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Coulombic and ring-shaped potentials treated in a unified way via a nonbijective canonical transformation

Maurice Kibler

Institut de Physique Nucléaire (et IN2P3), Université Claude Bernard Lyon 1, 43 Bd du 11 Novembre 1918, F-69622 Villeurbanne Cedex, France

Tidjani Négadi

Institut de Physique, Université d'Oran, Es-Sénia, Oran, Algérie

This paper is concerned with the three-dimensional potential $V_q = \eta\sigma^2(2a_0/r - q\eta a_0^2/r^2 \sin^2\theta)\varepsilon_0$ which comprises as particular cases the ring-shaped potential ($q = 1$) and the Coulomb potential ($q = 0$). The Schrödinger equation for the potential V_q is transformed via a nonbijective canonical transformation, viz., the Kustaanheimo–Stiefel transformation, into a coupled pair of Schrödinger equations for two-dimensional harmonic oscillators with inverse-square potentials. As a consequence, the discrete spectrum for the potential V_q is obtained in a straightforward way. A special attention is paid to the case $q = 0$. In particular, the coupled pair of Schrödinger equations for two-dimensional harmonic oscillators is tackled in the situations where the spectrum for the potential V_0 is discrete, continuous, or reduced to the zero point. Finally, some group-theoretical questions about the potential V_q are mentioned as well as a connection, via the Kustaanheimo–Stiefel and the Levi–Civita transformations, between the quantum-mechanical problems for the potential V_q and the Sommerfeld and Kratzer potentials.

Key words: Coulomb, Kratzer, Sommerfeld, and Hartmann potentials—canonical transformations

1. Introduction

We consider in this paper the three-dimensional potential

$$V_q = \eta\sigma^2\left(\frac{2a_0}{r} - q\eta\frac{a_0^2}{r^2\sin^2\theta}\right)\varepsilon_0 \tag{1}$$

where q is a real (dimensionless) parameter. The potential defined by Eq. (1) constitutes a slightly modified form of the ring-shaped potential introduced by Hartmann [1, 2] and further worked out by Hartmann and coworkers [3–5]. Indeed, the Hartmann potential corresponds to the case $q = 1$. The potential (energy) V_q is a function of the ordinary spherical coordinates r and θ and does not present the spherical symmetry except for the case $q = 0$. In Eq. (1), a_0 stands for the radius of the first Bohr orbit, ε_0 the energy of the ground level of the hydrogen atom, and η and σ are two positive real (dimensionless) parameters the values of which range from about 1 up to 10 in problems of chemical interest [5]. In the particular case $q = 0$, Eq. (1) gives the potential energy of a hydrogenlike atom with nucleus charge Ze provided we take $\eta\sigma^2 = Z$. Consequently, Eq. (1) makes it possible to describe both the hydrogen atom potential (case V_0 with $\eta\sigma^2 = 1$) and the Hartmann potential (case V_1). Note that, however, the parameter q is not really necessary to obtain the Coulomb potential as a limiting case of the Hartmann potential [4].

The Schrödinger equation for a particle in the ring-shaped potential V_1 has been solved by using standard polynomial methods [1, 2, 5] and equally well by using the so-called Kustaanheimo–Stiefel (KS) transformation [6]. Of course, the Schrödinger equation for a particle in the potential V_0 admits eigenvalues and eigenfunctions that are essentially the ones related to the Coulomb problem. It is one of the aims of this paper to achieve a unified quantum-mechanical treatment of V_0 and V_1, i.e. a treatment of V_q, by means of the KS transformation.

The KS transformation was introduced by Kustaanheimo and Stiefel [7], as an extension of the (conformal) Levi–Civita transformation, for the regularisation of the Kepler problem. This transformation was independently considered by Ikeda and Miyachi [8] in the framework of a unified treatment of the four-dimensional isotropic harmonic oscillator, the three-dimensional hydrogen atom, and the three-dimensional spherical rotator. The KS transformation corresponds to a surjection of the four-dimensional Euclidean space R^4 into the three-dimensional physical space R^3 and gives rise, from a quantum-mechanical viewpoint, to a nonbijective canonical transformation [7–9]. Such a canonical transformation permits to convert an eigenvalue problem in R^3 into an eigenvalue problem in R^4 subjected to a constraint condition. The interest in the KS transformation for theoretical physics has been continuously growing in recent years. The KS map has been used to connect various quantization cases in the language of either the Schrödinger equation [8–17] or the Feynman path integral [11, 18, 19]. Furthermore, the relevance of the KS bundle for a complete geometrical description of the magnetic monopole of Wu–Yang [20] and for a characterisation of a new class of instantons [21] has been recently underlined. The KS transformation has been also introduced in quantum chemistry. In fact, this transformation has been used in a study of the hydrogen atom via the path integral formalism [22]. In addition, the authors have shown in a short communication [6] how the KS transformation allows to transform the Schrödinger equation for the Hartmann potential V_1 into a coupled pair of Schrödinger equations for two-dimensional harmonic oscillators with inverse quadratic potentials supplemented by two constraint equations.

