The Coulomb – harmonic oscillator correspondence in $\mathcal{PT}$ symmetric quantum mechanics

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Abstract

We show that and how the Coulomb potential $V(x) = Z e^2/x$ can be regularized and solved exactly at the imaginary coupling $Ze^2$. The new spectrum of energies is real and bounded as expected, but its explicit form proves totally different from the usual real-coupling case.


1 Introduction

Quantum mechanics often works with the exactly solvable simplified models. For the precise fits of data or for some more subtle quantitative analyses, unfortunately, the number of solvable models is too limited. In $D$ dimensions, the only really useful and easily tractable interactions are harmonic oscillators and/or the central Coulomb well $V^{(Z)}(\vec{r}) = -Z e^2/|\vec{r}|$. A new way out of this deadlock emerges within the framework of the alternative, so called "$\mathcal{PT}$ symmetric" quantum mechanics. With its complex Hamiltonians $H$ breaking both the parity $\mathcal{P}$ and the time-reflection symmetry $\mathcal{T}$ and commuting only with their product $\mathcal{PT}$, this formalism was proposed by Bessis [1] and by Bender et al [2, 3] as a possible way towards weakening of the standard requirements of Hermiticity.

Several new exactly solvable $\mathcal{PT}$ symmetric models have been proposed recently [4]. This is a promising development with possible applications ranging from field theories [5] to supersymmetric models [6] and from quasi-classical methods [3] to perturbation theory [7].

Even the solvable harmonic oscillator itself acquires a richer spectrum after its consequent $\mathcal{PT}$ symmetric regularization in $D$ dimensions [8]. The detailed structure of spectrum of this prominent example does not in fact offer any really serious surprise. A manifest violation of the parity $\mathcal{P}$ is compensated by an emergence of the so called quasi-parity $q = \pm 1$ tractable as a signature of two equidistant subspectra. The new quantum number $q$ degenerates back to the eigenvalue of parity after a return to the standard Hermitean and one-dimensional oscillator.

No immediate surprise emerges also for the quartic anharmonic oscillator [9]. The situation only becomes less clear after one moves towards the asymptotically vanishing models. They exhibit several counterintuitive properties and open new mathematical challenges [10]. In particular, the popular Coulomb potential did not not even seem particularly suitable for any immediate $\mathcal{PT}$ symmetric regularization.
A psychological barrier has been created by the numerical and semiclassical studies of the general power-law forces $V(x) \sim -(ix)^{\delta}$. They may be well defined everywhere near the harmonic exponents $\delta = 2, \delta = 6$ etc [12]. At the same time, the related analyses hinted that it is apparently difficult to move beyond the Herbst’s singularity located at $\delta = 1$ [13].

In what follows, we intend to employ a slightly different strategy and try to study the Coulomb problem directly, via its well known correspondence to the harmonic oscillator. This correspondence is based on an elementary change of variables. Its background dates back to the nineteenth century mathematics and, in particular, to the work of Liouville [14]. The Newton’s monograph [15] cites also Fivel [16] as a newer source of the idea. In the contemporary literature (cf., e.g., [17] for further references) people usually speak about the Kustaanheimo - Steifel (KS) transformation [18]. In all the implementations of this idea the parameters appearing in the Coulombic and oscillator problems are interrelated of course. Details will be mentioned below. Preliminarily, let us only warn the reader that all the KS-type mappings can also change the dimensions and angular momenta and that the energies of one problem are related to the coupling constants of the other one and vice versa. Within the ”normal” quantum mechanics, all this has already been thoroughly discussed elsewhere: In ref. [19] for $D = 3$ and in ref. [20] for the continuous transformation between Coulomb problems and harmonic oscillators in various dimensions.

2 Liouvillean changes of variables

The change-of-variable approach to the Coulombic bound-state problem enables us to start directly from the harmonic oscillator potential $W(r) = r^2$ or, in the present less traditional context, from its $PT$ symmetric radial Schrödinger equation

$$\left[-\frac{d^2}{dr^2} + \frac{l(l + 1)}{r^2} + W(r)\right] \chi(r) = \varepsilon^2 \chi(r) \quad (1)$$
of ref. [8], using the complex coordinate \( r = x - ic \) with real \( x \in (-\infty, \infty) \) and with, say, positive \( c > 0 \). This means that the integration path has been shifted down from the position where it would cross the strong centrifugal singularity. Such a regularization preserves the asymptotic decrease of the normalizable solutions. Only in the limit \( c \to 0 \) and beyond the trivial one-dimensional case one has to omit all the so called irregular solutions \([21]\) defined by their “physically unacceptable” \( \chi(r) \sim r^{-l} \) behaviour near the origin.

