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Families of interrelated Schrödinger equations

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Abstract. We discuss an interesting property of the Schrödinger equation under the repeated application of a particular transformation, namely we show how this leads to a family of Schrödinger equations with related analytic solutions. These solutions may, in turn, be used to check computer codes for N-dimensional Schrödinger equations with potentials that do not admit analytic solutions.

Analytic solutions of the three- (and more generally N-) dimensional Schrödinger equation are of considerable interest in quantum mechanics.

Consider the N-dimensional radial Schrödinger equation [1, 2]

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\mathrm{d}^2}{\mathrm{d}s^2}-\frac{(k_0-1)(k_0-3)}{4s^2}\right)+V(s)-E\right]u_0(s)=0 \tag{1}$$

where $k_0 = N + 2l$, and $\int_0^\infty u_0^2(s)\,\mathrm{d}s = 1$.

Applying the operations $s = \rho^2$, $u_0(s) = \rho^{1/2}u_1(\rho)$, on equation (1), the resulting equation is again a Schrödinger equation, namely

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\mathrm{d}^2}{\mathrm{d}\rho^2}-\frac{(k_1-1)(k_1-3)}{4\rho^2}\right)+4\rho^2V(\rho)-4\rho^2E\right]u_1(\rho)=0 \tag{2}$$

where $k_1 = 2k_0 - 2$.

A second application of this transformation (this time on equation (2)) yields

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\mathrm{d}^2}{\mathrm{d}q^2}-\frac{(k_2-1)(k_2-3)}{4q^2}\right)+4^2q^6V(q)-4^2q^6E\right]u_2(q)=0 \tag{3}$$

with $k_2 = 2k_1 - 2$, and $s = q^4$.

The result of third, identical operation (on equation (3)) is

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2}-\frac{(k_3-1)(k_3-3)}{4r^2}\right)+4^3r^{14}V(r)-4^3r^{14}E\right]u_3(r)=0 \tag{4}$$

with $k_3 = 2k_2 - 2$, and $s = r^8$. Generally after n such operations, $k_n = 2k_{n-1} - 2$, and the last two terms in the resulting equation involve 4^n times a power of r given by 2, 6, 14, 30, for $n = 1, 2, 3, 4$, etc.

It is clear from the above four equations (1)–(4) that repeated application of this particular transformation on a radial Schrödinger equation retains the form of the original equation. One thus obtains a collection, constituting a class of different but related

Schrödinger equations. The above operations are independent of the details of $V(s)$ and hence of $u_0(s)$, and E. To obtain a family of related, analytically solvable Schrödinger equations one must begin with a potential $V(s)$ in equation (1), whose eigenfunctions $u_0(s)$ and eigenvalues E are known.

If $V(s)$ is chosen to be a Coulomb potential $V(s) = -A/s$, then (with $m = c = \hbar = 1$), $E_{nl} = -A^2/(2n^2)$, and

$$u_0(s) = Cs^{(k_0-1)/2}\,\mathrm{e}^{-As/n}\,{}_1F_1\left(-n + \frac{k_0-1}{2}; k_0 - 1; \frac{2As}{n}\right) \tag{5}$$

where $n = (k_0 - 1)/2$, $(k_0 + 1)/2, \ldots$.

For this choice of $V(s)$, the ground-state (i.e. $n = (k_0 - 1)/2$) wavefunction is

$$u_0(s) = Cs^n\,\mathrm{e}^{-As/n}. \tag{6}$$

One thus has the exactly solvable Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\mathrm{d}^2}{\mathrm{d}s^2} - \frac{(k_0-1)(k_0-3)}{4s^2}\right) - \frac{A}{s} + \frac{A^2}{2n^2}\right]u_0(s) = 0 \tag{7}$$

with $k_0 = 2n + 1$.

For this choice of $V(s)$, equation (2) becomes

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\mathrm{d}^2}{\mathrm{d}\rho^2} - \frac{(k_1-1)(k_1-3)}{4\rho^2}\right) - 4A + \frac{2A^2}{n^2}\rho^2\right]u_1(\rho) = 0 \tag{8}$$

with ground-state wavefunction

$$u_1(\rho) = C\rho^{2n-1/2}\,\mathrm{e}^{-A\rho^2/n} \tag{9}$$

where $k_1 = 4n$.