A second goal of this work is to further contribute to the penetration of the KS transformation in theoretical chemistry. Therefore, this transformation is introduced in Sect. 2 in a way that amalgamates results taken from Refs. [7] and [8]. Sect. 3 deals with the treatment of the Schrödinger equation for the potential V_q with the help of the KS transformation. As a last motivation of this paper, we want to render precisely the connection between the Kepler and harmonic oscillator (quantum-mechanical) problems recently revisited in Ref. [14]. In this regard, the Schrödinger equation for the particular case of the potential V_0 is investigated in Sect. 4 by means of the KS transformation. Finally, in Sect. 5 some group-theoretical considerations and an unexpected connection between the Hartmann and the Kratzer and Sommerfeld potentials are pointed out.

2. The KS transformation

We proceed by looking for a matrix of $SO_d \times R^+$, i.e. a $d \times d$ real matrix $A(\boldsymbol{u})$ whose elements are linear and homogeneous functions of $u_\alpha \in R$ $(\alpha = 1, 2, \dots, d)$ such that its rows and columns are orthogonal and have the norm $(\sum_{\alpha=1}^{d} u_\alpha^2)^{1/2}$. According to a theorem by Hurwitz, this problem has solutions only for $d = 1, 2, 4$, and 8. Indeed, such a problem may be connected to the product of two numbers (real numbers for $d = 1$, complex numbers of Cardan and Girard for $d = 2$, quaternionic numbers of Hamilton for $d = 4$, and octonionic numbers of Cayley for $d = 8$). The case $d = 2$ corresponds to the so-called Levi-Civita transformation and $d = 4$ to the KS transformation [7].

We limit ourselves to the case $d = 4$. The solution of the corresponding problem is given (up to row, column, and S_4 permutations) by

$$A(\boldsymbol{u}) = \begin{bmatrix} u_3 & -u_4 & u_1 & -u_2 \\ u_4 & u_3 & u_2 & u_1 \\ u_1 & u_2 & -u_3 & -u_4 \\ u_2 & -u_1 & -u_4 & u_3 \end{bmatrix}. \tag{2}$$

Following Kustaanheimo and Stiefel [7], we now consider

$$2A(\boldsymbol{u}) \begin{bmatrix} du_1 \\ du_2 \\ du_3 \\ du_4 \end{bmatrix} = \begin{bmatrix} 2(u_3\, du_1 - u_4\, du_2 + u_1\, du_3 - u_2\, du_4) \\ 2(u_4\, du_1 + u_3\, du_2 + u_2\, du_3 + u_1\, du_4) \\ 2(u_1\, du_1 + u_2\, du_2 - u_3\, du_3 - u_4\, du_4) \\ 2(u_2\, du_1 - u_1\, du_2 - u_4\, du_3 + u_3\, du_4) \end{bmatrix} \tag{3}$$

which can be rewritten as

$$2A(\boldsymbol{u})\begin{bmatrix} du_1 \\ du_2 \\ du_3 \\ du_4 \end{bmatrix} = \begin{bmatrix} d[2(u_1u_3-u_2u_4)] \\ d[2(u_1u_4+u_2u_3)] \\ d(u_1^2+u_2^2-u_3^2-u_4^2) \\ 2(u_2\,du_1-u_1\,du_2-u_4\,du_3+u_3\,du_4) \end{bmatrix} \tag{4}$$

so that the first three entries of the column-matrix (4) are seen to be total differentials. Then, we put

$$\begin{aligned} x &= 2(u_1u_3-u_2u_4) \\ y &= 2(u_1u_4+u_2u_3) \\ z &= u_1^2+u_2^2-u_3^2-u_4^2 \end{aligned} \tag{5}$$