Within the framework of the general Liouville method the change of variables mediates a transition to the different potential \( V(t) \). It is easy to show that once we forget about boundary conditions one merely has to demand the existence of an invertible function \( r = r(t) \) and its few derivatives \( r'(t), r''(t), \ldots \). Then, the explicit correspondence between the two bound state problems may be \textit{explicitly} given by the elementary formulae. From our original eq. (1) (i.e., in our case, harmonic oscillator) one obtains the new (i.e., in our case, Coulombic) Schrödinger equation

\[
\left[ -\frac{d^2}{dt^2} + \frac{L(L+1)}{t^2} + V(t) \right] \Psi(t) = E \Psi(t) \tag{2}
\]

with the new wave functions

\[
\Psi(t) = \chi[r(t)]/\sqrt{r'(t)} \tag{3}
\]

and with the new interaction and the new energies \([14]\),

\[
\frac{L(L+1)}{t^2} + V(t) - E = [r'(t)]^2 \left\{ \frac{l(l+1)}{r^2(t)} + W[r(t)] - \varepsilon^2 \right\} + \frac{3}{4} \left[ \frac{r''(t)}{r'(t)} \right]^2 - \frac{1}{2} \left[ \frac{r'''(t)}{r'(t)} \right].
\]

Thus, it only remains for us to re-analyse the boundary conditions.

### 3 \( \mathcal{PT} \) symmetric KS transformation

Without any serious formal difficulties let us extend the scope of the present considerations to all the singular forces \( \hat{W}(r) = W(r) + f/r^2 \) and and/or \( \hat{V}(t) = V(t) + F/t^2 \).
Both these central forces may act in the respective $d$ and $D$ dimensions. This means that

$$l(l + 1) = \{[j + (d - 3)/2][j + (d - 1)/2] + f\}$$

or rather

$$(l + 1/2)^2 (= \alpha^2) = [j + (d - 2)/2]^2 + f$$

(with $\text{Re} \, \alpha > 0$) and

$$(L + 1/2)^2 (= A^2) = [J + (D - 2)/2]^2 + F$$

(with $\text{Re} \, A > 0$) where the partial waves are numbered by the respective integers $j = 0, 1, \ldots$ and $J = 0, 1, \ldots$.

An important simplification of our effort is provided by our knowledge of the complete harmonic oscillator solution as derived in ref. [8]. Its two equidistant subsets of energies

$$\varepsilon^2 = \varepsilon^2_{(n,q)} = 4n + 2 - 2q \alpha, \quad q = \pm 1, \quad n = 0, 1, \ldots$$

correspond to the two families of the Laguerre-polynomial wave functions

$$\chi_{(n,q)}(r) = N r^{1/2-q \alpha} e^{-r^2/2} L_n^{(-q \alpha)}(r^2).$$

Integration path $r = x - i c$ lies in the lower half of the complex plane and does not change after the subsequent $\mathcal{P}$ and $\mathcal{T}$ transformations $r = r(x) \rightarrow -r$ and $-r \rightarrow -r^* = r(-x)$.

In the spirit of the above-mentioned KS mapping of harmonic oscillators on Coulombic bound states we now have to define a complex variable $t$ as a re-scaled square of $r(x)$ such that the resulting path $t(x)$ remains $\mathcal{PT}$ invariant. Our requirement implies that the complex plane of $r$ will cover twice the complex plane of $t$. In such an arrangement, our lower half plane of $r$ should cover the Riemann sheet given as a whole plane of $t$ which is cut upwards from the origin. In the polar representation, one has $r \sim \exp(-i \varphi)$ mapped upon $t \sim \exp(-2 i \varphi)$ with $\varphi \in (0, \pi)$. 

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Once we introduce a suitable free parameter $\kappa > 0$ we can put, say, $r^2 = 2 \kappa^2 z$ and then rotate the $z-$plane (which is cut, by construction, along the real and positive semi-axis) by the angle $\pi/2$ giving $t = i z$. Our final recipe

$$r^2 = -2 \kappa^2 t$$

maps the above-mentioned straight line $r(x) = x - i c$ upon a curve $t(x) = u + i v$. Its real part $u = u(x) = x c/\kappa^2$ and imaginary part $v = v(x) = (x^2 - c^2)/2 \kappa^2$ form, as required, a $\mathcal{PT}$ symmetric and upwards-oriented parabola $v = -c^2/2 \kappa^2 + (\kappa^2/2 c^2) u^2$ in complex plane. Obviously, a small asymptotic deformation of our original curve $r(x)$ with the modified shifts $c = c(x) \sim 1/x^{1+n}$ would transform the parabola to a pair of lines which are parallel to the cut in the asymptotic domain of $|x| \gg 1$.

Having achieved a $\mathcal{PT}$ symmetry in the complex plane of $t$, we may move to the (trivial) insertions and conclude that all the above-mentioned harmonic oscillator bound-state solutions are in a one-to-one correspondence to the solutions of the Coulombic Schrödinger equation (5),

$$\left[ -\frac{d^2}{dt^2} + \frac{L(L+1)}{t^2} + i \frac{Z e^2}{t} \right] \Psi(t) = E \Psi(t), \quad t = u(x) + i v(x), \quad x \in \mathbb{R}. \quad (5)$$

The underlying assignment of constants is such that $\alpha = 2 A$ while $\kappa$ itself becomes $n-$dependent, $\kappa^2 = 2 Z e^2/\varepsilon^2 = Z e^2/(2n + 1 - 2q A)$. In full detail one gets the new, Laguerre-polynomial wave functions

$$\Psi_{(n,q)}(t) = \mathcal{M} t^{1/2-q A} e^{i \kappa^2 t} L_n^{(2q A)}(-2 i \kappa^2 t) \quad (6)$$

and their energy spectrum specified by the elementary formula

$$E_{(n,q)} = \kappa_{(n,q)}^4 = \frac{Z^2 e^4}{(2n + 1 - 2q A)^2}, \quad q = \pm 1, \quad n = 0, 1, \ldots. \quad (7)$$

This is our main result.

