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Quasi-algebraic treatment of bound states of simple one-electron systems

Francisco M. Fernández and Eduardo A. Castro

División Química Teórica,
Instituto de Investigaciones Fisicoquímicas Teóricas y Aplicades (INIFTA),
Sucursal 4, Casilla de Correo 16, 1900 La Plata, Argentina

We present a straightforward, quasi-algebraic treatment of simple one-particle quantum-mechanical systems. The method consists primarily of a canonical transformation that changes the Schrödinger equation into a first-order differential equation, thus allowing an easier derivation of the eigenvalues and eigenfunctions. We express the latter in a way which is not commonly encountered in the standard literature on quantum mechanics and quantum chemistry. The derivation of generating functions for the eigenfunctions offers no difficulty because the method is formulated in the coordinate representation. As illustrative examples, we consider the harmonic oscillator and a particle in a Kratzer potential.

1. Introduction

Lie algebraic methods prove to be useful in treating a wide variety of physical problems. Typically, reviews, textbooks and monographs about such methods assume that the reader is familiar with the main features of Lie algebras and groups. Čížek and Paldus [1] pointed out that such preliminary knowledge is not necessary and proposed a motivating construction of the generators of the so(2, 1) algebra. They exploited a resemblance between this algebra and the well-known angular momentum algebra described in most standard textbooks on quantum chemistry [2,3].

The purpose of the present communication is an alternative approach to the motivating treatment of the so(2, 1) Lie algebra given in ref. [1]. We work in the coordinate representation and construct generating functions for the eigenfunctions of simple one-electron systems. The key of our method is a canonical transformation of the Schrödinger equation into a more easily solvable first-order differential equation. The general method is outlined in section 2. In section 3, we apply it to the harmonic oscillator and in section 4, we treat a particle moving in Kratzer potential. In section 5, we discuss the main results and mention additional applications of the present procedure.

2. The method

In what follows, x represents an arbitrary coordinate and D stands for d/dx. We use the standard notation $[A, B]$ to represent the commutator between the operators A and B. An important commutator in our approach is $[xD, x^iD^j] = (i-j)x^iD^j$, which follows from straightforward application of $[x, D] = 1$. We say that an operator O is of degree n if $[xD, O] = nO$. If O' is of degree $-n$, we have that $[xD, [O, O']] = 0$. In particular, the quite general operator

$$X_{mn} = \sum_{k=0}^{\min\{m,n\}} C_k x^{m-k} D^{n-k} \tag{1}$$

is of degree $m-n$. This simple criterion enables one to construct the algebra for one-electron systems very easily. Since we are interested in the treatment of second-order differential equations, it is sufficient for our purposes to consider the operators $X_1 = -x^{2-n}D^2/2 + \lambda/(2x^n)$ and $X_2 = -x^n/2$. Because they are, respectively, of degree $-n$ and n, their commutator has to be a function of xD. A straightforward calculation leads to $X_3 = [X_2, X_1] = nxD/2 + n(n-1)/4$. Furthermore, since $[X_3, X_2] = n^2X_2/2$ and $[X_3, X_1] = -n^2X_1/2$, we find it convenient to define the new set of operators

$$K_0 = 2X_3/n^2 = xD/n + (n-1)/(2n), \tag{2a}$$

$$K_+ = 2X_2/(cn^2) = x^n/(cn^2), \tag{2b}$$

$$K_- = cX_1 = c(-x^{2-n}D^2 + \lambda/x^n)/2, \tag{2c}$$

where c is a real number to be determined according to the form of the Schrödinger equation. These operators satisfy the commutation relations

$$[K_0, K_\pm] = \pm K_\pm, \quad [K_+, K_-] = K_0. \tag{3}$$

Upon using the well-known expression

$$e^A B e^{-A} = B + [A, B] + \tfrac{1}{2}[A,[A, B]] + \ldots, \tag{4}$$

which holds for any pair of linear operators A and B, we find that

$$\exp(\theta K_\pm) K_0 \exp(-\theta K_\pm) = K_0 \mp \theta K_\pm, \tag{5a}$$

$$\exp(\alpha K_+) K_- \exp(-\alpha K_+) = K_- + \alpha K_0 - \alpha^2 K_+/2, \tag{5b}$$

$$\exp(\beta K_-) K_+ \exp(-\beta K_-) = K_+ + \beta K_0 - \beta^2 K_-/2, \tag{5c}$$

$$\exp(\theta K_0) K_\pm \exp(-\theta K_0) = e^{\pm\theta} K_\pm, \tag{5d}$$

where θ, α, and β are arbitrary constants.