which coincides with Eq. (A.1) in Ref. [8] and constitutes a rewriting, up to S_3 (on the labels x, y, z) and S_4 (on the labels u_1, u_2, u_3, u_4) permutations, of Eq. (6) in Ref. [7]. Further, the last entry in the column-matrix (4) is not a total differential and we follow Kustaanheimo and Stiefel [7] by requiring

$$u_2\,du_1-u_1\,du_2-u_4\,du_3+u_3\,du_4=0. \tag{6}$$

The KS transformation is therefore the $R^4 \to R^3$ surjection defined by relations (5) supplemented by the constraint condition (6). Following Ikeda and Miyachi [8], we note that the KS transformation may be parametrized as

$$\begin{aligned} u_1 &= \sqrt{r}\cos\frac{\theta}{2}\cos\frac{\varphi+\psi}{2}, \\ u_2 &= \sqrt{r}\cos\frac{\theta}{2}\sin\frac{\varphi+\psi}{2}, \\ u_3 &= \sqrt{r}\sin\frac{\theta}{2}\cos\frac{\varphi-\psi}{2}, \\ u_4 &= \sqrt{r}\sin\frac{\theta}{2}\sin\frac{\varphi-\psi}{2}, \end{aligned} \tag{7}$$

since this (Cayley–Klein) parametrization, well-known in the study of R^4, by the aid of Eq. (5) leads to the spherical coordinates of R^3:

$$\begin{aligned} x &= r\sin\theta\cos\varphi, \\ y &= r\sin\theta\sin\varphi, \\ z &= r\cos\theta. \end{aligned} \tag{8}$$

We close this section by giving some properties to be used in the next section.

Property 1. We have

$$r=(x^2+y^2+z^2)^{1/2}=u_1^2+u_2^2+u_3^2+u_4^2. \tag{9}$$

Property 2. We have

$$dx^2+dy^2+dz^2=4r(du_1^2+du_2^2+du_3^2+du_4^2). \tag{10}$$

Property 3. We have

$$\begin{bmatrix} \dfrac{\partial}{\partial x} \\ \dfrac{\partial}{\partial y} \\ \dfrac{\partial}{\partial z} \\ \dfrac{1}{2r}X \end{bmatrix} = \frac{1}{2r}A(\boldsymbol{u}) \begin{bmatrix} \dfrac{\partial}{\partial u_1} \\ \dfrac{\partial}{\partial u_2} \\ \dfrac{\partial}{\partial u_3} \\ \dfrac{\partial}{\partial u_4} \end{bmatrix}, \tag{11}$$

where the operator

$$X=u_2\frac{\partial}{\partial u_1}-u_1\frac{\partial}{\partial u_2}-u_4\frac{\partial}{\partial u_3}+u_3\frac{\partial}{\partial u_4} \tag{12}$$

turns out to be the infinitesimal operator of a subgroup of type $U_1 \sim SO_2$ of the group O_4 that leaves the form $u_1^2+u_2^2+u_3^2+u_4^2$ invariant.

Property 4. As a corollary of Property 3, we can express the three-dimensional Laplacian Δ as

$$\Delta=\frac{1}{4r}\left(\Delta_u-\frac{1}{r}X^2\right) \tag{13}$$

in terms of the four-dimensional Laplacian Δ_u and the operator X.

3. The V_q potential

We start from the three-dimensional Schrödinger equation

$$\Delta\Psi+\frac{2\mu}{\hbar^2}\left[E-\eta\sigma^2\left(\frac{2a_0}{r}-q\eta\frac{a_0^2}{r^2\sin^2\theta}\right)\varepsilon_0\right]\Psi=0 \tag{14}$$

for the potential energy V_q. By using Property 4 and Eqs. (5) and (8), Eq. (14) may be transformed into

$$\Delta_u\Psi-\frac{1}{r}X^2\Psi+\frac{2\mu}{\hbar^2}\left[-8\eta\sigma^2a_0\varepsilon_0+4Er+q\left(\frac{1}{u_1^2+u_2^2}+\frac{1}{u_3^2+u_4^2}\right)\eta^2\sigma^2a_0^2\varepsilon_0\right]\Psi=0. \tag{15}$$

Following the line of reasoning adopted in Ref. [6], we take $X\Psi=0$ in order that the wave function Ψ is a univalued function of the coordinates

