a superposition of Yukawa potentials (Martin potential)

$$V=-g\int_{\mu_0}^{\infty}d\mu\, f(\mu)e^{-\mu r}/r\,.$$

The secular equation (44) would become

$$\det\left[[(k+l+1)(k'+l+1)]^{-1/2}\frac{2p_0}{\hbar}\times\int_{\beta_0}^{\infty}d\beta\, f\left(\frac{2p_0\beta}{\hbar}\right)\tau_{k,k'}^{-(l+1)}(g(\beta))-\frac{\delta_{kk'}}{\nu}\right]=0\,.$$

In a similar way resolvent or Green's functions, useful, for instance, in perturbation expansion, may be easily derived within the framework of the formalism developed here.[42] Eventually we should also mention the possibility of resorting to the powerful moment method[48] for performing similar calculations.

APPENDIX A: EXPRESSION OF THE MATRIX ELEMENTS $\tau_{kk'}^{u}(g)$

$\tau_{kk'}^{u}(g)$ is the matrix element of a local multiplier representation of SL$(2,R)$.[43] The latter can be defined for $u\in C-N_+^*$ on the complex vector space of all functions analytic in some neighborhood of zero, i.e., the space of all functions f of the form

$$f(t)=\sum_{n=0}^{+\infty}a_n t^n,\quad a_n\in C\,,$$

where the power series converges in a nonzero neighborhood of $t=0$:

$$\tau^{u}(g)F(t)=(ct+d)^{2u}F((at+b)(ct+d)^{-1})\quad\text{for } g^{-1}=\begin{bmatrix}a & b\\ c & d\end{bmatrix}. \tag{A1}$$

The matrix elements of the operator $\tau^u(g)$ are defined with reference to the basis functions

$$e_k(t)=[\Gamma(k-2u)/\Gamma(k+1)]^{1/2}t^k,\quad k\geqslant 0\,.$$

Their expression can be easily established in terms of hypergeometric polynomials

$$\tau_{kk'}^{u}(g)=\left(\frac{\Gamma(k_>+1)\Gamma(k_>-2u)}{\Gamma(k_<+1)\Gamma(k_<-2u)}\right)^{1/2}d^{2u-k_>}a^{k_<}\times\frac{(\gamma(b,c))^{k_>-k_<}}{(k_>-k_<)!}\,{}_2F_1\left(-k_<,k_>-2u;k_>-k_<+1;\frac{bc}{ad}\right), \tag{A2}$$

$$\gamma(b,c)=\begin{cases}b, & k_>=k'\\ -c, & k_>=k\end{cases}$$

$$k_{\gtrless}=\begin{matrix}\sup\\ \inf\end{matrix}(k,k')\geqslant 0\,,\quad 2u\in C-N\,.$$

This expression may be transformed further by noting that the hypergeometric polynomials are in fact Jacobi polynomials. In the specific case of the Yukawa potential, one has

$$\tau_{n-l-1,n'-l-1}^{-(l+1)}(g(\beta))=\left(\frac{(n_<-l-1)!(n_>+l)!}{(n_>-l-1)!(n_<+l)!}\right)^{1/2}(1+\beta)^{-(n+n')}\times(-\beta)^{n_>-n_<}P_{n_<-l-1}^{(n_>-n_<,\,-n-n')}(1-2\beta^2); \tag{A3}$$

$$n_{\gtrless}=\begin{matrix}\sup\\ \inf\end{matrix}(n,n')\geqslant 1\,.$$

APPENDIX B: COMPUTATION OF TRACES (Tr)

In the following, we shall put

$$\chi(g)=\mathrm{Tr}\,\mathcal{T}(g)\,,\quad x^u(g)=\mathrm{Tr}\,\tau^u(g)\,; \tag{B1}$$

we have, from the relation (38),

$$\chi(g)=\sum_{l=0}^{+\infty}(2l+1)x^{-(l+1)}(g)\,.$$

Now, for all triangular matrix

$$v^{-1}=\begin{bmatrix}\lambda & \rho\\ 0 & \mu\end{bmatrix}$$

it is straightforward to show that $\tau_{kk}^{u}(v)=\mu^{2u}(\lambda/\mu)^k$, see Eq. (A3). Thus, if $|\lambda|<|\mu|$, then

