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Bound states of hydrogen atom in a theory with minimal length uncertainty relations

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The following properties of bound states of hydrogen atom in a theory with noncommuting position operators are investigated: their number, multiplicities, accidental degeneracy, localization, and dependence on the values of deformation parameters. © *2007 American Institute of Physics.* [DOI: 10.1063/1.2423221]

I. INTRODUCTION AND PRELIMINARIES

This is a continuation of our work[14] on quantum mechanics of a system with noncommuting position operators [Eq. (1) below]; we refer to it for a discussion of the framework and for calculations involving the distance operator R. While Ref. 14 was concerned with kinematics of the system, here we discuss problems of dynamics of hydrogen-like atoms. Namely, we address the question of how much the properties of bound states of hydrogenlike atoms change when fundamental length is introduced through a modification of the kinematics of the system.

Since one has here both ultraviolet and infrared (large and small momentum) modifications of the standard quantum mechanics (stQM), it is *a priori* not clear how the spectrum of the system will change. To clarify this, we address the following questions: Is the number of bound states finite or infinite? What are the multiplicities of the eigenvalues of the Hamiltonian? Is the accidental degeneracy of its point spectrum removed or not? What are the localization properties of the eigenfunctions? How do the properties of the system depend on the values of the deformation parameters?

In stQM many of these questions are answered through position-space considerations. Since the position operators do not commute here, the position-space formulation of stQM is no longer available. In its place, we base our analysis on an extensive use of eigenvectors of the length operator R (R-basis) of Ref. 14.

For example, to discuss (and to define) space localization properties of a vector of the Hilbert space of the system, we consider the rate at which components of the vector in R-basis tend to zero, as the eigenvalues of R tend to infinity. Similarly, in our use of the Birman-Schwinger-type argument we use matrix elements with respect to an R-basis.

We refer to Refs. 3, 1, and 2 for earlier publications on bound states of the system under consideration, and to this introduction and Secs. II B and IV C for a few comments on the last two of these references.

We will now describe the content of the paper.

Since the operator $1/R$ is compact, the Hamiltonian is a compact perturbation of the kinetic energy operator and one easily locates its essential spectrum and, as a result of the scaling properties [Eqs. (6) and (7)], one obtains analyticity properties of the Hamiltonian as a function of the deformation parameter $\sqrt{\alpha}$ of Eq. (3) (Sec. II A). Using these analyticity properties and a result

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of Sec. IV B about nondegeneracy of the spectrum of the reduced Hamiltonian, we show in Sec. II B that the deformation lifts the accidental degeneracy of hydrogenlike atoms of stQM, and that a formula of Ref. 1 for energy eigenvalues cannot be true.

In Sec. III, it is shown that the system has an infinite number of bound states for any angular momentum. Since in our analysis of the Birman-Schwinger operator [Eq. (32)] we use an R-basis and for zero angular momentum elements of the basis are not in the domain of P^2, we use there the quadratic form associated with the operators.

Unlike in the case of stQM, the reduced Hamiltonians are not described by ordinary differential equations. However, we show in Sec. IV A that the coordinates of bound states with respect to an R-basis satisfy a second order difference equation. This equation differs from an eigenvalue equation of a Jacobi matrix in that the diagonal term of the equation can be written as $(q_1(n)-E)/(q_2(n)-E)$ instead of $(q(n)-E)$, where E is the eigenvalue. In addition, the equation becomes singular for some values of parameters. Nevertheless it is well adapted to numerical computation, providing a very useful heuristic tool (see Sec. IV C and Ref. 2), and it yields rigorous results, nondegeneracy of the spectrum of the reduced Hamiltonians, and exponential localization of the bound states.

The localization rate of energy eigenfunctions has here interesting properties, not encountered in stQM. As the energy tends to zero, the decay rate tends to zero, as in stQM. However, with decrease of the energy, the decay rate at first increases and then decreases again, passing through a point of a superexponential decay of the eigenfunctions. Furthermore, for energies close to zero, the eigenfunctions themselves are of constant sign at large distances, as in stQM. However, when one passes the point of superexponential decay the eigenfunctions become oscillatory at large distance. These features are related to the duality properties of the system, discussed in Ref. 14. We hope to write more on this in the future.

In the rest of this introduction we recall basic properties of the system and collect formulas for eigenvalues and eigenfunctions of the operator R^2.

Position operators,[8,9,4]

$$X_j = i\hbar\left((1+\beta\mathbf{P}^2)\partial_j + \beta' P_j\left(\sum_k P_k\partial_k\right)\right), \quad j=1,\ldots,D, \tag{1}$$

act on functions of $\mathbf{p}\in\mathbb{R}^D$; here β and β' are non-negative constants, $\partial_k=\partial/\partial p_k$, and P_j, $P_j f(\mathbf{p})=p_j f(\mathbf{p})$, are the momentum operators. The operators [Eq. (1)] are symmetric when acting in the Hilbert space $L^2(\mathbb{R}^D, w_0(p)\mathrm{d}^D\mathbf{p})$ with scalar product

$$(f|g) = \int \mathrm{d}^D\mathbf{p}\, w_0(p) f^*(\mathbf{p}) g(\mathbf{p}), \quad w_0(p) = \frac{1}{(1+\alpha p^2)^{1+\chi}}, \quad \chi = \frac{\beta'}{2\alpha}\bar{D}; \tag{2}$$

here and below

$$\alpha = \beta + \beta' \quad \text{and } \bar{D} = D-1. \tag{3}$$

In most of the present paper we assume that $D\geqslant 2$.

In three (space) dimensions, the Hamiltonian is

$$H = \frac{1}{2M}\mathbf{P}^2 - \frac{k}{R}, \quad \text{where } R = \left(\sum_j X_j^2\right)^{1/2}, \quad k = k_e e^2, \tag{4}$$

and M is the (reduced) mass. More generally, in dimension $D\geqslant 3$, one should consider

$$H = H_0 + V, \quad H_0 = \frac{1}{2M}\mathbf{P}^2, \quad V = -\frac{k}{R^{D-2}}. \tag{5}$$

However, we will work with the Hamiltonian [Eq. (4)] and in most of the work we assume that $D\geqslant 2$.

Change of variables $\mathbf{p}\mapsto\bar{\mathbf{p}}=\sqrt{\alpha}\mathbf{p}$, leads to dimensionless operators $\bar{X}_j$, $\bar{R}^2$, and $\bar{H}$:

$$X_j=\sqrt{\alpha}\hbar\bar{X}_j,\quad \bar{X}_j=i\left[(1+\eta\bar{\mathbf{P}}^2)\bar{\partial}_j+(1-\eta)\bar{P}_j\left(\sum_k\bar{P}_k\bar{\partial}_k\right)\right],\quad 1\leqslant j\leqslant D, \tag{6}$$

$$R=\sqrt{\alpha}\hbar\bar{R},\quad \bar{R}^2=\sum_j\bar{X}_j^2\quad\text{and } H=\frac{1}{2\alpha M}\bar{H},\quad \bar{H}=\bar{\mathbf{P}}^2-\frac{\vartheta}{\bar{R}}, \tag{7}$$

where $\bar{P}_j$ is the operator of multiplication by $\bar{p}_j$ and we introduced the dimensionless quantities

$$\eta=\frac{\beta}{\alpha},\quad \vartheta=\frac{2\sqrt{\alpha}Mk}{\hbar};\quad \bar{\partial}_j=\frac{\partial}{\partial\bar{p}_j}=\frac{1}{\sqrt{\alpha}}\frac{\partial}{\partial p_j}$$

[$\sqrt{\alpha}\hbar$ is closely related to the minimal length of the theory (see Ref. 14, Sec. II B)]. Furthermore, considering (α,η) instead of (β,β') of Eq. (1) as the parameters of the system, we see that $\bar{\mathbf{X}}$, $\bar{R}$, and $\bar{H}$ depend on η but not on α.

These formulas explain the form of the α dependence (scaling) of the eigenvalues [Eq. (11)] of R, of the change of variables [Eq. (8)] below, of the way α enters into the reduced Hamiltonian [Eq. (14)], and of the fact that the Hilbert space depends on the parameters only through η. However, we work with the variable $\mathbf{p}$ in most of the paper.