$u_\alpha (\alpha = 1, 2, 3, 4)$. Consequently, Eq. (15) can be replaced by the system

$$u_1 \frac{\partial \Psi}{\partial u_2} - u_2 \frac{\partial \Psi}{\partial u_1} - u_3 \frac{\partial \Psi}{\partial u_4} + u_4 \frac{\partial \Psi}{\partial u_3} = 0, \tag{16}$$

$$\Delta_u \Psi + \frac{2\mu}{\hbar^2} \left[-8\eta\sigma^2 a_0 \varepsilon_0 + 4E(u_1^2 + u_2^2 + u_3^2 + u_4^2) + q\left(\frac{1}{u_1^2 + u_2^2} + \frac{1}{u_3^2 + u_4^2} \right) \eta^2 \sigma^2 a_0^2 \varepsilon_0 \right] \Psi = 0. \tag{17}$$

We therefore have the result:

Result 1. The Schrödinger equation (Eq. (14)) for the potential V_q is equivalent to the Schrödinger equation (Eq. (17)) for a four-dimensional nonharmonic oscillator with the energy $-8\eta\sigma^2 a_0 \varepsilon_0$ accompanied by a constraint condition (Eq. (16)).

Proceeding as in Ref. [6], we use the d'Alembert method of separation of variables by trying a solution of the type

$$\Psi = f(u_1, u_2) g(u_3, u_4). \tag{18}$$

Then, both Eqs. (16) and (17) may be separated. This leads to the system

$$\frac{\partial^2 f}{\partial u_1^2} + \frac{\partial^2 f}{\partial u_2^2} + \frac{2\mu}{\hbar^2} [\alpha + 4E(u_1^2 + u_2^2) + q\eta^2\sigma^2 a_0^2 \varepsilon_0 (u_1^2 + u_2^2)^{-1}] f = 0, \tag{19}$$

$$\frac{\partial^2 g}{\partial u_3^2} + \frac{\partial^2 g}{\partial u_4^2} + \frac{2\mu}{\hbar^2} [\beta + 4E(u_3^2 + u_4^2) + q\eta^2\sigma^2 a_0^2 \varepsilon_0 (u_3^2 + u_4^2)^{-1}] g = 0, \tag{20}$$

$$\alpha + \beta = -8\eta\sigma^2 a_0 \varepsilon_0, \tag{21}$$

$$u_1 \frac{\partial f}{\partial u_2} - u_2 \frac{\partial f}{\partial u_1} = \gamma f, \tag{22}$$

$$u_3 \frac{\partial g}{\partial u_4} - u_4 \frac{\partial g}{\partial u_3} = \gamma g, \tag{23}$$

where α, β, and γ denote separation constants. Eqs. (19) and (20) exhibit the same structure and correspond to the Schrödinger equation for a two-dimensional harmonic oscillator with an inverse-square potential. Hence, Result 1 can be further precised by the result:

Result 2. The Schrödinger equation (Eq. (14)) for the potential V_q is equivalent to the set of (i) a pair of Schrödinger equations (Eqs. (19) and (20) connected by Eq. (21)) for two two-dimensional isotropic harmonic oscillators with isotropic inverse-square potentials and (ii) a pair of constraint conditions (Eqs. (22) and (23)).

The system of Eqs. (19)–(23) may be solved for $E < 0$ and $q > 0$ in exactly the same way as the corresponding system with $q = 1$ in Ref. [6]. It is thus possible to derive the discrete values of E from the system (19)–(23). As a net result, we obtain that the energy E is given by the formula

$$E=(\eta^2\sigma^4/N^2)\varepsilon_0 \tag{24}$$

where N has the form

$$\begin{aligned} &N=(m^2+q\eta^2\sigma^2)^{1/2}+n_r+n_r'+1\\ &m=0,\pm1,\pm2,\dots\\ &n_r=0,1,2,\dots\\ &n_r'=0,1,2,\dots. \end{aligned} \tag{25}$$

(The quantum numbers m, n_r, and n_r' have been defined in Ref. [6]. For a full understanding of what follows it is enough to note their range of variation.) For N and $|m|$ fixed, i.e. for a fixed value of

$$n=N-[(m^2+q\eta^2\sigma^2)^{1/2}-|m|], \tag{26}$$

the number of corresponding wave functions is equal to the number of values taken by n_r and n_r' with the restriction that n_r+n_r' has a fixed value. From ordinary combinatorics, this number is seen to be $n-|m|$, a result that coincides with the one obtained in Ref. [5] for the potential V_1.