Many quantum-mechanical problems can be reduced to an eigenvalue equation of the form

$$W\Psi = w\Psi, \quad W = aK_- + bK_+, \tag{6}$$

where $ab > 0$. For any operator U having an inverse U^{-1}, we can rewrite this eigenvalue equation as $UWU^{-1}\Phi = w\Phi$, in which $\Phi = U\Psi$. If we choose U so that UWU^{-1} is proportional to K_0, then the eigenvalue equation (6) becomes a first-order differential equation. This is the main reason why we explicitly select the coordinate representation and choose K_0 as in eq. (2a). The simplication just mentioned can be achieved by means of an operator

$$U = \exp(\beta K_-)\ \exp(\alpha K_+) \tag{7}$$

if the constants α and β are conveniently set. Straightforward application of the canonical transformations (5) shows that when

$$\alpha = (2b/a)^{1/2}, \quad \beta = -1/\alpha, \tag{8}$$

we have

$$UWU^{-1} = (2ab)^{1/2} K_0. \tag{9}$$

In eq. (8), we choose α to be the positive root in order to rule out the unphysical solution from the very beginning (cf. the examples below). The problem reduces to the solution of the first-order differential equation

$$K_0\Phi = x\Phi'/n + (n-1)\Phi/(2n) = k\Phi, \tag{10}$$

in which $k = w(2ab)^{-1/2}$ and the prime stands for differentiation with respect to x. The result up to a constant factor is

$$\Phi = x^s, \quad s = kn + (1-n)/2, \tag{11}$$

so that any eigenfunction Ψ of W reads

$$\Psi = \exp(-\alpha K_+)\ \exp(-\beta K_-)x^s. \tag{12}$$

Successive application of the operator K_- to x^s,

$$K_-^j x^s = (c/2)^j [\lambda - s(s-1)][\lambda - (s-n)(s-n-1)]$$
$$\ldots [\lambda - (s-jn+n)(s-jn+n-1)]x^{s-jn}, \qquad j = 1, 2, \ldots, \tag{13}$$

reveals that Ψ is not regular at the origin unless $K_-^j x^s$ vanishes for a certain j value such that $g = s - jn + n > 0$. These two conditions determine the eigenvalues

$$k = k_{j-1} = j - 1/2 \pm n^{-1}(\lambda + 1/4)^{1/2}, \quad j = 1, 2, \ldots, \tag{14a}$$

$$\gamma = 1/2 \pm (\lambda + 1/4)^{1/2} > 0. \tag{14b}$$

Clearly, if $\lambda > 0$, only the plus sign in eq. (14b) is admissible.

In order to construct a generating function for the solutions of the general problem (6), we define

$$\Phi_\nu = K_+^\nu x^\gamma, \; u_\nu = \exp(-\beta K_-)\Phi_\nu, \quad \nu = 0, \ldots, \tag{15}$$

so that

$$K_-\Phi_0 = 0. \tag{16}$$

Therefore,

$$G(t, x) = \sum_{\nu=0}^{\infty} u_\nu t^\nu/\nu! = \exp(-\beta K_-)\psi_t, \quad \psi_t = \exp(tK_+)\Phi_0. \tag{17}$$

It follows from

$$\begin{aligned} K_-\psi_t &= \exp(tK_+)\exp(-tK_+)K_- \exp(tK_+)\Phi_0 \\ &= \exp(tK_+)(K_- - tK_0 - t^2K_+/2)\Phi_0 \\ &= -[k_0 t + (t^2/2)K_+]\psi_t \end{aligned} \tag{18}$$

that

$$K\psi_t = -k_0 t\psi_t, \quad K = K_- + t^2K_+/2. \tag{19}$$

Therefore, if we find numbers c_1, c_2, and c_3 that satisfy

$$\exp(-\beta K_-) = \exp(-c_1K_+)\exp(c_2K_0)\exp(c_3K), \tag{20}$$

and take into account that

$$\begin{aligned} \exp(c_2K_0)\psi_t &= \exp(c_2K_0)\exp(tK_+)\exp(-c_2K_0)\exp(c_2K_0)\Phi_0 \\ &= \exp(c_2k_0)\exp(t\,e^{c_2}K_+)\Phi_0, \end{aligned} \tag{21}$$

then we conclude that the generating function is given by

$$G(t, x) = \exp[k_0(c_2 - tc_3)]\exp[(t\,e^{c_2} - c_1)K_+]\Phi_0. \tag{22}$$

One can determine c_1, c_2, and c_3 by means of any of the methods for disentangling exponential operators, some of which have been recently reviewed [4]. However, as we are here interested in G and not in the particular values of c_1, c_2, and c_3, we

can use a much simpler procedure. Equation (22) shows that the generating function is of the form

$$\exp(-\beta K_-)\psi_t = A(\beta)\exp[B(\beta)K_+]\Phi_0, \quad A(0)=1, \quad B(0)=t. \tag{23}$$