We will use below formulas of Ref. 14 [Eqs. (46) and (47)] for the spectrum of the radial part R_L^2 of the R^2 operator at angular momentum L, or more precisely, of its Friedrichs version. After passing to the z variable,

$$p=\frac{1}{\sqrt{\alpha}}\sqrt{\frac{1+z}{1-z}},\quad -1<z<1,\quad z=\frac{\alpha p^2-1}{\alpha p^2+1}, \tag{8}$$

setting

$$D_1=\frac{1}{2}\bar{D}-\frac{1}{2},\quad D_2=\frac{1}{2}\eta\bar{D}+\frac{1}{2}, \tag{9}$$

$$c=a+b+1,\quad a=a(\eta,L)=\sqrt{D_2^2+\eta^2L^2},\quad b=b(\eta,L)=\sqrt{D_1^2+L^2},$$

$$\sigma_1=-\frac{1}{2}D_1+\frac{1}{2}b(\eta,L),\quad \sigma_2=\frac{1}{2}D_2+\frac{1}{2}a(\eta,L), \tag{10}$$

and performing the gauge transformation $\Psi\mapsto\Phi$, $\Phi(z)=(1+z)^{\sigma_1}(1-z)^{\sigma_2}\Psi(z)$, i.e., setting $f(p)=(1+z)^{\sigma_1}(1-z)^{\sigma_2}\Psi(z)$ for a function f of the radial variable p, p and z related by Eq. (8), one obtains

$$\Psi_{L,n}(z)=P_n^{(a,b)}(z),\quad r_{L,n}=2\hbar\sqrt{\alpha}\sqrt{\rho_{L,n}} \tag{11}$$

for eigenfunctions and eigenvalues of the operator R_L^2, the reduction of the Friedrichs version of R^2 at angular momentum L, where $P_n^{(a,b)}$ are the Jacobi polynomials and

$$\rho_{L,n}=\left(n+\frac{c}{2}\right)^2-\frac{1}{4}(\chi^2+(1-\eta)^2L^2)=\left(n+\frac{c}{2}\right)^2-\frac{1}{16}(1-\eta)^2((D-1)^2+4L^2), \tag{12}$$

$n=0,1,\ldots$. Here R_L^2 acts in the Hilbert space

$$\mathcal{H} = \mathcal{H}^{(a,b)} = L^2([-1,1], w^{(a,b)}(z)\mathrm{d}z), \quad w^{(a,b)}(z) = (1-z)^a(1+z)^b \tag{13}$$

of the radial degrees of freedom.

Given these formulas, this paper is essentially independent from that of Ref. 14.

II. THE REDUCED HAMILTONIAN, BOUND STATES, AND THEIR PROPERTIES

The Hamiltonian. We turn now to an analysis of the Hamiltonian [Eq. (4)] in any dimension $D \geqslant 2$. For reasons explained,[14] the radial operator R used below is the one defined by the Friedrichs version of R^2. While most of the following applies to general spherically symmetric potentials with suitable behavior at infinity, the potentials of Eq. (5), in particular, to streamline the paper we restrict our attention to the Coulomb potential.

Since the spectrum of R is bounded away from zero, the operator $V = -k/R$ is bounded and therefore the domain of H coincides with that of $\mathbf{P}^2$. In fact, V is a compact operator, as can be seen from its spectrum. Hence, by Weyl's theorem,[12] $\sigma_{\mathrm{ess}}(H) = [0, +\infty[$, and the negative part of the spectrum of H consists of eigenvalues of finite multiplicity, with zero as their only possible accumulation point.

Boundedness of V leads to a simple definition of H and of its domain. However, some of the eigenfunctions of V are not in the domain of H_0, or H_0^{-1}, while being in the domain of quadratic forms associated with these operators. This explains the appearance of quadratic form arguments in this and the following section.

A. Basic properties of the reduced Hamiltonian

More precise information about H is obtained from consideration of the reduced Hamiltonians,

$$H_L = H_{L,0} + V_L, \tag{14}$$

where

$$H_{L,0} = H_{L,0}(\alpha, \eta) = \frac{1}{2\alpha M}\frac{1+Z}{1-Z}, \quad V_L = V_L(\alpha, \eta) = -\frac{k}{r_L(N)}, \tag{15}$$

and $r_L(N)\Psi_{L,n} = r_{L,n}\Psi_{L,n}$, $r_{L,n} \geqslant 0$ as in Eq. (11), and Z is the operator of multiplication by the variable z. H_L acts in the Hilbert space of Eq. (13).

From the expression [Ref. 14, Eq. (15)] of the reduced R^2 operator, it follows that R_L^2 is an increasing function of L and that therefore eigenvalues of H_L have also this property. Also, Eq. (12) implies that $r_{L,n}$ has a lower bound proportional to L and that therefore the lowest eigenvalue of H_L is bounded below by a number proportional to $-1/L$, a situation similar to that of stQM.

The eigenvalue problem for Eq. (14) can be rewritten as

$$\left[\frac{1+Z}{1-Z} + \varepsilon - \frac{\vartheta}{r_L(N)}\right]\Phi = 0, \quad \text{where } \varepsilon = -2\alpha M E > 0, \quad \vartheta = \frac{Mk\sqrt{\alpha}}{\hbar}, \tag{16}$$

i.e., as an eigenvalue problem for the Hamiltonian,

$$\bar{H} = \bar{H}(\vartheta) = \bar{H}_0 + \bar{V}, \quad \bar{H}_0 = \frac{1+Z}{1-Z}, \quad \bar{V} = \bar{V}_L(\vartheta) = -\frac{\vartheta}{\bar{r}_L(N)}, \quad \bar{r}_{L,n} = \frac{r_{L,n}}{2\hbar\sqrt{\alpha}}, \tag{17}$$

the dimensionless version of Eq. (14). We show in Sec. IV B that the discrete spectrum of Eq. (17) is nondegenerate, i.e., eigenvalues $\{\varepsilon_i\}$ of $\bar{H}$ can be so labeled that

$$\varepsilon_1 > \varepsilon_2 > \cdots, \quad \varepsilon_n \to 0 \quad \text{as } n \to \infty;$$

ε_n depend on (L, α, η). We now fix η and L, so that the Hilbert space on which the operators $\bar{H}(\vartheta)$ act is fixed; we consider ϑ to be the parameter of the problem and we look at the properties of $\vartheta \mapsto \varepsilon_n(\vartheta)$.

$\vartheta \mapsto \bar{H}(\vartheta)$, $\vartheta \in \mathbb{C}$, is an analytic family of type (A) in the sense of Ref. 7, p. 375 and Ref. 12, p. 16, since its domain is independent of ϑ and for each Φ in the domain of $\bar{H}_0$, $\bar{H}(\vartheta)\Phi$ is an analytic (linear) function of ϑ [this argument can be applied directly to Eq. (7)]. Since for each $\vartheta \in]0, +\infty[$ and each n the eigenvalue $\varepsilon_n(\vartheta) = \varepsilon_{L,n}(\vartheta)$ is isolated and nondegenerate, by Ref. 12, p. 17, Theorem XII.9, $\vartheta \mapsto \varepsilon_n(\vartheta)$ extends to an analytic function, denoted again by ε_n, in some open subset Ω of $\mathbb{C}$ containing $]0, +\infty[$. We also note that Eq. (16) implies that for fixed η, $\varepsilon_{L,n}$ is an increasing function of $\alpha \in]0, +\infty[$, and since $\varepsilon_{L,n}$ is not identically zero, it has no zero in $]0, +\infty[$.

B. Lifting accidental degeneracy and another corollary of analyticity

We will now use the information about analyticity properties of $\vartheta \mapsto \varepsilon_n(\vartheta)$ to prove two facts: first, that for $\beta' = 0$, generically in $\alpha > 0$, the spectrum of Eq. (4) is not L-degenerate (this is an answer to a question of Yosi Avron about lifting of accidental degeneracy of the spectrum of a Hydrogen atom), and second, that a formula of Ref. 1 for the ground state energy $E_{0,1}(\alpha)$ cannot be true.

Proposition: *For* $\beta' = 0$ (i.e., $\eta = 1$) *if* $(L, n) \neq (L', n')$ *then for any* $\alpha_0 > 0$ *the set of* α *larger than* α_0 *for which* $E_{L,n}(\alpha) = E_{L',n'}(\alpha)$ *is finite. In other words, the set of* $\alpha > 0$ *for which* $E_{L,n}(\alpha) = E_{L',n'}(\alpha)$ *can have only* 0 *as accumulation point. This statement holds also for any fixed* $\eta \neq 1$, *possibly apart from a countable number of values of* η.

To prove the Proposition, we show first that, for any η,

$$\varepsilon_{L,n}(\vartheta)/\vartheta \to 1/\bar{r}_{L,n} \quad \text{as } \vartheta \to \infty, \tag{18}$$

then use the analyticity to reduce the proof to show that $\bar{r}_{L,n} \neq \bar{r}_{L',n'}$ if $(L, n) \neq (L', n')$, which in turn is demonstrated using an elementary argument.