This illustrates the known connection between the Coulomb and oscillator systems [3, 4] where, in equation (8),

$$v(\rho) = \frac{2A^2}{n^2}\rho^2 \qquad E = 4A.$$

For this choice of $V(s)$, equation (3) becomes

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\mathrm{d}^2}{\mathrm{d}q^2} - \frac{(k_2-1)(k_2-3)}{4q^2}\right) - 16Aq^2 + \frac{8A^2}{n^2}q^6\right]u_2(q) = 0 \tag{10}$$

with $k_2 = 8n-2$, i.e. it involves a quantum mechanical system with the polynomial potential

$$v(q) = \frac{8A^2}{n^2}q^6 - 16Aq^2 \tag{11}$$

(a repulsive oscillator, plus an attractive sextic term), eigenvalue $E = 0$, and ground-state wavefunction

$$u_2(q) = Cq^{4n-3/2}\,\mathrm{e}^{-Aq^4/n}. \tag{12}$$

Similarly equation (4) becomes

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\mathrm{d}^2}{\mathrm{d}\rho^2} - \frac{(k_3-1)(k_3-3)}{4\rho^2}\right) - 64A\rho^6 + \frac{32A^2}{n^2}\rho^{14}\right]u_3(\rho) = 0 \tag{13}$$

with $k_3 = 16n - 6$, i.e. it corresponds to the potential

$$v(q) = \frac{32A^2}{n^2}\rho^{14} - 64A\rho^6 \tag{14}$$

energy eigenvalue $E = 0$, and ground-state wavefunction

$$u_3(\rho) = Cq\rho^{8n-7/2}\,\mathrm{e}^{-A\rho^8/n} \tag{15}$$

and so on.

These connections are useful, among other things because such exact solutions may be used to test numerical Schrödinger equation solutions for polynomial potentials that cannot be solved analytically. For instance, to see if the numerical solutions for an arbitrary $(G > 0)$ potential $v(\rho) = G\rho^{14} + H\rho^6$ are accurate, one may substitute the values for G, and H given in equation (14) and see how close E (ground-state numerical) is to 0, and the numerical ground-state wavefunction is to equation (15). One has here a class of solutions for arbitrary dimension, where the one-dimensional systems constitute a simple special case. These may be compared to the one-dimensional quasi-exactly-soluble polynomial Schrödinger equations discussed by Turbiner and co-worker [5]

There are an infinite number of analytic solutions, equation (5), of equation (7) and these may each be converted into solutions of the related equations (8), (10), and (13) as was illustrated above for the lowest eigenfunction (equation (6)).

An interesting observation in this connection is that given equation (1), one can also proceed in the opposite direction from that involved in obtaining equations (2)–(4). Thus, it is clear that the equation

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{(k_{-1}-1)(k_{-1}-3)}{4r^2}\right) + \frac{V(r)}{4r} - \frac{E}{4r}\right]u_{-1}(r) = 0 \tag{16}$$

transforms into equation (1) under the above operations, with $r = s^2$, and $k_0 = 2k_{-1} - 2$.

For the choices leading to equations (7), (8), (10), and (13), equation (16) becomes the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{(k_{-1}-1)(k_{-1}-3)}{4r^2}\right) - \frac{A}{4r^{3/2}} + \frac{A^2}{8n^2 r}\right]u_{-1}(r) = 0 \tag{17}$$

a system subject to the repulsive Coulomb potential $v_1(r) = A^2/(8n^2r)$ plus the attractive $r^{-3/2}$ power potential $v_2(r) = -A/(4r^{3/2})$, where $k_{-1} = n + 3/2$, $E = 0$, and the ground-state wavefunction is

$$u_{-1}(r) = Cr^{(2n+1)/4}\,\mathrm{e}^{-A\sqrt{r}/n}. \tag{18}$$

Other choices for $V(s)$ in equation (1) yield different analytically soluble families of related Schrödinger equations.

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