Product Wavefunction and the Nikiforov-Uvarov Method for the Schrodinger Equation

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In a series of notes (1) , we suggested one may compare the Schrodinger equation, with the ground state solution removed, to a general hypergeometric equation:
p(x) d/dx d/dx W1(x) + q(x) d/dx W1(x) + C1 W(1x) = 0 ((1)) where p(x) is at most quadratic in x and q(x) is at most linear. Such an equation has known Rodrigues polynomial solutions (2).To remove the ground state, we write W(x)=Wo(x)W1(x) where W(x) is the full wavefunction of a bound state and Wo(x), the ground state (or another state). Inserting into the time-independent Schrodinger equation leads to the coupled equation:

-1/2m d/dx d/dx W1(x) - 1/m d/dx W1(x) [d/dx Wo(x) / Wo(x)] = (E-Eo) W1(x) ((2))

Recently in 2006, a more general method was presented in the literature (3). In this method, W(x)=f(x)F(x), E=Ef + EF and V=Vf + VF. These values arre inserted into the time-independent Schrodinger equation and compared with the Nikiforov-Uvarov method equation. This general method was applied to a specific case of Jacobi polynomials and VF found to be 0.
In the case that VF=0, f(x) is a solution of the time-independent Schrodinger equation and this general method is the same as the one presented in (1). In fact, it seems in the example in (3), VF is forced to equal 0 which may imply the more general method is very similar to the method of (1) The objective of this note is to compare the two methods.

Method of (3)

In (3), the Nikiforov-Uvarov (NU) approach and not the general hypergeometric DE ((1)) is the starting point. The NU approach yields solutions for a DE of the form:

d/dy d/dy F(y=s(x)) + t1(s)/s1(s) d/dy F + s2/(s1*s1) F= 0 ((3))

s1 and s2 are at most quadratic polynomials in y=s(x) and t1 is linear.

The authors of (3) use W(x)=f(x)F(s(x)), where y=s(x) is a transformation, which they insert into the time-independent Schrodinger equation obtaining:

d/dy d/dy F(s) + { (d/dx d/dx s) / (d/dx s)^2 + 2 d/d f / [(d/dx s) f] } d/dy F(s) + { (d/dx d/dx f) / [f (d/dx s) ^{2} + (E-V)/[(d/dx s)^2] } F(s) = 0 ((4))

They then identify:

(d/dx d/dx f) / f= Vf-Ef (a Schrodinger equation result containing Vf i.e. part of the potential)

VF-EF = - s1/ (s2*s2) (d/dx s) ^{2}

and f(x) = (d/dx s) $^{-½}$ exp [½ integral (upper bound s(x) t1/s1 ds]

Thus, it seems the authors of (3) are not looking upon f(x) as a solution of the Schrodinger equation, although it becomes one if VF=0.

This general approach is then applied to a Jacobi polynomial problem where:

VF-EF= C2 (d/dx s)2 / [1-s*s]

(See details in (3).)

The authors of (3) argue: "Since we have a constant (EF) on the left-hand side, there must be at least one term on the right-hand side, from which a constant arises." (3)

They then set: C1= C2 (d/dx s)2 / [1-s*s] ((5)) or VF=0. In the approach of (1), VF=0 right at the beginning. It seems that VF=0 is being forced to zero. If that is the case, the general method of (3) seems to collapse to the method of (1).

If VF is forced to 0, then f(x) is a solution of the Schrodinger equation and the coefficient of F(x) in ((4)) becomes:

{ (d/dx d/dx f) / [f (d/dx s) ^{2} + (E-V)/[(d/dx s)^{2}] } = (E-Eo)

because f(x) is a solution of the Schrodinger equation with energy Eo. Thus, the coefficient of F(x) is a constant forcing the coefficient of d/dy F in ((4)) to be of the form: c s(x) + b where c and b are unknown constants. Thus, ((4)) is compared to the general hypergeometric DE ((1)).

The authors of (3) choose s(x)= cos(ax) where C=a*a as a solution of ((5)) but point out there are other solutions. They then obtain a potential:

Vf = C3 csc2(ax) + C4 csc(a) cot(a) ((6)) where C3 and C4 are constants.

Method of (1)

We compare the method of (3) with that of (1). In (1), VF=0 automatically and f(x)=Wo(x). The Schrodinger equation with W(x)=Wo(x)W1(s(x)) where s(x)=y is a transformation leads to the equation:

$-1/2m\ [d/dx\ s]^2\ d/dy\ d/dy\ W1 + (\ \{\ (d/dx\ d/dx\ s) + 2\ (d/dx\ s)\ d/dx\ f / [\ f]\ \}\ ) - (E-Eo)\ W1 = 0$
((7))

In order for ((7)) to be of hypergeometric form ((1)):

$\{\ (d/dx\ d/dx\ s) + 2\ (d/dx\ s)\ d/dx\ f / [\ f]\ \} = cy + b$ ((8))

and $(d/dx\ s)^2$ must be a quadratic or lower in s. If s(x)= cos(ax) as in (3), then

$(d/dx\ s)^2 = a*a\ \sin(ax)\ \sin(ax) = a*a\ (1- s*s)$ ((8))

Thus, the quadratic condition is met. The goal becomes to solve ((8)) where:

$d/dx\ d/dx\ s(x) = -a*a\ \cos(ax) = -a*a\ y$ and $d/dx\ s = -a\ \sin(ax) = -a\ \mathrm{sqrt}(1-y*y)$

Note:

$d/dx(\ d/d\ f / f) + (d/dx\ f / f)^2 = d/d\ d/dx\ f / f$ and ((9))

$d/d\ d/dx\ f = -2m(Eo-V)\ f$ ((10))

Let $g(x)= d/dx\ f /f$ then:

$-a*a\ y - 2\ a\ \mathrm{sqrt}(1-y*y)\ \mathrm{sqrt}\ \{\ -2m(Eo-V) - d/dx\ g\} = c\ y + b$ ((11))

$4a*a\ (1-y*y)\ \{\ -2m(Eo-V) - d/dx\ g\} = [a*ay + (cy+b)]^2$ ((12))

One may obtain g from ((8)) and hence d/dx g i.e.

$g= (C1\ \cos(ax) + C2\ ) / \sin(ax)$ and $d/dx\ g = C3\ \cot^2(ax) + C4\csc2(ax) + C5$

Equation ((11)) then yields:

$V(x)= \mathrm{constant} + C6\ \cot^2(ax) + C7\ \csc^2(ax) + C8\ \cos(ax) / [\sin^2(ax)]$ ((12))

Noting : $1+ \cot^2(ax) = \csc^2(ax)$ one has a potential of the same form as in (3).

Conclusion

In conclusion, it seems the method of (1) is identical to that of (3) if VF=0. If one forces VF to be zero, it seems this is the equivalent to model (1) with VF=0 as an initial conditoin. The results of the two methods yield the same result for the example considered in (3).

References

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