Consider the operator

$$\hat{H}(\vartheta) = \frac{1}{\vartheta}\frac{1+Z}{1-Z} - \frac{1}{\bar{r}(N)} = \hat{H}_0(\vartheta) - \frac{1}{\bar{r}(N)}.$$

Its eigenvalues are $\hat{\varepsilon}_{L,n}(\vartheta) = -\varepsilon_{L,n}(\vartheta)/\vartheta$. To prove that

$$\hat{\varepsilon}_{L,n}(\vartheta) \to -1/\bar{r}_{L,n} \quad \text{as } \vartheta \to \infty, \tag{19}$$

we note first that since $\hat{H}_0(\vartheta)$ is a positive operator, one has

$$\hat{\varepsilon}_{L,n}(\vartheta) \geqslant -1/\bar{r}_{L,n} \quad \text{for any } \vartheta > 0. \tag{20}$$

On the other hand, a slight extension of Ref. 12, p. 83, Theorem XIII.3, "the Rayleigh-Ritz technique," yields an upper bound on $\hat{\varepsilon}_{L,n}(\vartheta)$ which converges to $-1/\bar{r}_{L,n}$. Namely, we want P of this theorem to be the projection on the linear span of the first q eigenvectors $\Phi_1, \ldots, \Phi_q$ of $1/\bar{r}(N)$. The slight extension consists in letting the V of the proof of Ref. 12, p. 83, Theorem XIII.3, to be a finite dimensional subspace of the domain of the quadratic form associated with H and then letting H_V of the proof be the restriction of this quadratic form to V. (This can be proven in the same way as the quadratic form version of Theorem XIII.1, i.e., Theorem XIII.2, is proven.) The quadratic form version is needed since, as is easy to see, for $L=0$ the vectors $\Phi_{L,n}$ are not in the domain of $\hat{H}_0(\vartheta)$ but are in the domain of the quadratic form associated with this operator (Ref. 11 p. 277).

If $Q_{i,j}$, $i,j=1,\ldots,q$, are the (Φ_i,Φ_j)-matrix elements of the quadratic form associated with $(1+Z)/(1-Z)$, the (Φ_i,Φ_j)-matrix elements of the quadratic form associated with $\hat{H}_0(\vartheta)$ are

$$\frac{1}{\vartheta}Q_{i,j}-\frac{1}{\bar{r}_{L,i}}\delta_{i,j}, \quad i,j=1,\ldots,q. \tag{21}$$

According to the quadratic form version of Ref. 12, p. 83, Theorem XIII.3, denoting by $\hat{\varepsilon}^q_{L,n}(\vartheta)$ eigenvalues of this matrix, one has

$$\hat{\varepsilon}^q_{L,n}(\vartheta) \geqslant \hat{\varepsilon}_{L,n}(ta), \quad n=1,\ldots,q. \tag{22}$$

On the other hand, since one deals here with a finite dimensional case, $\hat{\varepsilon}^q_{L,n}(\vartheta)\to -1/\bar{r}_{L,n}$ as $\vartheta\to\infty$. Since q is arbitrary, combining bounds (20) and (22), one obtains Eq. (19).

Since $\varepsilon_{L,n}(\vartheta)/\vartheta$ are analytic functions of ϑ in open sets containing $]0,+\infty[$, to prove the Proposition it is enough to show that $\varepsilon_{L,n}(\vartheta)/\vartheta\neq\varepsilon_{L,n}(\vartheta)/\vartheta$ for large ϑ, or by Eq. (18), that $\bar{r}_{L,n}\neq\bar{r}_{L',n'}$.

We deal first with the case of $\eta=1$. Since then $\bar{r}_{L,n}=n+c(L)/2$, it is enough to show that for $m\neq n$, $c(m)-c(n)$ is not an integer. We prove it here for $D=3$ only: in general, if D is odd the proof goes through almost verbatim whereas for even D the argument is somewhat different.

Since [see Eq. (9)]

$$c(\ell)=\sqrt{9/4+\ell(\ell+1)}+\sqrt{1/4+\ell(\ell+1)}+1/2=\sqrt{2+\left(\ell+\frac{1}{2}\right)^2}+\ell+1,$$

it is enough to show that K defined by

$$K=\sqrt{2+\left(n+\frac{1}{2}\right)^2}-\sqrt{2+\left(m+\frac{1}{2}\right)^2} \tag{23}$$

is not an integer for any integers m,n, $m\neq n$.

Now, since

$$\sqrt{2+\left(n+\frac{1}{2}\right)^2}-\sqrt{2+\left(m+\frac{1}{2}\right)^2}=\frac{(n+m+1)(n-m)}{\sqrt{2+\left(n+\frac{1}{2}\right)^2}+\sqrt{2+\left(m+\frac{1}{2}\right)^2}},$$

one has

$$\sqrt{2+\left(n+\frac{1}{2}\right)^2}+\sqrt{2+\left(m+\frac{1}{2}\right)^2}=\frac{(n+m+1)(n-m)}{K}. \tag{24}$$

Assuming that K is an integer and solving Eqs. (23) and (24) for the square roots, one obtains that $\sqrt{2+(n+1/2)^2}$ is a rational number, say, $\sqrt{2+(n+1/2)^2}=p/q$, where the integers p,q are relatively prime. Then

$$\frac{(2n+1)^2}{4}=\frac{p^2-2q^2}{q^2}. \tag{25}$$

But if p,q are relatively prime then so are p^2-2q^2 and q^2, and therefore Eq. (25) implies that q is an even integer, say, $q=2m$. It follows that $(p^2-8m^2)/m^2$ is an odd integer, which in turn implies that p^2/m^2 is an odd integer, contradicting the assumption that p,q are relatively prime, and proving the Proposition for $\eta=1$.

Passing to arbitrary η, $0<\eta\leqslant 1$, our problem is again in determining when $\bar{r}_{L,n}\neq\bar{r}_{L',n'}$ for $(L,n)\neq(L',n')$, or, equivalently, when $\rho_{L,n}\neq\rho_{L',n'}$ for $(L,n)\neq(L',n')$, $\rho_{L,n}$ given by Eq. (12). Since

$$4(\rho_{L,n}-\rho_{L',n'}) = ((2n+c(L))^2-(1-\eta)^2L^2)-((2n'+c(L'))^2-(1-\eta)^2L'^2), \tag{26}$$

where c is as in Eq. (9), it is enough to find η for which the right hand side of identity (26) is zero. Now, it is easy to see that the last condition is equivalent to η being a zero of a (degree 8) nonzero polynomial in η. Therefore for each (L,n,L',n'), $\bar{r}_{L,n}=\bar{r}_{L',n'}$ for a finite number of values of η. Combining these values for all possible (L,n,L',n') we obtain the denumerable set of the Proposition.

As another corollary of analyticity of eigenvalues we will show that a formula of Ref. 1 for zero angular momentum bound state energies cannot be true. According to Ref. 1, the nth energy level can be obtained from the equation

$$\kappa(1-\alpha\kappa^2) = \frac{Z\tilde{\alpha}Mc}{n}, \quad \kappa = \sqrt{2M|E|}, \tag{27}$$

where $\tilde{\alpha}$ is the fine structure constant and c is the speed of light, supplemented by a rule for the choice of the root of the cubic equation [Eq. (27)]. It is not hard to show that this leads to discontinuity of κ at

$$\alpha_n = \frac{4}{27}\frac{n^2}{Z^2\tilde{\alpha}m^2c^2}, \quad n=1,2,\ldots .$$

Since these discontinuities occur at relatively large values of α, and one is interested mainly in small α, it has been argued that these discontinuities are not relevant to the present problem. However, we will prove now that one has here a more troubling difficulty: we will show that if $\kappa=\kappa(\alpha,n)$ satisfies Eq. (27) for small values of α then one cannot have the analyticity properties of $E_{0,n}$ described above. More precisely, one has the following.

If there exists $\alpha'>0$ such that $\chi=\chi(\alpha,n)$ satisfies Eq. (27) for $\alpha<\alpha'$ and $\sqrt{\alpha}\chi(\alpha,n)\to 0$ as $\alpha\to 0$, then $E_{0,n}$ cannot be a smooth function of α.

Let $x=\sqrt{\alpha}\kappa$. Then $x=\sqrt{\varepsilon}$ and Eq. (27) can be rewritten as

$$x(1-x^2) = a\vartheta, \quad \text{where } a=a_n=Z\tilde{\alpha}c\hbar/(kn). \tag{28}$$

That something is wrong here can be seen by plotting the left hand side of Eq. (28). The graph shows that there is no positive solution of Eq. (28) for $a\sqrt{\alpha}>0.4$ (more precisely, for $a\sqrt{\alpha}>2\sqrt{3}/9$). We now proceed with a proof of the statement.

