Notes concerning some

Quantum Applications of the Riccati Equation

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Introduction. I have today (22 June 2004) received for review, from the editor of the American Journal of Physics, a manuscript by J. Morales, J. J. Peña, M. A. Ropmero-Romo & J. L. López-Bonilla which they entitle "A direct method to solve the one-dimensional Schrödinger equation." The authors' command of English is quite imperfect, which makes their work a little hard to read. My intent here will be to see if I can construct a brief encapsulation of their essential technical idea . . . which seems on first glance to be of some interest.

1. The essential idea. It was known already to Euler (1769)[1] that if $u(x)$ is a solution of the linear 2$^{\text{nd}}$ order differential equation (Sturm-Liouville equation)

$$\alpha(x)u''(x) + \beta(x)u'(x) + \gamma(x)u(x) = 0$$

then

$$y(x) \equiv \tfrac{d}{dx}\log u(x) = \frac{u'(x)}{u(x)}$$

is a solution of the non-linear 1$^{\text{st}}$ order differential equation (Riccati equation)

$$y' + y^2 + \frac{\beta y + \gamma}{\alpha} = 0$$

From this general observation it follows in particular that if $\psi(x)$ is a solution of the time-independent Schrödinger equation

$$-\tfrac{\hbar^2}{2m}\psi'' + V(x)\psi = E\psi$$

[1] See Keisuke Hasegawa, "The Riccati equation & its applications in physics" (Reed College thesis, 2001), §1.6.

then[2] $\sigma(x) \equiv \psi'/\psi$ is a solution of

$$\sigma' + \sigma^2 - \tfrac{2m}{\hbar^2}\big[V(x) - E\big] = 0 \tag{1}$$

This is sometimes written

$$\begin{aligned} V(x) &= E_n + \tfrac{\hbar^2}{2m}(\sigma_n' + \sigma_n^2) \\ &= E_n + \tfrac{\hbar^2}{2m}(\psi_n''/\psi_n) \end{aligned} \tag{2}$$

to emphasize that from any particular eigenpair $\big\{E_n, \psi_n(x)\big\}$ one can recover the potential—a proposition most commonly encountered in reference to the groundstate: $\big\{E_0, \psi_0(x)\big\}$.

Morales *et al* note that supersymmetric quantum mechanics (SSQM) proceeds from the observation that the operator $\mathbf{H} - E\,\mathbf{I}$ can be factored

$$\tfrac{1}{2m}\,\mathbf{p}^2 + V(x) - E = \big[-i\tfrac{1}{\sqrt{2m}}\,\mathbf{p} + W(x)\big]\big[+i\tfrac{1}{\sqrt{2m}}\,\mathbf{p} + W(x)\big]$$

by requiring of the "superpotential" $W(x)$ that[3]

$$W^2 - \tfrac{\hbar}{\sqrt{2m}}W' = V - E$$

Here again we have encountered an instance of the Riccati equation (an instance which is again most commonly encountered in the case $E = E_0$) and indeed: if we were to set

$$W = -\tfrac{\hbar}{\sqrt{2m}}\sigma$$

we would recover precisely (1).

Look now to (2) in the instance $n = 0$:

$$V(x) = E_0 + \tfrac{\hbar^2}{2m}(\sigma_0' + \sigma_0^2) \tag{3}$$

Morales *et al* would have us **guess** the $\sigma_0(x)$ that leads, by (3), to the $V(x)$ we have in mind. Looking by way of example to the harmonic oscillator, they pluck $\sigma_0(x) = -Bx$ out of their sombreros, compute

$$\begin{aligned} V(x) &= E_0 + \frac{\hbar^2 B^2}{2m}x^2 - \frac{\hbar^2 B}{2m} \\ &\downarrow \\ &= E_0 + \tfrac{1}{2}m\omega^2 x^2 - \tfrac{1}{2}\hbar\omega \quad \text{if set} \quad B = m\omega/\hbar \end{aligned}$$

and observe that they arrive at their intended destination $V(x) = \tfrac{1}{2}m\omega^2 x^2$ if they set $E_0 = \tfrac{1}{2}\hbar\omega$. To obtain $\psi_0(x)$ they use

$$\psi(x) = A\exp\Big\{\int^x \sigma(\xi)\,d\xi\Big\} \tag{4}$$

[2] See Hasegawa, §3.1.