In the particular case where $q=1$, Eqs. (24) and (25) are in complete agreement with the corresponding results in Refs. [1, 2, 5]. In addition, in the particular case where $q=0$ and $\eta\sigma^2=Z$, Eqs. (24) and (25) give back the Balmer–Bohr formula

$$E=(Z^2/n^2)\varepsilon_0 \quad \text{with } n=1,2,3,\dots \tag{27}$$

for the bound states of a hydrogenlike atom.

4. The Coulomb Potential

At this stage, it is to be noticed that the approach developed in Sect. 3 leads to the discrete spectrum of V_q (Eq. (25)) but tells nothing about its continuous spectrum when there is any. Therefore, Results 1 and 2 demand further specifications as far as questions concerning the continuous spectrum (when any) of the operator $H_q=(-\hbar^2/2\mu)\Delta+V_q$ are addressed. We now give an outline of the specifications it is possible to bring to Result 2 in the special case $q=0$ and $\eta\sigma^2=Z$ and reserve more mathematical considerations (for any value of q) concerning Results 1 and 2 for a future publication in a journal of mathematical physics.

By taking $\eta\sigma^2=Z$ and $q=0$, Eqs. (19)–(23) may be rewritten as

$$-\frac{\hbar^2}{2\mu}\left(\frac{\partial^2 f}{\partial u_1^2}+\frac{\partial^2 f}{\partial u_2^2}\right)-4E(u_1^2+u_2^2)f=4Z_1e^2f, \tag{28}$$

$$-\frac{\hbar^2}{2\mu}\left(\frac{\partial^2 g}{\partial u_3^2}+\frac{\partial^2 g}{\partial u_4^2}\right)-4E(u_3^2+u_4^2)g=4Z_2e^2g, \tag{29}$$

$$Z_1+Z_2=Z, \tag{30}$$

$$u_1 \frac{\partial f}{\partial u_2} - u_2 \frac{\partial f}{\partial u_1} = \gamma f, \tag{31}$$

$$u_3 \frac{\partial g}{\partial u_4} - u_4 \frac{\partial g}{\partial u_3} = \gamma g. \tag{32}$$

At first glance, both Eqs. (28) and (29) correspond to the Schrödinger equation for a two-dimensional isotropic harmonic oscillator. Indeed, care must be exercised according to whether as $E = 0$, $E > 0$, or $E < 0$. This yields the following results.

Result 3. The Schrödinger equation for a hydrogenlike atom with zero energy ($E = 0$, i.e. zero-energy case) is equivalent to the set of (i) a pair of Schrödinger equations

$$-\frac{\hbar^2}{2\mu}\left(\frac{\partial^2 f}{\partial u_1^2} + \frac{\partial^2 f}{\partial u_2^2}\right) = 4Z_1 e^2 f \tag{33}$$

$$-\frac{\hbar^2}{2\mu}\left(\frac{\partial^2 g}{\partial u_3^2} + \frac{\partial^2 g}{\partial u_4^2}\right) = 4Z_2 e^2 g \tag{34}$$

for two two-dimensional free-particle systems, with fixed energies $4Z_1e^2$ and $4Z_2e^2$, connected by Eq. (30) and (ii) a pair or constraint conditions (Eqs. (31) and (32)).

Result 4. The Schrödinger equation for a hydrogenlike atom with *positive* energy ($E > 0$, i.e. continuous spectrum case) is equivalent to the set of (i) a pair of Schrödinger equations (Eqs. (28) and (29)) for two-dimensional isotropic harmonic oscillators, with *repulsive* potentials $-4E(u_1^2 + u_2^2) < 0$ and $-4E(u_3^2 + u_4^2) < 0$ and fixed energies $4Z_1e^2$ and $4Z_2e^2$, connected by Eq. (30) and (ii) a pair of constraint conditions (Eqs. (31) and (32)).

Result 5. The Schrödinger equation for a hydrogenlike atom with *negative* energy ($E < 0$, i.e. discrete spectrum case) is equivalent to the set of (i) a pair of Schrödinger equations (Eqs. (28) and (29)) for two two-dimensional isotropic harmonic oscillators, with *attractive* potentials $-4E(u_1^2 + u_2^2) > 0$ and $-4E(u_3^2 + u_4^2) > 0$ and fixed energies $4Z_1e^2$ and $4Z_2e^2$, connected by Eq. (30) and (ii) a pair of constraint conditions (Eqs. (31) and (32)).