4 Discussion
4.1 Consequences of the curvature of our integration path

The latter two formulae exhibit several unusual features. The first concerns the asymptotics of the wave functions which are determined by the decreasing exponential $\exp(i \kappa^2 t)$. Its form re-confirms the correctness of the above, slightly counter-intuitive KS-dictated choice of our $\mathcal{PT}$ symmetric integration path. Asymptotically, it encircles more or less closely the positive imaginary axis in $t$ plane. This clarifies the apparent paradox.

The second unexpected result is the positivity and unusual $n-$dependence of the energies. This can be related to the choice of the KS integration path $t(x)$ again. In the very vicinity of the origin, one can visualize this path as a circle with radius $\sigma$,

$$u^2(x) + v^2(x) = \sigma^2, \quad |x| \ll 1.$$

From the appropriate definitions we get the formula

$$\sigma = c^2(0)/2 \kappa^2_{(n,q)} + \mathcal{O}(x^2)$$

and see that this radius is $n-$dependent and increases with the growth of this principal quantum number, $\sigma \sim n \, c^2(0)/Z \, e^2, \, n \gg 1$. As a consequence, an “effective charge” of our $\mathcal{PT}$ symmetric Coulomb potential appears to decrease with $n$ since

$$\left| \frac{i \, Z \, e^2}{t} \right| \sim \frac{Z \, e^2}{\sigma} + \mathcal{O}(t) = \mathcal{O}(1/n).$$

This offers a “rule-of-thumb” guide to the unusual and certainly counterintuitive $n-$dependence of the energy levels (4). Of course, in practice, a preferred integration path will be $n-$independent. In such a case, the $n-$dependence re-appears in the small-$x$ deformation of the initial harmonic-oscillator path with $c = c_n(x) = \mathcal{O}(1/n)$. Such a flexible transfer of the excitation-dependence throws also a new light on the complexified KS transformation itself.
4.2 “Flown-away” energies and unavoided crossings

Let us return in more detail to the $A-$dependence of our energies (7). Firstly, we notice their power-law dependence on $n$ and $A$ (with exponent = -2) as somewhat similar to the spectra in $\mathcal{PT}$ symmetric oscillator well (with exponent = +1) and in the Morse potential of ref. (with exponent = +2).

In the present case, obviously, we have to distinguish between the two separate families $E(n,q)$ with $q = +1$ (cf. Figure 1) and $q = -1$ (cf. Figure 2). The latter set is, up to its sign, analogous to the ordinary Coulombic spectrum. By far not so the former one. Its energies enrich and dominate the spectrum. The $n_{\text{div}}-$th energy “flies away” and disappears from the spectrum at $A_{\text{div}} = n_{\text{div}} + 1/2$. Moreover, at all the positive integers and half-integers $A$ one encounters the unavoidable level crossings. In contrast to the harmonic case, they appear at both the opposite and identical (viz., positive) quasiparities $q$. The former case takes place at $A = A_{\text{crit}} = (n - n')/2$ while in the latter case we must fulfill the condition $A = A_{\text{crit}} = (n + n' + 1)/2$. A sample of this phenomenon is given in Figure 3.

Formally the unavoided crossings generate certain identities which connect different Laguerre polynomials (cf. their sample in ref. 8). In applications, these “critical” cases are not exceptional at all. For $F = 0$ forces without a spike, the critical integer or half-integer coordinates $A_{\text{crit}} = J - 1 + D/2$ correspond precisely to the physical (namely, integer) dimensions $D$ and partial waves $J$.

In the conclusion, let us not forget about many open questions. Pars pro toto, one could mention a not yet clear possibility of re-interpretation of our bound states, say, in the limit $t \to \text{real}$, i.e., beyond the mathematical and apparently natural boundaries of our present approach. Moreover, we must keep in mind that via our complexification of the coordinates we of course broke their immediate connection to any standard $D-$dimensional problem. In this sense, our $F = 0$ and $F \neq 0$ Hamiltonians differ just in an inessential way. One could even prefer the latter, Kratzer-like option as a model which is formally simpler, due to the generic absence.
of the puzzling unavoidable crossings. At $F \neq 0$ the structure of the spectrum of our present Coulomb model becomes also richer and, in this sense, more interesting.

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Figure 1. Quasi-even levels (n,q) (units Z=e=1)
Figure 2. Quasi-odd levels (n=0-5, units Z=e=1)
Figure 3. Sample of unavoidable crossings