[3] See Christopher Lee, "Supersymmetric quantum mechanics" (Reed College thesis, 2001), §1.1.

and get

$$\psi_0(x) = A\exp\Big\{-\tfrac{m\omega}{2\hbar}x^2\Big\}$$

Because this function is node-free we know we have in fact nailed the ground state.

Morales *et al* turn at this point to the question: How—having computed $\{E_0, \psi_0(x)\}$—to compute $\{E_n, \psi_n(x)\} : n > 0$? To that end they use

$$\psi_n(x) \equiv \psi_0(x)\cdot g_n(x) \tag{5}$$

to define new functions $g_n(x)$[4] and from

$$\sigma_n(x) = \frac{g_n'(x)}{g_n(x)} + \frac{\psi_0'(x)}{\psi_0(x)} = \frac{g_n'(x)}{g_n(x)} + \sigma_0(x)$$

obtain

$$\begin{aligned}\sigma_n' + \sigma_n^2 &= \sigma_0' + \frac{g_n g_n'' - g_n' g_n'}{g_n^2} + \sigma_0^2 + \frac{2\sigma_0 g_n'}{g_n} + \frac{g_n' g_n'}{g_n^2}\\ &= \sigma_0' + \sigma_0^2 + \frac{g_n'' + 2\sigma_0 g_n'}{g_n}\\ &= \tfrac{2m}{\hbar^2}\big[V(x) - E_0\big] + \frac{g_n'' + 2\sigma_0 g_n'}{g_n}\\ &= \tfrac{2m}{\hbar^2}\big[V(x) - E_n\big]\end{aligned}$$

whence finally

$$E_n = E_0 - \tfrac{\hbar^2}{2m}\frac{g_n'' + 2\sigma_0 g_n'}{g_n}$$

which upon multiplication by g_n becomes

$$g_n'' + 2\sigma_0\, g_n' + \tfrac{2m}{\hbar^2}(E_n - E_0)\, g_n = 0 \tag{6}$$

An initial Sturm-Liouville problem (Schrödinger equation) has by this point been converted into an alternative Sturm-Liouville problem, the advantage (such as it is) being that

- whereas it was $V(x)$ that had to be specified to render the Schrödinger equation precise
- $V(x)$ is entirely absent from (6); one is asked instead to specify $\sigma_0(x)$. But this, by $V(x) = E_0 + \hbar^2(\sigma_0' + \sigma_0^2)/2m$, is simply an alternative presentation of the same essential information.

Our non-trivial assignment, according to Morales *et al*, is to identify the constants E_n endowed with the property that the associated solutions $g_n(x)$ of (6) engender functions $\psi_n(x) \equiv \psi_0(x)\cdot g_n(x)$ that conform to the familiar physical side conditions. It is not at all clear that the problem thus posed will, in general, be any more tractable than the problem posed by Schrödinger, and I

[4] Note that necessarily $g_0(x) = 1$ (all x).

fail to understand the grounds on which Morales *et al* assert that "[the method] guarantees that the quantum mechanical problem. . . is exactly solvable."