To convince the reader of the interest of these results, let us show how Result 5 allows to readily recover the Balmer-Bohr formula. Each isotropic harmonic oscillator with attractive potential has a frequency ($\nu = \omega/2\pi$) such that

$$-4E = (1/2)\mu\omega^2. \tag{35}$$

Further, the energies of the two oscillators under consideration are given by

$$\begin{aligned} 4Z_1e^2 &= (n_1 + n_2 + 1)\hbar\omega, \\ 4Z_2e^2 &= (n_3 + n_4 + 1)\hbar\omega, \end{aligned} \tag{36}$$

where $n_\alpha = 0, 1, 2, \ldots$ for $\alpha = 1, 2, 3, 4$. By combining Eqs. (30), (35), and (36) we get

$$E = -2\mu Z^2 e^4/\hbar^2(n_1 + n_2 + n_3 + n_4 + 2)^2. \qquad (37)$$

The last step amounts to employ the constraint conditions (31) and (32) to prove that $n_1 + n_2 = n_3 + n_4$. This may be achieved by looking for solutions of the type

$$\begin{aligned} f &= \sum_{n_1 n_2} C_{n_1 n_2} \varphi_{n_1}(u_1) \varphi_{n_2}(u_2), \\ g &= \sum_{n_3 n_4} C_{n_3 n_4} \varphi_{n_3}(u_3) \varphi_{n_4}(u_4), \end{aligned} \qquad (38)$$

where $\varphi_{n_\alpha}(u_\alpha)$ denotes an eigenfunction of a one-dimensional harmonic oscillator and $C_{n_\alpha n_\beta}$ are expansion coefficients. Inserting Eq. (38) into Eqs. (31) and (32) leads to the following recursion formulas

$$\begin{aligned} C_{n_1-1,n_2+1}[n_1(n_2+1)]^{1/2} - C_{n_1+1,n_2-1}[(n_1+1)n_2]^{1/2} &= \gamma C_{n_1 n_2}, \\ C_{n_3-1,n_4+1}[n_3(n_4+1)]^{1/2} - C_{n_3+1,n_4-1}[(n_3+1)n_4]^{1/2} &= \gamma C_{n_3 n_4}, \end{aligned} \qquad (39)$$

which may be proved to admit a solution for $n_1 + n_2 = n_3 + n_4$. Thus, Eq. (37) reads

$$\begin{aligned} &E = -\mu Z^2 e^4/2\hbar^2 n^2 \\ &n = n_1 + n_2 + 1 = n_3 + n_4 + 1 = 1, 2, 3, \ldots \end{aligned} \qquad (40)$$

in accordance with Eq. (27). Finally, we observe that the present treatment of the case $E < 0$ yields the known degeneracy of the energy level $E \sim -1/n^2$. As a matter of fact, the degeneracy of the energy level $(n_1 + n_2 + 1)\hbar\omega = (n_3 + n_4 + 1)\hbar\omega$ is n (see Eq. (40)) so that the degeneracy of the energy level $E \sim -1/n^2$ is $n \times n = n^2$, i.e. just the Stone number.

To close this section, it has to be mentioned that Result 5 was obtained [14] in a completely different way by finding and solving a boson realization of the algebra derived by Pauli, in the early days of quantum mechanics, for the angular momentum operator and the quantum-mechanical analog of the Laplace–Runge–Lenz vector.

5. Related matters

At this point, it may be worthwhile to consider two pending questions that could possibly pave the way for future investigations.