Let $F(x,\vartheta)=x(1-x^2)-a\vartheta$. Noting that $F(0,0)=0$ and $F_x(0,0)=1$ and then applying implicit function theorem, one obtains that a solution of Eq. (28) which tends to zero with α is an analytic function of ϑ for small $|\vartheta|$. By positivity and analyticity of ε for $\alpha>0$, $\vartheta\mapsto x(\vartheta)$ extends to an analytic function of $\vartheta>0$ and by permanence property of algebraic equations, this analytic function, denoted again by x, satisfies the equation

$$x(1-x^2)-a\vartheta = 0 \tag{29}$$

for all $\vartheta>0$. Now, differentiating Eq. (29) with respect to ϑ, one obtains

$$x'(1-3x^2) = a, \quad \text{where } x' = \frac{\mathrm{d}x}{\mathrm{d}\vartheta}. \tag{30}$$

But, as is not hard to see, Eqs. (29) and (30) imply that for $\vartheta<\vartheta_1:=2x/(a3\sqrt{3})$ is an increasing function of ϑ and that $x\to\infty$ as $\vartheta\nearrow\vartheta_1$. This contradiction with analyticity proves our statement.

We refer the reader to Ref. 2, Fig. 1, for a graphical illustration of the above (the graph is obtained from a numerical solution of the difference equation of [Eq. (51)] below).

III. INFINITE NUMBER OF BOUND STATES FOR ANY ANGULAR MOMENTUM

Birman-Schwinger principle (method). With the notation of Eq. (17), Eq. (16) is

$$(\bar{H}_0 + \varepsilon + \bar{V})\Phi = 0,$$

which can be rewritten as

$$(|\bar{V}|^{1/2}(\bar{H}_0 + \varepsilon)^{-1}|\bar{V}|^{1/2})(|\bar{V}|^{1/2}\Phi) = |\bar{V}|^{1/2}\Phi. \tag{31}$$

According to the Birman-Schwinger principle (Ref. 13, p. 86 and Ref. 12, p.99), the number of eigenvalues of $\bar{H}$ smaller than $-\varepsilon$ is equal to the number of eigenvalues of

$$K_\varepsilon \coloneqq |\bar{V}|^{1/2}(\bar{H}_0 + \varepsilon)^{-1}|\bar{V}|^{1/2}, \tag{32}$$

which are larger than 1. (Proof of this fact is especially easy in our case, since negative eigenvalues are nondegenerate, as will be shown in Sec. IV B.)

Here are two elementary but important properties of K_ε, $\varepsilon > 0$,

Property $(K1)$. K_ε is a compact operator: $(\bar{H}_0+\varepsilon)^{-1}$ is bounded and $\bar{V}$ is compact.

Property $(K2)$. (Strict) Positivity and monotonicity: for any nonzero Φ, $(\Phi|K_\varepsilon\Phi) > 0$ and

$$(\Phi|K_\varepsilon\Phi) < (\Phi|K_{\varepsilon'}\Phi) \quad \text{for } \varepsilon > \varepsilon'.$$

It would be not hard to show at this point that there is at least one negative eigenvalue for any α: as $\varepsilon \to 0$, the norm of the positive compact operator K_ε tends to infinity, in any dimension; and the norm of a positive compact operator is an eigenvalue. However, a much stronger result is obtained below.

A. Zero-energy ($\varepsilon \searrow 0$) limits of matrix elements of K_ε

We work here with general $a > -1$, $b > 0$. The assumption on b, which holds for any L if $D > 2$, is used in taking the limit of $(\Phi_m|K_\varepsilon\Phi_n)$ as $\varepsilon \searrow 0$: singularity appears at $p=0$ ($z=-1$, i.e., at the b end of the interval), since the middle term of the right hand side of Eq. (32) is proportional to P^{-2}. The case of $b=0$ requires a separate consideration. With the above values of b, the calculations below show that the $(\varepsilon \searrow 0)$ limit of quadratic form defined by K_ε exists; for nonzero angular momentum one obtains also an operator limit.

We will compute now

$$K_{m,n} \coloneqq \lim_{\varepsilon \searrow 0} (\hat{P}_m|K_\varepsilon \hat{P}_n), \quad \text{where } \hat{P}_n = P_n^{(a,b)}/\|P_n^{(a,b)}\| \tag{33}$$

are the normalized eigenfunctions of R_L^2, and $m,n=0,1,\ldots$; $K_{m,n}$ will be used in a proof of the fact that the limit of K_ε as $\varepsilon \searrow 0$ defines an unbounded operator.

Since

$$(\hat{P}_m|K_\varepsilon \hat{P}_n) = \sqrt{\frac{\vartheta_m\vartheta_n}{h_m h_n}} \int_{-1}^{1} \mathrm{d}z\, w^{(a,b)}(z) \frac{1-z}{1+\varepsilon+z(1-\varepsilon)} P_m^{(a,b)}(z) P_n^{(a,b)}(z), \tag{34}$$

where

$$\vartheta_n = \vartheta/\sqrt{\rho_n} = \vartheta/\bar{r}_n, \quad h_n = \int_{-1}^{1} \mathrm{d}z\, w^{(a,b)}(z) |P_n^{(a,b)}(z)|^2,$$

for $b > 0$, the $(\varepsilon \searrow 0)$ limit of Eq. (34) exists:

$$K_{m,n} = \sqrt{\frac{\vartheta_m \vartheta_n}{h_m h_n}} \int_{-1}^{1} \mathrm{d}z w^{(a,b)}(z) \frac{1-z}{1+z} P_m^{(a,b)}(z) P_n^{(a,b)}(z).$$

We will first compute the matrix elements of the quadratic form associated with $(\bar{H}_0)^{-1}$:

$$k_{m,n} := \frac{1}{\sqrt{h_m h_n}} \int_{-1}^{1} \mathrm{d}z w^{(a,b)}(z) \frac{1-z}{1+z} P_m^{(a,b)}(z) P_n^{(a,b)}(z);$$

we will do this for arbitrary $a > -1$, $b > 0$. Since the matrix $(k_{m,n})$ is symmetric, it is enough to consider the case of $n \geqslant m$.

The following formulas will be used in the computation: for general a, b, $\mathrm{Re}\, a > -1$, $\mathrm{Re}\, b > -1$, one has the orthogonality relations

$$\int_{-1}^{1} (1-z)^a (1+z)^b P_m^{(a,b)}(z) P_n^{(a,b)}(z) \mathrm{d}z = \delta_{m,n} \frac{2^{a+b+1} \Gamma(n+a+1) \Gamma(n+b+1)}{n!(2n+a+b+1) \Gamma(n+a+b+1)}, \tag{35}$$

(Ref. 6, p. 1036, 8.962.1), which yields normalization constants h_n for Jacobi polynomials,

$$h_n = \int_{-1}^{1} \mathrm{d}z (1-z)^a (1+z)^b [P_n^{(a,b)}(z)]^2 = \frac{2^{a+b+1} \Gamma(n+a+1) \Gamma(n+b+1)}{n!(2n+a+b+1) \Gamma(n+a+b+1)}; \tag{36}$$

and

$$\int_{-1}^{1} \mathrm{d}z (1-z)^a (1+z)^c P_n^{(a,b)}(z) = \frac{2^{a+c+1} \Gamma(c+1) \Gamma(a+n+1) \Gamma(c-b+1)}{n! \Gamma(c-b-n+1) \Gamma(c+a+n+2)}, \tag{37}$$

[Ref. 5, p. 284, 16.4(1)], which holds for $\mathrm{Re}\, a > -1$ and $\mathrm{Re}\, c > -1$ and under the condition that no argument of the Γ functions on the right hand sides is a negative integer. In the latter case the values of the integrals are obtained by taking a limit, as is done below. [The factorial $n!$ of Eq. (37) is missing in Ref. 5.]

To compute $k_{m,n}$ for arbitrary $n \geqslant m$ we proceed as follows. By Ref. 6, p. 1036, 8.962,

$$P_n^{(a,b)}(-1) = (-1)^n \frac{\Gamma(n+b+1)}{n! \Gamma(b+1)}.$$

Since the polynomial $P_n^{(a,b)}(z) - P_n^{(a,b)}(-1)$ is equal zero at $z=-1$, it is divisible by $z+1$. Hence, one can write

$$P_n^{(a,b)}(z) = (-1)^n \frac{\Gamma(n+b+1)}{n! \Gamma(b+1)} + (z+1) Q_{n-1}(z), \tag{38}$$

where Q_{n-1} is a polynomial of order $n-1$.