Let's see how the method works when applied to the harmonic oscillator. Setting $\sigma_0(x) = -m\omega x/\hbar$, as we learned to do on the preceding page, equation (6) becomes

$$g_n'' - 2\tfrac{m\omega}{\hbar} x\, g_n' + \tfrac{2m}{\hbar^2}(E_n - \tfrac{1}{2}\hbar\omega)\, g_n = 0$$

Introduce the dimensionless variable

$$y = \sqrt{\tfrac{m\omega}{\hbar}}\, x$$

write $G(y) \equiv g(x)$ and obtain

$$\begin{aligned} G''(y) - 2y\,G'(y) + 2n\,G(y) &= 0 \\ 2n \equiv \tfrac{2}{\hbar\omega}(E_n - \tfrac{\hbar\omega}{2}) \end{aligned} \tag{7}$$

Mathematica is quick to inform us that the general solution of (7) can be described $G(y) = A \cdot \mathrm{HermiteH}[n, y] + B \cdot \mathrm{Hypergeometric1F1}[-\frac{1}{2}n, \frac{1}{2}, y^2]$. We seek solutions such that

$$G(y) \cdot e^{-\frac{1}{2}y^2} \to 0 \quad \text{as} \quad y \to \pm\infty$$

which (after some tedious argument) forces us to set $B = 0$ and to insist that n be an integer. We are brought thus to the familiar conclusion that

$$E_n = (n + \tfrac{1}{2})\hbar\omega \quad \text{and} \quad G_n(y) = A \cdot \text{Hermite polynomial } H_n(y)$$

This argument is—compared to the standard textbook argument—pretty clean, I have to admit. But the oscillator is, in all respects, an exceptionally friendly system.

Morales *et al* look similarly to the charged oscillator in a constant electric field, the charged oscillator in an external dipole field, the free particle, the particle in a Morse potential, a particle in a Hulthén potential. I remain unconvinced, however, that their method—particularly since it proceeds from some informed guesswork (their "Ansatz")—can be applied with equal ease to "*any* exactly solvable potential."

All of the above examples refer to motion on the unrestricted line. It is by way of contrast that I look now, therefore, to details of the method as they arise in connection with its. . .

2. Application to the particle-in-a-box problem. Let a particle of mass m be constrained to the interior of the interval $0 \leqslant x \leqslant a$, within which it moves freely. The problem, as posed by Schrödinger, is to solve

$$-\tfrac{\hbar^2}{2m}\psi'' = E\psi$$

subject to the conditions $\psi(0) = \psi(a) = 0$ and $\int_0^a |\psi(x)|^2\, dx = 1$. It is, of course, already well known in advance that[5]

$$E_n = E_0 \cdot (n+1)^2 \quad \text{with} \quad E_0 = \tfrac{\pi^2\hbar^2}{2ma^2} \quad : \quad n = 0, 1, 2, \ldots$$

and

$$\psi_n(x) = \sqrt{2/a} \cdot \sin[(n+1)\pi x/a]$$

We know, therefore, that

$$\sigma_0(x) = \pi/a \cdot \frac{\cos[\pi x/a]}{\sin[\pi x/a]} = \pi/a \cdot \cot[\pi x/a] \tag{8}$$

By calculation

$$\sigma_0' + \sigma_0^2 + \tfrac{2m}{\hbar^2}E_0 = \tfrac{2m}{\hbar^2}E_0 - \tfrac{\pi^2}{a^2}$$

so to satisfy Morales' "fundamental equation" (3) we must assign to E_0 precisely the value already stated. Note that Morales and his friends are obligated to *guess* (8), which I don't think they would find easy. But if they enlisted the assistance of *Mathematica* they would be led to functions of the design

$$\sigma(x) = -k\tan[k(x-\xi)] \quad \text{with} \quad k \equiv \tfrac{\sqrt{2mE_0}}{\hbar}$$