In order to determine the form of the functions A and B, we simply differentiate both sides of this last equation with respect to β and rewrite the result according to

$$\begin{aligned} -K_-G &= -A\exp(BK_+)\exp(-BK_+)K_- \exp(BK_+)\Phi_0 = (k_0B + B^2K_+/2)G \\ &= [A^{-1}\mathrm{d}A/\mathrm{d}\beta + (\mathrm{d}B/\mathrm{d}\beta)K_+]G, \end{aligned} \tag{24}$$

thus obtaining the differential equations

$$\mathrm{d}A/\mathrm{d}\beta = k_0BA, \quad \mathrm{d}B/\mathrm{d}\beta = B^2/2, \tag{25}$$

the solutions of which are

$$A = (1-\beta t/2)^{-2k_0}, \quad B = 2t/(2-\beta t). \tag{26}$$

Therefore, the generating function is

$$G(t,x) = (1-\beta t/2)^{-2k_0}\, x^\gamma \exp\{2tx^n/[cn^2(2-\beta t)]\}, \tag{27}$$

from which one can obtain the polynomials u_ν according to eq. (17). Although one commonly derives such polynomials more easily from their definition [15], the generating functions are extremely useful to obtain normalization factors and other integrals involving them.

3. The harmonic oscillator

The first illustrative example is the Schrödinger equation for the simple one-dimensional harmonic oscillator, which we write in dimensionless form as

$$H\Psi = E\Psi, \quad H = \tfrac{1}{2}(-D^2 + x^2). \tag{28}$$

We can treat this problem easily by means of the operators in eqs. (2) with $n=2$, $\lambda = 0$ and $c = 1$, so that

$$K_0 = \tfrac{1}{2}xD + \tfrac{1}{4}, \quad K_+ = \tfrac{1}{4}x^2, \quad K_- = -\tfrac{1}{2}D^2. \tag{29}$$

It follows from

$$W = H = K_- + 2K_+, \tag{30}$$

that $a = 1$ and $b = 2$ (notice that $ab > 0$ as assumed in section 2). Therefore, we have $\alpha = 2$ and $\beta = -1/2$, so that

$$U = \exp(D^2/4)\exp(x^2/2), \tag{31}$$

and the canonical transforation is $UHU^{-1} = 2K_0$. According to the general equations in the previous section, the eigenvalues and eigenfunctions are given, respectively, by

$$E_\nu = 2k_\nu = \{2j - 3/2,\ 2j - 1/2,\ j = 1, 2, \ldots\} = \{\nu + 1/2,\ \nu = 0, 1, \ldots\} \tag{32}$$

and

$$\Psi_\nu = \exp(-x^2/2)\exp(-D^2/4)\Phi_\nu,\quad \Phi_\nu = K_+^\nu x^\gamma,\quad \gamma(\gamma - 1) = 0. \tag{33}$$

The two possible values of γ, $\gamma = 0$ and $\gamma = 1$, give rise to the even and odd states, respectively. The generating functions for these states are, respectively,

$$G_e(t, x) = 2(4 + t)^{-1/2}\exp[tx^2/(4 + t)] \tag{34a}$$

and

$$G_o(t, x) = 8(4 + t)^{-3/2}\exp[tx^2/(4 + t)]x. \tag{34b}$$

These two generating functions come from the two solutions of the annihilation condition $D^2x^\gamma = 0$, $\gamma = 0$ and $\gamma = 1$, and can be reduced to only one expression in terms of γ.

The results just obtained can be greatly simplified by reordering the set of functions $\{x^{2\nu+\gamma},\ \gamma = 0, 1,\ \nu = 0, 1, \ldots\}$ as $\{x^\nu,\ \nu = 0, 1, \ldots\}$. Hence, we can redefine Φ_ν and u_ν as

$$u_\nu = \exp(-D^2/4)\Phi_\nu,\quad \Phi_\nu = x^\nu, \tag{35}$$

so that the eigenfunctions of H become

$$\Psi_\nu = \exp(-x^2/2)\exp(-D^2/4)x^\nu. \tag{36}$$

The polynomials $u_\nu(x)$ are related to the Hermite polynomials $H_\nu(x)$ by

$$u_\nu(x) = 2^{-\nu}H_\nu(x). \tag{37}$$

Therefore, the latter can be obtained from

$$H_\nu(x) = \exp(-\mathrm{d}^2/\mathrm{d}y^2)y^\nu,\quad y = 2x. \tag{38}$$

Furthermore, the generating function for the new polynomials u_ν is much simpler than an of those in eqs. (34):

$$G(t, x) = \sum_{\nu=0}^{\infty} t^\nu u_\nu(x)/\nu! = \exp(-D^2/4)\exp(tx) = \exp(tx - t^2/4). \tag{39}$$

The expression (38) for the Hermite polynomials does not commonly appear in special function tables. It has been derived by Wolf [5] in the realm of canonical transforms. Our treatment is much simpler and more straightfoward. Here, we leave the discussion of the well-known solutions of the harmonic oscillator to consider a slightly more complicated problem which better illustrated the capability of the quasi-algebraic method developed in the previous section.