$$x^u(v)=\mu^{2u+1}/(\mu-\lambda)=\lambda^{-(2u+1)}/(\mu-\lambda)\,. \tag{B3}$$

It follows from (B2) and (B3) that

$$\chi(v)=(\mu+\lambda)/(\mu-\lambda)^3\,. \tag{B4}$$

Afterwards, any element $g^{-1}=\left(\begin{smallmatrix}a & b\\ c & d\end{smallmatrix}\right)\in$ SL$(2,C)$ can be triangularized: $g^{-1}=\hat{s}v^{-1}\hat{s}^{-1}$, with

$$\left\{\begin{matrix}\lambda\\ \mu\end{matrix}\right\}=\tfrac{1}{2}\left\{\mathrm{Tr}g^{-1}\pm[(\mathrm{Tr}g^{-1})^2-4]^{1/2}\right\}, \tag{B5}$$

and, if $|\lambda|<|\mu|$, in some neighborhood of the identity in SL$(2,C)$, we obtain

$$x^u(g)=x^u(v)=2^{2u+1}\frac{\{\mathrm{Tr}g^{-1}-[(\mathrm{Tr}g^{-1})^2-4]^{1/2}\}^{-(2u+1)}}{[(\mathrm{Tr}g^{-1})^2-4]^{1/2}}, \tag{B6}$$

$$\chi(g)=\chi(v)=\mathrm{Tr}g^{-1}/[(\mathrm{Tr}g^{-1})^2-4]^{3/2}\,. \tag{B7}$$

The above expressions allow us to calculate three important norms for operators Σ and Σ_l. The trace norm of Σ_l and the Hilbert-Schmidt norms of Σ_l and Σ,

$$\mathrm{Tr}\Sigma_l = \int_0^{+\infty} dt\, x^{-(l+1)}(g(\beta)d(t))\,; \tag{B8}$$

$$\mathrm{Tr}(\Sigma_l)^2 = \|\Sigma_l\|^2_{L^2} = \int_0^{+\infty} dt \int_0^{+\infty} dt'\, x^{-(l+1)}(g(\beta)d(t)g(\beta)d(t'))\,; \tag{B9}$$

$$\mathrm{Tr}(\Sigma)^2 = \|\Sigma\|^2_{L^2} = \int_0^{\infty} dt \int_0^{\infty} dt'\, \chi(g(\beta)d(t)g(\beta)d(t'))\,. \tag{B10}$$

The first integral [Eq. (B8)] may be expressed in terms of tabulated integrals by noting that

$$\mathrm{Tr}[\,g(-\beta)d(-t)\,] = 2(\cosh(\tfrac{1}{2}t) + \beta\sinh(\tfrac{1}{2}t))$$

and using the following variable change:

$$z^{1/2} + z^{-1/2} = 4(\cosh(\tfrac{1}{2}t) + \beta\sinh(\tfrac{1}{2}t))$$

we get

$$\mathrm{Tr}(\Sigma_l) \equiv I_l(\beta) = \int_0^1 dz\, z^l (z^2 - 2(1-2\beta^2)z + 1)^{-1/2}. \tag{B11}$$

This latter integral is easily recurrently evaluated, and one has eventually ($l > 0$) (Ref. 49):

$$I_l(\beta) = -[2l(1-2\beta^2)]^{-1} + \frac{(2l-1)(1-2\beta^2)}{l} \times I_{l-1}(\beta) - \frac{l-1}{l}\, I_{l-2}(\beta)\,, \tag{B12}$$

with

$$I_0 = \ln|(1+\beta)/\beta|\,.$$

The analysis is somewhat more complicated for the Hilbert-Schmidt norms. However, since

$$\mathrm{Tr}[d(-t)g(-\beta)d(-t')g(-\beta)] = e^{t/2}e^{t'/2}[(1-\beta)^2 e^{-t}e^{-t'} - \beta^2(e^{-t} + e^{-t'}) + (l+\beta)^2]\,,$$

and making the variable change

$$z = e^{-t}\,, \quad z' = e^{-t}\,,$$

Eq. (B10) is reduced to the following double integral:

$$\|\Sigma\|^2_{L^2} \equiv J_l(\beta) = \int_0^1 dz \int_0^1 dz'\, A(\beta; z, z') \times [A^2(\beta, z, z') - 4zz']^{-3/2}\,, \tag{B13}$$

where

$$A(\beta; z, z') = (1-\beta)^2 zz' - \beta^2(z+z') + (1+\beta)^2\,.$$

Again this integral may be expressed in terms of known tabulated integrals,[49] and after some tedious algebra one recovers the well-known result

$$\|\Sigma\|^2_{L^2} = 1/2\beta(1+\beta) \tag{B14}$$

Evidently the things are much more intricate for the partial-wave Hilbert-Schmidt norm [Eq. (B9)] which may be ultimately expressed as follows:

$$\|\Sigma_l\|^2_{L^2} = 2^{-(2l+1)} \int_0^1 dz \int_0^1 dz' (zz')^{-(l+1)} \times \frac{\{A(\beta; z, z') - [A^2(\beta; z, z') - 4zz']\}^{2l+1}}{[A^2(\beta; z, z') - 4zz']^{1/2}}$$

This double integral is easily reduced to a single one,[49] which may be evaluated by using standard numerical techniques.

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*Laboratoire "Matiére et Rayonnement" Associé au Centre Nationale de la Recherche Scientifique.

[1]M. Yukawa, Proc. Phys. Math. Soc. Jpn. 17, 48 (1935).

[2]N. Kemmer, Proc. Cambridge Philos. Soc. 34, 354 (1938).

[3]A. H. Wilson, Proc. Cambridge Philos. Soc. 34, 365 (1938).

[4]R. G. Sachs and M. Goeppert-Mayer, Phys. Rev. 53, 991 (1938).

[5]L. Hulthen and K. V. Laurikainen, Rev. Mod. Phys. 23, 1 (1951).

[6]G. Ecker and W. Weizel, Ann. Phys. (Leipzig) 17, 126 (1956).

[7]H. Margenau and M. Lewis, Rev. Mod. Phys. 31, 569 (1959).

[8]G. M. Harris, Phys. Rev. 125, 1131 (1962).

[9]C. R. Smith, Phys. Rev. 134, A1235 (1964).

[10]H. Totsuji, J. Phys. Soc. Jpn. 31, 584 (1971).

[11]C. A. Rouse, Phys. Rev. 159, 41 (1967); 163, 62 (1967); see also, 176, 423 (1968).

[12]F. J. Rogers, H. C. Graboske, Jr., and D. J. Harwood, Phys. Rev. A 1, 1577 (1970); F. J. Rogers, *ibid.* 4, 1145 (1971).

[13]T. W. Preist, J. Phys. B 4, 1129 (1971).

[14]I. Z. Fisher and V. I. Krylovich, Zh. Tekh. Fiz. 27, 1289 (1956) [Sov. Phys. Tech. Phys. 2, 1184 (1957)].

[15]J. B. Krieger, Phys. Rev. 178, 1337 (1969).

[16]H. Rollnik, Z. Phys. 145, 639 (1956); J. Schwinger, Proc. Natl. Acad. Sci. U.S.A. 47, 122 (1961); more general discussions may be found in T. Kato, Prog. Theor. Phys. Suppl. 40, 3 (1967); M. Scadron, in *Symposium on Theoretical and Physical Mathematics*, edited by A. Ramakrishnan (Plenum, New York, 1968), Vol. 7; and especially in B. Simon, *Quantum Mechanics*

for Hamiltonians Defined as Quadratic Forms (Princeton University, Princeton, N.J., 1971), and references therein.

[17]M. Scadron and S. Weinberg, Phys. Rev. 133, B1589 (1964); M. Scadron, S. Weinberg, and J. Wright, *ibid.* 135, B202 (1964); J. Wright and M. Scadron; Nuovo Cimento 34, 1571 (1964).

[18]C. S. Lam and Y. P. Varshni, Phys. Rev. A 4, 1875 (1971); 6, 1391 (1972).

[19]K. M. Roussel and R. F. O'Connell, Phys. Rev. A 9, 52 (1974).

[20]R. L. Greene and C. Aldrich, Phys. Rev. A 14, 2363 (1976).