—*all* of which satisfy

$$\sigma' + \sigma^2 + k^2 = 0$$

To achieve box-confinement it seems natural to identify consecutive singularities of the tangent with the boundaries of the box: setting

$$\begin{aligned} k(0-\xi) &= -\tfrac{\pi}{2} \\ k(a-\xi) &= +\tfrac{\pi}{2} \end{aligned}$$

we obtain $\xi = \pi/2k$ and $ka = \pi$, the latter of which can be written $E_0 = \frac{\pi^2\hbar^2}{2ma^2}$. So we have

$$\sigma_0(x) = -k\tan[kx - \tfrac{1}{2}\pi] = k\cot[kx]$$

—in precise agreement with (8). Working now from (4) we obtain

$$\psi_0(x) = A\exp\Big\{\log\sin[kx]\Big\} = A\sin[\pi x/a]$$

and to achieve normalization are obliged to set $A = \sqrt{2/a}$. We have recovered precisely the boxed-particle ground state (no nodes on the physical interval) reported at the top of the page. We look now to the excited states:

Working from (6) we have

$$g_n'' + 2k\cot[kx]\,g_n' + k^2(\lambda_n - 1)\,g_n = 0 \quad : \quad \lambda_n \equiv E_n/E_0$$

Introduce the dimensionless variable $y \equiv kx$, write $G_n(y) \equiv g_n(x)$ and obtain n-subscripted differential equations of the form

$$G''(y) + 2\cot(y)\cdot G'(y) + (\lambda - 1)\,G(y) = 0$$

[5] See D. Griffiths, *Introduction to Quantum Mechanics* (1995), §2.2.

The general solution of this differential equation is, according to *Mathematica*, a hypergeometric mess. But if we use what we know from elementary quantum mechanics to construct test functions

$$G_n(y) \equiv \frac{\sin[(n+1)y]}{\sin[y]}$$

we find that

$$\begin{aligned}
&G_0''(y) + 2\cot(y)\cdot G_0'(y) + (\lambda-1)\,G_0(y) \text{ vanishes if } \lambda = 1\\
&G_1''(y) + 2\cot(y)\cdot G_1'(y) + (\lambda-1)\,G_1(y) \text{ vanishes if } \lambda = 4\\
&G_2''(y) + 2\cot(y)\cdot G_2'(y) + (\lambda-1)\,G_2(y) \text{ vanishes if } \lambda = 9\\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\vdots
\end{aligned}$$

This would appear to be a tediously *difficult* way to establish that

$$\lambda_n \equiv E_n/E_0 = (n+1)^2$$

and that

$$\psi_n(x) = A\sin[(N+1)\pi x/a]$$

The method hasn't exactly failed, but has been shown to be—at least in this simplest-of-all-cases—terribly clumsy and inefficient.

3. Status of the Morales "Ansatz." The problem of solving diverse instances of the "generalized Riccati equation"

$$\frac{dy}{dx} = P(x) + Q(x)y + R(x)y^2$$

—of which (1) provides a particular instance—is a problem to which many of the greatest mathematicians of the 18^{th} and 19^{th} Centuries gave close and productive attention.[6] It was within precisely this context that Liouville (1839) established that in many typical instances the solutions of nonlinear ordinary differential equations *cannot be described by finite combinations of elementary transcendental functions*. For Morales *et al* to ask us to *guess* the solution of (3)—of

$$V(x) = E_0 + \tfrac{\hbar^2}{2m}(\sigma_0' + \sigma_0^2)$$

with $V(x)$ preassigned and E_0 properly evaluated—is for them to ask quite a lot . . . particularly since there are *many* solutions: we are asked to guess the one that permits

$$\psi_0(x) = A\exp\left\{\int^x \sigma_0(\xi)\,d\xi\right\}$$

to be identified with the (nodeless) physical ground state.

[6] See E. Hille, *Ordinary Differential Equations in the Complex Domain* (1976), Chapter 4 and (especially) G. N. Watson, *A Treatise on the Theory of Bessel Functions* (2^{nd} edition, 1976), Chapters 1 & 4.