Now, for arbitrary (m,n),

$$k_{m,n} = (h_m h_n)^{-1/2} \int_{-1}^{1} \mathrm{d}z w^{(a,b)}(z) \frac{2-(1+z)}{1+z} P_m^{(a,b)}(z) P_n^{(a,b)}(z)$$

$$= \frac{2}{\sqrt{h_m h_n}} \int_{-1}^{1} \mathrm{d}z w^{(a,b-1)}(z) P_m^{(a,b)}(z) P_n^{(a,b)}(z) - \frac{1}{\sqrt{h_m h_n}} \int_{-1}^{1} \mathrm{d}z w^{(a,b)}(z) P_m^{(a,b)}(z) P_n^{(a,b)}(z) = k'_{m,n} - k''_{m,n}.$$

$k''_{m,n} = \delta_{m,n}$ by orthogonality relations [Eq. (35)]. As for $k'_{m,n}$, by Eq. (38),

$$k'_{m,n} = \frac{2(-1)^m\Gamma(m+b+1)}{m!\Gamma(b+1)\sqrt{h_m h_n}}\int_{-1}^{1} \mathrm{d}z w^{(a,b-1)}(z)P_n^{(a,b)}(z) + \frac{1}{\sqrt{h_m h_n}}\int_{-1}^{1} \mathrm{d}z w^{(a,b)}(z)Q_{m-1}(z)P_n^{(a,b)}(z).$$

The second term on the right hand side is zero for $n \geqslant m$ since Jacobi polynomial of order n is orthogonal to any polynomial of order smaller than n. To compute the first integral, we take the limit $c \to b-1$ in Eq. (37). Since $\Gamma(z)$ has simple poles at $z=-p$, $p=0,1,2,\ldots$, with residues $(-1)^p/p!$,

$$\lim_{\varepsilon\to 0} \varepsilon\Gamma(-p+\varepsilon) = \frac{(-1)^p}{p!}, \quad p = 0,1,2, \ldots ,$$

and one obtains

$$\int_{-1}^{1} \mathrm{d}z w^{(a,b-1)}(z)P_n^{(a,b)}(z) = (-1)^m \frac{2^{a+b}\Gamma(b)\Gamma(a+n+1)}{\Gamma(a+b+n+1)}. \tag{39}$$

Therefore

$$k'_{m,n} = 2^{a+b+1}(-1)^{m+n}\frac{\Gamma(m+b+1)}{m!b\sqrt{h_m h_n}}\frac{\Gamma(a+n+1)}{\Gamma(a+b+n+1)} \quad \text{for } n \geqslant m.$$

Substituting for h_n from Eq. (36) and setting $c=a+b+1$,

$$k'_{m,n} = \frac{(-1)^{m+n}}{b}\sqrt{(2m+c)(2n+c)}\sqrt{\frac{\Gamma(m+b+1)\Gamma(m+c)}{m!\Gamma(m+a+1)}\frac{n!\Gamma(n+a+1)}{\Gamma(n+b+1)\Gamma(n+c)}}.$$

Since $k''_{m,n}=\delta_{m,n}$ this yields

$$k_{m,n} = \frac{(-1)^{m+n}\sqrt{(2m+c)(2n+c)}}{b}\sqrt{\frac{\Gamma(m+b+1)\Gamma(m+c)}{m!\Gamma(m+a+1)}\frac{n!\Gamma(n+a+1)}{\Gamma(n+b+1)\Gamma(n+c)}} \tag{40}$$

for $n>m$ and $k_{n,n}=(2n+c)/b-1$, and then

$$K_{m,n} = \sqrt{\vartheta_m}k_{m,n}\sqrt{\vartheta_n}, \quad K_{n,m} = K_{m,n}. \tag{41}$$

We note that since $\sqrt{\vartheta_m} \geqslant \sqrt{\vartheta}/(n+c/2)$, one obtains that for $n>m$ the bound

$$(-1)^{m+n}K_{m,n} \geqslant 2\frac{\vartheta}{b}\frac{K_n}{K_m}, \quad \text{where} \quad K_n = \sqrt{\frac{n!\Gamma(n+a+1)}{\Gamma(n+b+1)\Gamma(n+c)}}. \tag{42}$$

B. K_ε, K, and infinite number of bound states

Let Q be the quadratic form defined as follows:

$$D(Q) = \{\Phi \in \mathcal{H}:(\Phi|K_\varepsilon\Phi) \leqslant c(\Phi) \quad \text{for all } \varepsilon > 0\}, \tag{43}$$

where $c(\Phi)$ is some (Φ-dependent) positive number, and for $\Phi \in D(Q)$, set

$$Q(\Phi) = \lim_{\varepsilon\searrow 0}(\Phi|K_\varepsilon\Phi).$$

The limit exists by the monotonicity property (K2) and the boundedness property of Eq. (43).

Lemma 1: Q is a densely defined strictly positive closed quadratic form.

That $D(Q)$ defined by Eq. (43) is a linear manifold follows from triangle inequality. Q is nondegenerate, since the kernel of K_ε is trivial and $Q(\Phi) \geqslant (\Phi|K_{\varepsilon(\Phi)}\Phi)$. $D(Q)$ is dense in $\mathcal{H}$ since it contains the orthogonal basis $\{\Phi_n\}$. It remains to show that the form Q is closed.

For $\Phi \in D(Q)$, set $\|\Phi\|_Q = \sqrt{Q(\Phi)}$, and suppose that for $\{\Psi_n\} \subset D(Q)$, $\|\Psi_n - \Psi\| \to 0$ and $\|\Psi_m - \Psi_n\|_Q \to 0$ as $m,n \to \infty$. Then since

$$\big| \|\Psi_n\|_Q - \|\Psi_m\|_Q \big| \leqslant \|\Psi_n - \Psi_m\|_Q$$

(true for any seminorm), the sequence $n \mapsto \|\Psi_n\|_Q$ is Cauchy, and therefore bounded. Thus, there exists a $c>0$ such that $\|\Psi_n\|_Q \leqslant c$ for all n. But then $\sqrt{(\Psi_n|K_\varepsilon \Psi_n)} \leqslant c$ for all n and all $\varepsilon>0$. Letting here $n \to \infty$, one obtains that $\sqrt{(\Psi|K_\varepsilon \Psi)} \leqslant c$ and that therefore $\Psi \in D(Q)$.

Since the quadratic form Q is densely defined closed and positive, it is a quadratic form associated with a unique self-adjoint operator. This operator, denoted by K, is characterized either by Ref. 7, p. 322, Theorem 2.1 or by Ref. 11, p. 277, Example 2.

Lemma 2: The operator K is unbounded.

Suppose that this is not the case, i.e., that K is a bounded operator. By Ref. 7, p. 322, the domain of K, $\mathcal{D}(K)$, is contained in the domain of Q. On the other hand, since K is closed and bounded, $\mathcal{D}(K)=\mathcal{H}$ and therefore $\mathcal{D}(Q)=\mathcal{H}$. It follows that $K_{m,n}=(\hat{\Phi}_m|K\hat{\Phi}_n)$. But then

$$\sum_m |K_{m,n}|^2 = \sum_m |(\hat{\Phi}_m|K\hat{\Phi}_n)|^2 = \|K\hat{\Phi}_n\|^2 \leqslant \|K\|^2.$$

Since

$$\sum_{m\geqslant 0} |K_{m,n}|^2 \geqslant \sum_{m>n}^{\infty} |K_{m,n}|^2 = \sum_{m>n}^{\infty} |K_{n,m}|^2,$$

to prove that the operator K is unbounded it is enough to show that either the series $\Sigma_{m>n}^{\infty}|K_{n,m}|^2$ is divergent or that it has a lower bound that tends to infinity with n.

Now, by Eq. (42),

$$\sum_{m>n}^{\infty} |K_{n,m}|^2 \geqslant \frac{4\vartheta^2}{b^2} \sum_{m>n} \frac{\Gamma(n+b+1)\Gamma(n+c)}{n!\Gamma(n+a+1)} \frac{m!\Gamma(m+a+1)}{\Gamma(m+b+1)\Gamma(m+c)}$$
$$= \frac{4\vartheta^2}{b^2} \frac{\Gamma(n+b+1)\Gamma(n+c)}{n!\Gamma(n+a+1)} \sum_{m>n} \frac{\Gamma(m+1)\Gamma(m+a+1)}{\Gamma(m+b+1)\Gamma(m+c)}. \tag{44}$$

As n tends to infinity, the asymptotic behavior of the sum on the right hand side of Eq. (44) is the same as that obtained by replacing in it gamma functions by the leading term in Stirling's formula, or, more precisely, to obtain a lower bound on the sum of Eq. (44) one can use a bound $\Gamma(z) \geqslant C_1 z^{z-1/2}e^{-z}$ for the Γ of the numerators and a bound $\Gamma(z) \leqslant C_2 z^{z-1/2}e^{-z}$ for the Γ of the denominators, where C_1 and C_2 are positive constants. Hence,

$$\sum_{m>n}^{\infty} \frac{\Gamma(m+1)\Gamma(m+a+1)}{\Gamma(m+b+1)\Gamma(m+c)} \geqslant A_1 \sum_{m>n} \frac{(m+1)^{(m+1)}(m+a+1)^{(m+a+1)}}{(m+b+1)^{(m+b+1)}(m+c)^{(m+c)}} \geqslant A_2 \sum_{m>n} m^{-2b};$$

A_1, A_2 here and A_3, A_4, A_5 below are positive constants which may depend on a,b but not on n. If $b \leqslant 1/2$ the series $\Sigma_{m>n}^{\infty} m^{-2b}$ is divergent, proving our statement. If $b>1/2$,

$$\sum_{m>n} m^{-2b} \geqslant A_3 \int_n^{+\infty} x^{-2b} \mathrm{d}x = A_3 \frac{1}{2b-1} n^{1-2b},$$

and therefore

$$\sum_{m>n}\frac{\Gamma(n+b+1)\Gamma(n+c)}{n!\Gamma(n+a+1)}\frac{m!\Gamma(m+a+1)}{\Gamma(m+b+1)\Gamma(m+c)} \geqslant A_4\frac{\Gamma(n+b+1)\Gamma(n+c)}{n!\Gamma(n+a+1)}\frac{1}{n^{2b-1}}$$

$$\geqslant A_5\frac{n^{b+1+c-1-a-1}}{n^{2b-1}} = A_5 n,$$

which is divergent as $n\to\infty$. Lemma 2 is proved.