[21]V. L. Bonch-Bruevich and V. B. Glasko, Fiz. Tverd. Tela 4, 510 (1962) [Sov. Phys. Solid. State 2, 371 (1962)]; Opt. Spectrosc. 14, 495 (1964) [Opt. and Spectrosc. 14, 264 (1964)].

[22]B. A. Trubnikov and Ya.N. Yavlinskii, Zh. Eksp. Teor. Fiz. 48, 1618 (1965) [Sov. Phys. JETP, 21, 1088 (1965)].

[23]H. M. Schey and J. L. Schwartz, Phys. Rev. 139, B1428 (1965).

[24]A. Ahmadzadeh, P. G. Burke, and C. Tate, Phys. Rev. 131, 1315 (1963).

[25]C. Lovelace and D. Masson, Nuovo Cimento 26, 472 (1962).

[26]G. J. Iafrate and L. B. Mendelsohn, Phys. Rev. 182, 244 (1969).

[27]E. Zauderer, J. Math. Phys. 13, 42 (1972).

[28]H. Cheng and T. T. Wu, Phys. Rev. D 5, 3189 (1972).

[29]H. J. W. Müller-Kirsten and N. Vahedi-Faridi, J. Math. Phys. 14, 1291 (1973).

[30]R. H. Pratt and H. K. Tseng, Phys. Rev. A 5, 1063 (1972); J. McEnnan, L. Kissel, and R. H. Pratt, *ibid.* 13, 532 (1976); J. McEnnan, D. J. Botto, R. H. Pratt, D. Bunaciu, and V. Florescu, *ibid.* 16, 1768 (1977).

[31]W. Bühring, J. Math. Phys. 18, 1121 (1977).

[32]M. Bednar, Ann. Phys. (N.Y.) 75, 305 (1973).

[33]B. I. Dunlap and L. Armstrong, Jr., Phys. Rev. A 6, 1370 (1972).

[34]J. P. Gazeau, C. R. Acad. Sci. Paris 273B, 1074 (1971).

[35]S. Kumei, Phys. Rev. A 9, 2306 (1974).

[36]M. Levy, Proc. R. Soc (London) Ser. A 204, 145 (1950).

[37]B. O. Enflo, Phys. Scr. 4, 11 (1971).

[38]V. Fock, Z. Phys. 98, 145 (1935); see also, M. Bander and C. Ytzyckson, Rev. Mod. Phys. 38, 330 (1966); J. Schwinger, J. Math. Phys. 5, 1606 (1964).

[39]M. Rotenberg, Ann. Phys. (N.Y.) 19, 262 (1962); in *Advances in Atomic and Molecular Physics*, edited by R. D. Bates and I. Estermann (Academic, New York, 1970), Vol. 6.

[40]The story of the Sturmian functions may be traced back to the papers by P. S. Epstein, Proc. Natl. Acad. Sci. U.S.A. 12, 630 (1926), and B. Podolski, *ibid.* 14, 253 (1928).

[41]J. P. Gazeau, J. Math. Phys. 19, 1041 (1978).

[42]J. P. Gazeau, thesis (Université Paris VI, 1978) unpublished; J. P. Gazeau, M. Cl. Dumont Lepage, and A. Ronveaux (unpublished).

[43]W. Miller, Jr., *Lie Theory and Special Functions*, (Academic, New York, 1968), Chaps. I and V.

[44]R. R. Coifman and G. Weiss, *Analyse Harmonique Non Commutative sur Certains Espaces Homogènes*, Lectures Notes in Math., No. 242, (Springer-Verlag, Berlin, 1971).

[45]F. W. Byron and R. W. Fuller, Mathematics of Classical and Quantum Physics, Vol. 2 (Addison-Wesley, Reading, Mass., 1970).

[46]W. Magnus, F. Oberhettinger, and R. P. Soni, *Formulas and Theorems for the Special Functions of Mathematical Physics* (Springer-Verlag, Berlin, 1966).

[47]See, for instance, H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms* (Springer-Verlag, Berlin, 1957), Appendix, p. 344.

[48]D. Masson, in *The Padé Approximant in Theoretical Physics*, edited by G. A. Baker and J. L. Gammel (Academic, New York, 1970), Sec. 7, p. 197.

[49]I. S. Gradshteyn and I. W. Ryshik, *Table of Integrals Series and Products* (Academic, New York, 1965).