To illustrate the point, look again to the harmonic oscillator, where (1) can be written

$$\sigma' + \sigma^2 - \tfrac{2m}{\hbar^2}\big[\tfrac{1}{2}m\omega^2x^2 - E\big] = 0$$

and becomes

$$f' + f^2 - [y^2 - \varepsilon] = 0 \tag{9}$$

if we define $y \equiv \sqrt{m\omega/\hbar}\,x$, $\varepsilon \equiv 2E/\hbar\omega$, $f(y) \equiv \sqrt{\hbar/m\omega}\,\sigma(x)$. *Mathematica* reports that the *general* solution of (9) can be described

$$f(y) = \frac{N(y,\varepsilon)}{D(y,\varepsilon)}$$

with

$$\begin{aligned} N(y,\varepsilon) &= ye^{-\frac{1}{2}y^2}\Big\{(\varepsilon-1)\texttt{HermiteH[}\tfrac{1}{2}(\varepsilon-3), y\texttt{]} - \texttt{HermiteH[}\tfrac{1}{2}(\varepsilon-1), y\texttt{]}\Big\} \\ &\quad - kye^{-\frac{1}{2}y^2}\Big\{(\varepsilon-1)\texttt{Hypergeometric1F1[}\tfrac{1}{4}(5-\varepsilon), \tfrac{3}{2}, y^2\texttt{]} \\ &\qquad + \texttt{Hypergeometric1F1[}\tfrac{1}{4}(1-\varepsilon), \tfrac{1}{2}, y^2\texttt{]}\Big\} \\ D(y,\varepsilon) &= e^{-\frac{1}{2}y^2}\Big\{\texttt{HermiteH[}\tfrac{1}{2}(\varepsilon-1), y\texttt{]} \\ &\qquad + k\,\texttt{Hypergeometric1F1[}\tfrac{1}{4}(1-\varepsilon), \tfrac{1}{2}, y^2\texttt{]}\Big\} \end{aligned}$$

where k is a constant of integration and where the $e^{-\frac{1}{2}y^2}$ factors can, in fact, be abandoned. Morales *et al* tacitly expect us, if we would get where they would have us go, to have the wit to set $k = 0$ and $\varepsilon = 1$. For then (according to *Mathematica*) we obtain the much simpler result

$$f(y) = -y$$

With this we do recover precisely the $\sigma_0(x) = m\omega x/\hbar$ and $E_0 = \frac{1}{2}\hbar\omega$ of page 2, but only by exercise of a fairly sophisticated command of higher function theory.

4. Concluding remarks. I am brought to the conclusion that the "Riccati method," as implemented by Morales *et al*, is pretty when it works, but that it can be expected to work only when one has prior knowledge (of $\psi_0(x)$, from some other source) sufficient to frame a sharp Ansatz. Even then, one can expect to be able to carry the method through to completion—to construction of *all* the eigenvalues/eigenstates—only in especially favorable cases.

It would be interesting to see where the method leads when one possesses only an *approximately* correct description of $\sigma_0(x)$, one which leads *via* (3) to an *approximate* description of $V(x)$. It would be interesting, more generally, to see what kind of perturbation theories can be constructed within the framework provided by the method.[7]

[7] See in this connection the Reed College thesis "Variational methods using supersymmetric quantum mechanics" by Douglas B. Beringer (2004).

While the methods sketched here and those standard to SSQM were seen on page 2 to be related—both assign importance to formally identical instances of the Riccati equation—no attempt has been made here to trace the deeper details of that relationship. We note in particular that "factorization of the Hamiltonian" has played no explicit role in the preceding discussion. Nor have we attempted to make use of any of the intricately lovely formal properties that have been known since classical times to interrelate diverse solutions of the Riccati equation.[8]

I think Morales *et al* would not have bothered to write their paper had they been familiar with S. B. Haley's "An underrated entanglement: Riccati and Schrödinger equations," AJP **65**, 237 (1997), which provides a more carefully reasoned account of exactly the same subject, and which in his Chapter 3 was taken as Hasegawa's point of departure.

I am very deeply indebted to D. Strickland for discussions which took place while this work was in progress.

[8] See Chapter 1 in Hasegawa's thesis.[1]