Theorem: *In three or more dimensions (for $D>2$), for any positive α and any angular momentum L, the reduced Hamiltonian* [Eq. (14)] *has an infinite number of negative energy eigenstates. In two dimensions the statement is true for $L>0$.*

Pick any two positive numbers, say, 2 and 3. Since K is a positive unbounded operator, $P_{[3,+\infty[}\mathcal{D}(K)$ is an infinite dimensional subspace of $\mathcal{D}(K)$ (here $P_{[3,+\infty[}$ is the spectral projection of K corresponding to $[3,+\infty[\subset\mathbb{R}$). Thus for any natural number n there exists an n-dimensional subspace $\mathcal{D}_n$ of $\mathcal{D}(K)$

$$(\Phi|K\Phi) \geqslant 3(\Phi|\Phi) \quad \text{for any } \Phi\in\mathcal{D}_n.$$

By continuity (choosing a basis of $\mathcal{D}_n\cdots$), it follows that there exists $\varepsilon(n)$ such that

$$(\Phi|K_{\varepsilon(n)}\Phi) \geqslant 2(\Phi|\Phi) \quad \text{for any } \Phi\in\mathcal{D}_n$$

[in fact this is true for any $\varepsilon\leqslant\varepsilon(n)$]. But this implies that each $K_{\varepsilon(n)}$ has at least n eigenvalues larger than 1, i.e., that H has at least n eigenvalues below $-\varepsilon(n)$. Since this is true for any natural n, the theorem holds.

C. Matrix elements of P^2

(this is not used in the following)

We note that $k_{m,n}$ are essentially the matrix elements of $(P^2)^{-1}$ in the basis $(\hat{\Phi}_n)$. To obtain the matrix elements of P^2, one could repeat with a minor change the calculations that yield $k_{m,n}$. Here is an easier way, using the duality between $p=0$ and $p=\infty$.

Making dependence on (a,b) explicit, the matrix elements of P^2 are

$$\hat{p}_{m,n} = \hat{p}^{(a,b)}_{m,n} = \frac{1}{\sqrt{h_m h_n}}\int_{-1}^{1}\mathrm{d}z(1-z)^a(1+z)^b\frac{1+z}{1-z}P_m^{(a,b)}(z)P_n^{(a,b)}(z).$$

Performing the change of variables $z\mapsto -z$, using the fact that $P_n^{(a,b)}(-z)=(-1)^nP_n^{(b,a)}(z)$ and that the normalization constants h_n are symmetric in a,b, one obtains

$$\hat{p}^{(a,b)}_{m,n} = (-1)^{m+n}\frac{1}{\sqrt{h_m h_n}}\int_{-1}^{1}\mathrm{d}z(1+z)^a(1-z)^b\frac{1-z}{1+z}P_m^{(b,a)}(z)P_n^{(b,a)}(z) = (-1)^{m+n}k^{(b,a)}_{m,n},$$

i.e.,

$$\hat{p}_{m,n} = \frac{\sqrt{(2m+c)(2n+c)}}{b}\sqrt{\frac{\Gamma(m+b+1)\Gamma(m+c)}{m!\Gamma(m+a+1)}\frac{n!\Gamma(n+a+1)}{\Gamma(n+b+1)\Gamma(n+c)}} \quad \text{for} \quad n<m,$$

$$\hat{p}_{n,n} = \frac{2n+c}{b} - 1.$$

IV. DIFFERENCE EQUATION AND PROPERTIES OF BOUND STATES

Using the difference equation derived below, we prove here the nondegeneracy of spectra of the reduced Hamiltonians and (exponential or better) localization properties of their eigenvectors.

A. Recursion relations

With $c=a+b+1$, a,b arbitrary, and P_{-1} set equal to zero, Jacobi polynomials satisfy the following recursion relations:

$$2(n+1)(n+c)(2n+c-1)P_{n+1}(z) = (2n+c)[(2n+c-1)(2n+c+1)z+a^2-b^2] \times P_n(z) - 2(n+a)(n+b)(2n+c+1)P_{n-1}(z)$$

for $n \geqslant 1$ and

$$2(n+1)(n+c)(2n+c-1)P_{n+1}(z) = (2n+c)[(2n+c-1)(2n+c+1)z+a^2-b^2]P_n(z)$$

for $n=0$, a special case of contiguity relations for the hypergeometric function [Ref. 6, p. 1035, 8.961.2]; for $n=0$ one has to drop the P_{n-1} term. For $c>1$, as in the case at hand, this is equivalent to

$$ZP_n = a_n P_{n+1} + b_n P_n + c_n P_{n-1}, \tag{45}$$

where

$$a_n = \frac{2(n+1)(n+c)}{(2n+c)(2n+c+1)}, \quad b_n = \frac{b^2-a^2}{(2n+c-1)(2n+c+1)}, \quad c_n = \frac{2(n+a)(n+b)}{(2n+c)(2n+c-1)}. \tag{46}$$

With $\hat{P}_n = P_n/\sqrt{h_n}$ and $h_n = \|P_n\|^2$ [see Eqs. (33) and (36)], Eq. (45) is

$$Z\hat{P}_n = \hat{a}_n \hat{P}_{n+1} + b_n \hat{P}_n + \hat{c}_n \hat{P}_{n-1}, \quad \text{where } \hat{a}_n = a_n \frac{\sqrt{h_{n+1}}}{\sqrt{h_n}}, \quad \hat{c}_n = c_n \frac{\sqrt{h_{n-1}}}{\sqrt{h_n}}. \tag{47}$$

We note that since Z is a symmetric operator, one has $(\hat{P}_n | Z\hat{P}_{n+1}) = (Z\hat{P}_n | \hat{P}_{n+1})$, i.e., $\hat{a}_n = \hat{c}_{n+1}$.

Let

$$\Phi = \sum_{n \geqslant 0} f_n \hat{P}_n \tag{48}$$

be the expansion of an eigenvector Φ of H in terms of normalized Jacobi polynomials $\hat{P}_n$. Since $1-Z$ is a bounded operator with trivial kernel, Eq. (16) implies that

$$[1+Z+(1-Z)(\varepsilon - \vartheta/\bar{r}(N))]\Phi = 0; \tag{49}$$

and since the operator in the square bracket is bounded, one has

$$\sum_{n \geqslant 0} f_n[(1+z)+(1-z)(\varepsilon-\vartheta_n)]\hat{P}_n = 0, \quad \text{i.e.,} \sum_{n \geqslant 0} f_n[(1+\varepsilon-\vartheta_n)+(1-\varepsilon+\vartheta_n)z]\hat{P}_n = 0.$$

By Eq. (47), with $P_{-1}=0$, this is

$$\sum_{n \geqslant 0} f_n[(1+\varepsilon-\vartheta_n)\hat{P}_n + (1-\varepsilon+\vartheta_n)(\hat{a}_n\hat{P}_{n+1} + b_n\hat{P}_n + \hat{c}_n\hat{P}_{n-1})] = 0,$$

or

$$\sum_{n \geqslant 0} f_n[(1-\varepsilon+\vartheta_n)(\hat{a}_n\hat{P}_{n+1} + \hat{c}_n\hat{P}_{n-1}) + ((1+\varepsilon-\vartheta_n)+(1-\varepsilon+\vartheta_n)b_n)\hat{P}_n] = 0,$$

which, on setting

$$s_n = 1-\varepsilon+\vartheta_n \quad \left(\lim_{n\to+\infty} s_n = 1-\varepsilon\right), \tag{50a}$$

$$t_n = (1 + \varepsilon - \vartheta_n) + (1 - \varepsilon + \vartheta_n)b_n = s_n(b_n - 1) + 2 \quad (\lim_{n\to+\infty} t_n = 1 + \varepsilon) \tag{50b}$$

is

$$\sum_n f_n[s_n(\hat{a}_n\hat{P}_{n+1} + \hat{c}_n\hat{P}_{n-1}) + t_n\hat{P}_n] = 0.$$

Finally, taking a scalar product with $\hat{P}_n$, one obtains the difference equation

$$\hat{c}_{n+1}s_{n+1}f_{n+1} + t_nf_n + \hat{a}_{n-1}s_{n-1}f_{n-1} = 0, \quad n = 0,1, \ldots, \quad f_{-1} = 0. \tag{51}$$

In fact, with $(f_n) \in \ell^2$, Eq. (51) is equivalent to the eigenvalue equation [Eq. (16)]: for Eq. (49) shows that $(1+Z)\Phi$ is in the range of $1-Z$, and since the latter operator has trivial kernel, it is easy to see that Eq. (49) implies Eq. (16).