The first question is devoted to group-theoretical considerations about the potential V_q and the associated Hamiltonian H_q. We note that $V_q \sim 1/(x^2+y^2+z^2)^{1/2} - q\eta a_0/2(x^2+y^2)$ so that the potential V_q is invariant under the point symmetry group $C_{\infty v}$. [The interaction term V_q presents the same symmetries as the diamagnetic term $H_d \sim (x^2+y^2)\mathcal{H}^2$ for a hydrogenlike atom under the influence of a magnetic field $\mathcal{H}$.] Consequently, according to a famous theorem by Wigner, we may expect that the energy levels of H_q should be *at least* one-fold or two-fold degenerate since $C_{\infty v}$ has only one- and two-dimensional irreducible representations. It is clear however that a higher degeneracy can occur in the discrete spectrum of H_q. In other words, some *accidental* degeneracies may appear besides the *essential* degeneracies (of degree 1 and 2) afforded by the symmetry group $C_{\infty v}$. The appearance of these accidental degeneracies might be an argument for guessing the relevance of a larger symmetry group in the study of the spectrum of H_q. Indeed, this point must be examined with attention because we know that (as a still open problem of theoretical physics): Given a (normal) operator H invariant under a group G, the occurrence of accidental degeneracies besides the essential degeneracies afforded by G does not necessarily imply the existence of a larger group $G'(G' \supset G)$ for which the degeneracies of H are essential (see, for instance, Ref. [23]). For the Hamiltonian H_q, we have $G_q \equiv C_{\infty v}$ and an answer to the problem of finding a group G'_q exists in some cases. As a matter of fact, the Lie algebras of the groups SO_4 (the special orthogonal group in 4 dimensions, isomorphic to the four-dimensional proper rotation group), $SO_{3,1}$ (the special pseudo-orthogonal group in 3 + 1 dimensions, isomorphic to the restricted Lorentz group), and E_3 (the rotation-translation Euclidean group in 3 dimensions, isomorphic to the restricted Galilean group) are of special interest for the discrete spectrum, continuous spectrum, and zero-energy cases of H_0 with $\eta\sigma^2 = Z$, respectively (cf. for example, Refs. [14–16]). Hence, we have $G'_0 \equiv SO_4$, $SO_{3,1}$, or E_3 according as we deal with the discrete spectrum, continuous spectrum, or zero-energy case of H_0, respectively. We may think of this result as being an encouragement to examine the very much involved problem of a group G'_q for $H_q(q \neq 0)$ and we hope to reach some (interesting) conclusions in future.

The second question concerns a captivating relation between the Hartmann potential problem and the Kratzer [24] and Sommerfeld [25] potential problems. Let us consider the three-dimensional potential

$$W_q = -2aD\left(\frac{1}{r} - q\frac{a}{2r^2}\right). \tag{41}$$

The case $q = 1$ corresponds to the Kratzer potential, the case $2aD = Ze^2$ and $qa^2D > 0$ to the Sommerfeld potential, and the case $2aD = Ze^2$ and $q = 0$ to the Coulomb potential. Needless to say that the study conducted in Sect. 3 for the potential V_q can be applied to the potential W_q too. We give here only the two central results of such a study.

Result 6. The Kustaanheimo–Stiefel transformation permits to convert the Schrödinger equation

$$\Delta\psi + \frac{2\mu}{\hbar^2}\left[E + 2aD\left(\frac{1}{r} - q\frac{a}{2r^2}\right)\right]\psi = 0 \tag{42}$$

for the potential W_q into the set of (i) the Schrödinger equation

$$\Delta_u\psi + \frac{2\mu}{\hbar^2}[8aD + 4E(u_1^2+u_2^2+u_3^2+u_4^2) - 4qa^2D(u_1^2+u_2^2+u_3^2+u_4^2)^{-1}]\psi = 0 \tag{43}$$

for a four-dimensional isotropic harmonic oscillator with inverse-square potential and (ii) a constraint condition

$$u_1\frac{\partial\psi}{\partial u_2}-u_2\frac{\partial\psi}{\partial u_1}-u_3\frac{\partial\psi}{\partial u_4}+u_4\frac{\partial\psi}{\partial u_3}=0. \tag{44}$$

We note the analogy between Eqs. (43) and (19) or (20). In fact, Eqs. (19) or (20) and (43) formally bear the same form. The main difference is that Eq. (43) is concerned with a motion in a four-dimensional space while Eqs. (19) and (20) with a motion in a two-dimensional space. This type of connection can be made even sharper owing to the following result.

Result 7. The Levi–Civita transformation ($x=u_1^2-u_2^2$, $y=2u_1u_2$) permits to convert the two-dimensional Schrödinger equation for a potential of type W_q with $r=(x^2+y^2)^{1/2}$ into an equation having exactly the same form as Eqs. (19) and (20).

It is one of the forthcoming assignments of the authors to further elaborate on the latter two results and the above-mentioned problem of the group G'_q.

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