4. The Kratzer potential

The radial part of the Schrödinger equation for a particle moving in a Kratzer potential $V(r) = A/(2r^2) - B/r$ can be written [6]

$$[-(1/2)\mathrm{d}^2/\mathrm{d}r^2 + \lambda/(2r^2) - B/r]F(r) = EF(r), \tag{40}$$

where $\lambda = A + l(l+1)$, $l = 0, 1, \ldots$ being the angular momentum quantum number. The physical solution $F(r)$ vanishes at the origin and at infinity. We have chosen the units so that both $\hbar$ and the mass of the particle are unity. By means of the change of variables $x = (-2E)^{1/2}r$, we can rewrite eq. (40) as

$$W\Psi = w\Psi, \quad W = -xD^2/2 + \lambda/(2x) + x/2, \quad w = B/(-2E)^{1/2}, \tag{41}$$

which is of the general form (6) with

$$K_0 = xD, \quad K_+ = x, \quad K_- = -xD^2/2 + \lambda/(2x), \tag{42}$$

$n = 1$, $a = 1$, $b = 1/2$ and $c = 1$. Therefore, $\alpha = 1$ and $\beta = -1$ so that the transformation operator is

$$U = \exp(-K_-)\mathrm{e}^x. \tag{43}$$

According to the general equations of section 2, we have

$$w_\nu = k_\nu = \nu + \gamma, \quad \gamma = 1/2 + [A + (l+1/2)^2]^{1/2}, \quad \nu = 0, 1, \ldots, \tag{44}$$

$$\Phi_\nu = x^{\nu+\gamma}, \quad u_\nu = \exp(K_-)x^{\nu+\gamma}, \quad \Psi_\nu = \mathrm{e}^{-x}\exp(K_-)x^{\nu+\gamma}. \tag{45}$$

The energy eigenvalues are given by $E_\nu = -B^2/(2w_\nu)^2$. The dependence of the eigenfunctions and eigenvalues on the angular momentum quantum number l is not explicitly indicated to make the notation simpler. The expression for the eigenfunctions Ψ_ν given in eq. (45) is not commonly found in the literature on quantum mechanics and quantum chemistry.

According to eq. (27), the generating function is

$$G(t,x) = 4^\gamma(2+t)^{-2\gamma}x^\gamma \exp[2tx/(2+t)], \tag{46}$$

from which one can obtain the polynomials u_ν according to the expansion (17).

5. Further comments and conclusions

Throughout this paper, we have presented a simple, straightforward, quasi-algebraic way of solving the Schrödinger equation for simple one-particle systems. The main ingredients of the present approach that make it different from standard algebraic treatments are the explicit use of the coordinate representation, the particular selection of the operator K_0, and the canonical transformation that reduces the eigenvalue equation to a first-order differential equation. In the standard algebraic approach, the annihilation condition (cf. eq. (16)) becomes a first-order differential equation in the coordinate representation, whereas here it is a second-order differential equation. Although the results obtained in this paper may not be entirely original, we have shown that one can exploit Lie algebraic methods without special knowledge of Lie algebra and Lie groups. This communication is intended to complement ref. [1] through the derivation of generating functions and alternative expressions for the eigenfunctions from a different, although closely related, approach. The expressions for the polynomials u_ν are most interesting, since they do not commonly appear in the literature on quantum mechanics and quantum chemistry.

The method can be easily applied to many other problems such as hydrogen-like atoms and the harmonic oscillator in an arbitrary number of dimensions, and to the Morse oscillator. One can also use the same strategy to solve some second-order differential equations that commonly appear in theoretical physics and chemistry, such as the one that produces the hypergeometric functions.

Some of our equations for the harmonic oscillator are reminiscent of the Bargmann representation for the creation and annihilation operators [7], thus disclosing a connection between this representation and the algebraic methods. Therefore, the results in section 2 can be thought of as a generalization of the Bargmann representation which may be useful, for instance, to extend the analysis of the anharmonic oscillator carried out by Hioe and Montroll [8] to a wider class of problems. Another example is the use of the canonical transformation described in this paper to facilitate the application of perturbation theory to nontrivial one-particle systems [9].

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