If one introduces $u(n)=(-1)^n s_n f_n$, then formally, the first nonzero term in the small-α expansion of Eq. (51) yields the usual equation

$$u''(r) + \frac{2M}{\hbar^2}\left(E - U(r) - \frac{\hbar^2}{2M}\frac{\ell(\ell+1)}{r^2}\right)u = 0 \tag{52}$$

for hydrogenlike atom.

B. Properties of bound states: Duality

Since in our case $\hat{a}_n$ and $\hat{c}_n$ are never (i.e., for $n=0,1,\ldots$) zero, if an eigenvalue ε is such that s_n is never zero, as it happens for $\varepsilon \leqslant 1$, the solution of Eq. (51) is obviously unique, up to a multiplicative constant. Hence, such eigenvalues are nondegenerate. We will show now that the other eigenvalues are also nondegenerate.

Suppose now that ε is a *singular* eigenvalue, i.e., that

$$s_n = 0, \quad \text{i.e.,} \ \varepsilon = \vartheta_n + 1 \quad \text{for some } n \geqslant 0. \tag{53}$$

We first note the following property of eigenvectors corresponding to singular eigenvalues.

Observation: *There is no eigenvector* $\Phi=(f_n)_{n=0}^{\infty}$ *such that* $f_0=0$.

If $f_0=0$ and $n\geqslant 1$ then $f_0=\cdots=f_{n-1}=0$. But this is impossible since under assumption (53) the eigenvalue equation [Eq. (16)] is

$$\left[\frac{1+Z}{1-Z} + 1 + \frac{\vartheta}{\bar{r}_n} - \frac{\vartheta}{\bar{r}(N)}\right]\Phi = 0,$$

and the operator

$$\frac{\vartheta}{\bar{r}_n} - \frac{\vartheta}{\bar{r}(N)}$$

has non-negative expectation value in the state defined by Φ, while the operator $(1+Z)/(1-Z)+1$ is positive definite. If $n=0$ the same argument applies.

Suppose then that $f_0 \neq 0$. Then one solution of Eq. (51) is obtained by setting $f_n+\hat{a}_{n-1}s_{n-1}f_{n-1}=0$ and $f_{n+1}=\cdots=0$. If there is another solution, say, $(g_n)_{n=0}^{\infty}$, then by the Observation, $g_0\neq 0$ and $g-(g_0/f_0)f$ is a nonzero eigenvector with zero component equal to 0, in contradiction with the Observation. This proves that singular eigenvalues, if any, are nondegenerate. Since the Observation is obviously valid for eigenvalues that are not singular, it is valid for all eigenvalues.

We note that since eigenvalues $\varepsilon \leq 1$ are nonsingular, and since, by Eq. (16), any eigenvalue ε satisfies $\varepsilon < \vartheta/\bar{r}_0$, one obtains that the eigenvalues are not singular for $\vartheta \leq \bar{r}_0$. It is also not hard to show that for each n there exists exactly one value of ϑ for which $\varepsilon_n(\vartheta)$ is a singular eigenvalue.

We now pass to a proof of exponential localization of the eigenfunctions.

Since

$$a_n \to \frac{1}{2}, \quad b_n \to 0, \quad c_n \to \frac{1}{2} \quad \text{as } n \to \infty, \tag{54}$$

and, from Eq. (36),

$$\frac{h_n}{h_{n+1}} = 1 + \frac{1}{n} + O\left(\frac{1}{n^2}\right) \quad \text{as } n \to \infty, \tag{55}$$

letting $n \to \infty$ in the coefficients of Eq. (51), one obtains that the indicial (characteristic) equation of Eq. (51) is

$$(1-\varepsilon)r^2 + 2(1+\varepsilon)r + (1-\varepsilon) = 0.$$

For $\varepsilon \neq 1$ this is

$$r^2 + 2\omega r + 1 = 0, \quad \text{where } \omega = \frac{1+\varepsilon}{1-\varepsilon}, \quad |\omega| > 1, \tag{56}$$

yielding the characteristic multipliers $r_\pm = -\omega \pm \sqrt{\omega^2 - 1}$. Since $|\omega| > 1$, the characteristic multipliers are real and of modulus different from 1; and since $r_+ r_- = 1$, only one of the characteristic multipliers has absolute values smaller than 1. A short computation shows that this characteristic multiplier is equal to

$$\lambda = \frac{\sqrt{\varepsilon} - 1}{\sqrt{\varepsilon} + 1}. \tag{57}$$

By Poincaré-Perron theory,[10] any solution f of Eq. (51) with $\varepsilon \neq 1$ and such that Eq. (51) is nonsingular can be written as a linear combination of two solutions, say, f'_n, f''_n, such that $f'_{n+1}/f'_n \to \lambda$ and $f''_{n+1}/f''_n \to 1/\lambda$ as $n \to +\infty$. For f to be square summable, its f''_n component has to be zero. Since f'_n is unique, up to a multiplicative constant, one obtains that for any nonsingular eigenvalue $\varepsilon \neq 1$ the corresponding eigenvector satisfies

$$f_{n+1}/f_n \to \lambda, \quad \text{as } n \to +\infty. \tag{58}$$

As $\varepsilon \to 1$ the characteristic multiplier λ approaches zero while the other characteristic multiplier tends to infinity. Since the usual formulation of Poincaré-Perron assumes both characteristic multipliers to be finite, it does not provide information for $\varepsilon = 1$. However, since $\lambda = 0$ for $\varepsilon = 1$, one would expect in this case faster than exponential decrease of f_n. An independent argument, which we skip, shows that this is indeed the case.

Thus we have the following.

Proposition: *Bound states* (f_n) *are nondegenerate and for* $\varepsilon \neq 1$ *exponentially localized, i.e.,* f_n *tends to zero exponentially fast as n tends to infinity. Also,* $(-1)^n f_n$ *is asymptotically* (*for large* n) *of a constant sign for* $\varepsilon < 1$ *and asymptotically alternating for* $\varepsilon > 1$. *The characteristic multipliers for eigenvalues* ε *and* ε^{-1} *are equal and they tend to zero as* $\varepsilon \to 1$. *If* $\varepsilon = 1$ *is an eigenvalue then the corresponding eigenvector* (f_n) *has stronger than exponential localization.*

The equality of characteristic multipliers for eigenvalues ε and ε^{-1} is an expression of the duality described in Ref. 14. We hope to discuss in the future the duality properties of eigenvectors.

The exponential localization of f_n can be also described by writing $|f_n| \sim \exp(-\xi r_n)$, $\xi = \xi(E)$, i.e., by setting

$$\xi = -\lim_{n\to\infty} \frac{\ln|f_n|}{r_n}.$$

Taking then Eqs. (11) and (12) into account, one obtains

$$\xi = \frac{-\ln|\lambda|}{2\hbar\sqrt{\alpha}} = \frac{1}{2\hbar\sqrt{\alpha}} \ln\left|\frac{1+\sqrt{\varepsilon}}{1-\sqrt{\varepsilon}}\right| = \frac{1}{2\hbar\sqrt{\alpha}} \ln \frac{1+\sqrt{-2\alpha ME}}{|1-\sqrt{-2\alpha ME}|}.$$

C. Numerical and perturbative calculations

Assuming that $s_n \neq 0$ for all n, which is true for $\varepsilon \leqslant 1$, in particular, we set

$$g_n = \frac{s_n}{\sqrt{h_n}} f_n$$

and rewrite Eq. (51) as

$$c_{n+1}g_{n+1} + \frac{t_n(E)}{s_n(E)} g_n + a_{n-1}g_{n-1} = 0, \quad n \geqslant 0, \quad g_{-1} = 0, \tag{59}$$

i.e.,

$$g_{n-1} = -\frac{1}{a_{n-1}}\left[\frac{t_n(E)}{s_n(E)} g_n + c_{n+1}g_{n+1}\right], \quad n \geqslant 0, \quad g_{-1} = 0,$$

where a_n and c_n are as in Eq. (46) and (s_n, t_n) as in Eq. (50a). The advantage of Eq. (59) over Eq. (51) is that, while the right hand side of the former does not define a symmetric operator in ℓ^2 and the latter does, numerical calculations using Eq. (51) are computationally much more demanding.

Introducing the ratio $r(n) = g_{n-1}/g_n$, Eq. (59) can be rewritten as

$$r(n) = p(n) + \frac{q(n)}{r(n+1)}, \quad \text{where } p(n) = -\frac{1}{a_{n-1}} \frac{t_n(E)}{s_n(E)}, \quad q(n) = -\frac{c_{n+1}}{a_{n-1}}. \tag{60}$$

The spectrum is found from the condition $r(0) = 0$ (recall that $g_{-1} = 0$ and $g_0 = 0$ imply that $g_n = 0$ for all n).

To use these formulas in numerical calculations one can proceed as follows. Since, by Eq. (58),

$$\lim_{n\to+\infty} r(n) = \frac{\sqrt{\varepsilon}+1}{\sqrt{\varepsilon}-1},$$

one can pick a "large" n, set $r(n) = (\sqrt{\varepsilon}+1)(\sqrt{\varepsilon}-1)$, iterate Eq. (60) backwards to obtain $r(0)$, and then solve the equation $r(0) = 0$ for ε. In this context, it is reassuring that the limit in Eq. (58) is approached exponentially fast. The convergence is fast for small characteristic multipliers and slows down when the characteristic multipliers are close to 1.

Figure 1 is an example of an application of this numerical scheme. The figure is a MATHEMATICA plot of $r(0)$ as a function of a variable proportional to ε^{-1} for $D=3$ and $L=0$, and for quite a large value of ϑ. The figure suggests that one has an infinite number of bound states, which is in agreement with the theorem of Sec. III B. It also indicates $\varepsilon_n \sim 1/n$, not $1/n^2$, so that one is presumably in the regime of the limiting behavior of Eq. (19). It would be interesting to see if indeed one has the $(\varepsilon_n \sim 1/n)$ behavior for large α and $(\varepsilon_n \sim 1/n^2)$ behavior for small α, and if the

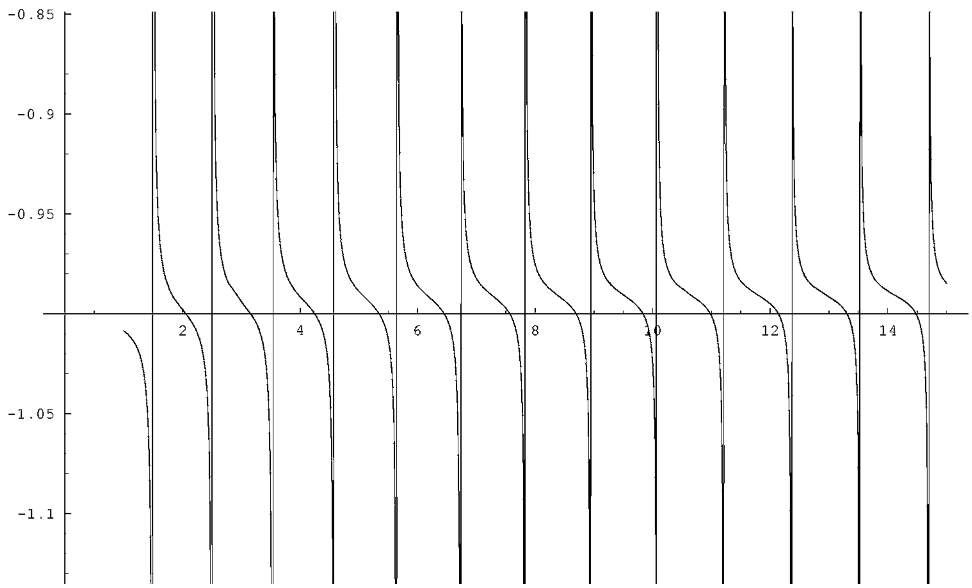

FIG. 1. $r(0)$ as a function of a variable proportional to ε^{-1}.

transition between these two asymptotics occurs at $\varepsilon=1$; the estimations in Sec. II B are not uniform in n and therefore do not provide this kind of information.

This and other numerical results, in particular, monotonicity properties of this graph and the fact that the zeros of g_0 and g_1 are interspaced, raise the question of which properties of the eigenvalue difference equations of Jacobi operators generalize to equations of the form of Eq. (51): after the transformation $f_n \mapsto s_n f_n$ one obtains here an equation with the eigenvalue appearing in a rational factor of the middle term while in the case of Jacobi operators one obtains a linear factor.

We now pass to the perturbative calculations. Fix η and denote by $\mathcal{H}^\alpha$ the Hilbert space defined by the scalar product [Eq. (2)], which we denote now by $(\cdots|\cdots)_\alpha$. Let f_α be an eigenvector of H_α with eigenvalue $E(\alpha)$. Then, formally,

$$\left.\frac{\mathrm{d}}{\mathrm{d}\alpha}E(\alpha)\right|_{\alpha=0} = (f_0|H_0' f_0)_0,$$

where H_0' is the derivative of H_α with respect to α at $\alpha=0$. This is the Hellman-Feynman theorem, which is usually stated in case all the Hilbert spaces $\mathcal{H}^\alpha$ coincide, but which holds also in the more general context of a smooth (Hilbert space) bundle, if suitably interpreted. We applied it to the family H_α of Eq. (4), which depends of α since R does, and to differentiation at $\alpha=0$, at the point where the functions are not smooth.

Formal calculations yield

$$-\hbar^{-2}R^2 = \partial^2 + \alpha[2\eta p^2\partial^2 + (2\eta + \eta'\bar{D})(\mathbf{p}\cdot\partial) + 2\eta'(\mathbf{p}\cdot\partial)^2] + O(\alpha^2),$$

where $\eta' = \beta'/\alpha = 1-\eta$, ∂^2 is the Laplace operator, and $\mathbf{p}\cdot\partial$ is the radial derivative, up to the factor p^{-1}. Thus, formally, one can write

$$R^2 = A + B\alpha + O(\alpha^2), \quad A = -\hbar^2\partial^2 = R^2|_{\alpha=0},$$

$$B = -\hbar^2[2\eta p^2\partial^2 + (2\eta + \eta'\bar{D})(\mathbf{p}\cdot\partial) + 2\eta'(\mathbf{p}\cdot\partial)^2], \tag{61}$$

and to find H_0' of

$$H_\alpha = H_0 + \alpha H_0' + O(\alpha^2),$$

one needs the first nontrivial term of the expansion of $(A+B\alpha)^{-1/2}$ in powers of α, for *noncommuting* A and B. We proceed as follows.

Squaring

$$\sqrt{A + \alpha B + O(\alpha^2)} = C + \alpha D + O(\alpha^2), \tag{62}$$

one obtains the equations

$$C^2 = A \text{ and } CD + DC = B \tag{63}$$

for operators C and D. For positive A, we will assume that expansion (62) is (perturbatively) positive, i.e., $C=\sqrt{A}$. The problem is in solving assuming that the operator C is invertible, the second equation of Eq. (63) can be solved, again formally, in representation in which C is diagonal: $(Cf)(x)=c(x)f(x)$, where f is a function of some variable x and B is an integral operator,

$$Bf(x) = \int b(x,y)f(y)\mathrm{d}y,$$

where $\mathrm{d}y$ is some measure. Then writing D as an integral operator D, $Df(x)=\int \mathrm{d}(x,y)f(y)\mathrm{d}y$, one obtains the solution

$$\mathrm{d}(x,y) = \frac{b(x,y)}{c(x)+c(y)} \tag{64}$$

of $CD+DC=B$. Finally, using

$$\frac{1}{C+\alpha D} = \frac{1}{C} - \alpha\frac{1}{C}D\frac{1}{C} + O(\alpha^2),$$

one obtains

$$H_0' = k\frac{1}{C}D\frac{1}{C}.$$

One can apply this to the case at hand, using for x either the position variable $(x_1,\ldots,x_D)$ or the radial variable r, if one works with the reduced Hamiltonian. In either case, one obtains a distribution for the kernel b. For zero angular momentum, our computations resulted in $(f_0|H_0'f_0)_0$ given by logarithmically divergent integrals, which agrees with our claim that expression (27) cannot hold.

While this scheme may prove useful also in another context, we skip details of the calculations, since all these are pretty formal and superseded by now by the results claimed in Ref. 2, which has not only perturbative formulas but also claims of a control of the $O(\alpha^2)$ term.

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