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PERTURBATION THEORY FOR ILLUSTRATION PURPOSES

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ABSTRACT

The general Laguerre equations provide the simplest examples for testing perturbation theories.

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PERTURBATION THEORY FOR ILLUSTRATION PURPOSES

The aim is to use simple equations with simple perturbation functions which allow for simple integration of both unperturbed and perturbed equations. The Laguerre functions are used in this manner.

Laguerre Functions

Let us consider a mathematical or artificial perturbation problem involving the general Laguerre functions. How such a perturbation could arise in connection with a two dimensional wave equation with a potential energy equal $-(\text{constant})/(x^2+y^2)^{\frac{1}{2}}$. Some of the properties of Laguerre functions are considered in the Appendix. The wave functions for harmonic oscillators correspond to Laguerre functions L^m_{n+m} with $m = -\frac{1}{2}$ for the symmetric solutions and $m = +\frac{1}{2}$ for the antisymmetric. The cases where m is an integer provide much simpler results when used in connection with perturbation theory.

The harmonic oscillator solutions are reduced to the Laguerre functions in the following manner

$$
\begin{aligned}
H &= -\frac{d^2}{dr^2} + (1+\alpha)^2 r^2 \quad , \quad H = H_o + V \quad , \\
H_o &= -\frac{d^2}{dr^2} + r^2 \quad , \quad V = (2\alpha + \alpha^2) r^2 \quad .
\end{aligned}
\tag{1}
$$

Replacing $\frac{1}{4}H$ by H, and introducing the new variable $x = r^2$, we find for the symmetric, antisymmetric solutions, respectively,

$$
\begin{aligned}
&\text{Symmetric} \quad H = -x\frac{d^2}{dx^2} - \frac{1}{2}\frac{d}{dx} + (1+\alpha)^2 \frac{x}{4} \quad , \quad E_n = (n+\tfrac{1}{4})(1+\alpha) \quad , \\
&\text{Antisymmetric} \quad H = -x\frac{d^2}{dx^2} - \frac{3}{2}\frac{d}{dx} + (1+\alpha)^2 \frac{x}{4} \quad , \quad E_n = (n+\tfrac{3}{4})(1+\alpha) \quad .
\end{aligned}
\tag{2}
$$

The general Laguerre example treated as a perturbation, proceeds as follows:

$$Hy = (H_o+V)y = Ey$$

$$H = -x\frac{d^2}{dx^2} - (m+1)\frac{d}{dx} + (1+\alpha)^2\frac{x}{4}, \quad E_n = (n+\frac{m+1}{2})(1+\alpha)$$

$$H_o = -x\frac{d^2}{dx^2} - (m+1)\frac{d}{dx} + \frac{x}{4}, \quad V = \frac{\alpha}{2}(1+\frac{\alpha}{2})x, \quad E_n^{(o)} = (n+\frac{m+1}{2}). \tag{3}$$

We shall define the unperturbed functions by

$$\psi(x,s) = \frac{e^{-\frac{x}{2}\frac{1+s}{1-s}}}{(1-s)^{m+1}} = \sum_{n=o}^{\infty} y_n(x)s^n \quad , \tag{4}$$

corresponding to the explicit expressions

$$y_n(x) = e^{-\frac{x}{2}}\sum_{k=o}^{n}\binom{n+m}{n-k}\frac{(-x)^k}{k!} \quad , \tag{4a}$$

$$y_o(x) = e^{-\frac{x}{2}} \quad ,$$

$$y_1(x) = e^{-\frac{x}{2}}\left[m+1-x\right] \quad , \tag{4b}$$

$$y_2(x) = e^{-\frac{x}{2}}\left[\binom{m+2}{2} - \binom{m+2}{1}x + \frac{x^2}{2}\right] \quad , \text{ etc.}$$

From (4) the normalization integral

$$\int_o^\infty y_n(x)y_\ell(x)x^m dx = \frac{(n+m)!}{n!} \quad , \tag{5}$$

whence we see that functions are normalized only in the case of $m = 0$.

The recurrence formula

$$xy_n = (2n+m+1)y_n - (n+1)y_{n+1} - (n+m)y_{n-1} \tag{6}$$

is also easily established. In the general case of arbitrary m we shall prefer these non-normalized functions.

We shall write

$$Hz = Ez \tag{7}$$

for the perturbed functions and expand them in terms of the y_n,

$$z(x) = \sum_{n=o}^{\infty} c_n y_n(x) \quad , \tag{7a}$$

which by means of (3) and (6) gives the linear equations

$$- n \frac{\alpha}{2} (1+\frac{\alpha}{2}) c_{n-1} + \left[(n+\frac{m+1}{2})(1+\alpha) + (2n+m+1)(\frac{\alpha}{2})^2 - E\right] c_n - (n+1+m) \frac{\alpha}{2} (1+\frac{\alpha}{2}) c_{n+1} = 0 \quad . \tag{8}$$

The true eigenvalues E_n of (3) can be found from the corresponding determinant; however, not quite easily. These eigenvalues being known, we may put, say, $E = E_\ell$ into (8) to obtain the coefficients of $z_\ell(x)$. We might take $z_\ell(x) = y_\ell((1+\alpha)x)$. For better conformity, however, we should have to add a factor $(1+\alpha)^{\frac{m+1}{2}}$. To the order of α^2 this corresponds to writing

$$z_\ell(x) = (1+\frac{\alpha}{2})^{m+1} y_\ell((1+\alpha)x) \quad . \tag{9}$$

Then putting (ℓ) as upper index in c_n of (7a) we have

$$c_n^{(\ell)} = \frac{n!}{\ell!} \frac{(\frac{\alpha}{2})^{n-\ell}}{(1+\frac{\alpha}{2})^{n-\ell}} \sum_{k=o}^{\ell} \binom{\ell}{k} \frac{(-1)^k (n+m+k)!}{(n-\ell+k)!(n+m)!} \left(\frac{\frac{\alpha}{2}}{1+\frac{\alpha}{2}}\right)^{2k} \quad . \tag{10}$$

For small α then approximately $c^{(\ell)} = 1$. The coefficients are not, however, easily found in this way.

We shall, therefore, write

$$\sum_{\ell=o}^{\infty} z_\ell(x) t^\ell = (1+\frac{\alpha}{2})^{m+1} \psi((1+\alpha)x,t) \tag{11}$$

The transition to the harmonic oscillator, whether for non-normalized or normalized functions are easily performed by putting $m = \mp \frac{1}{2}$ for symmetric and antisymmetric solutions, respectively.

For general illustration purposes, however, the simplest case of $m = o$, with normalized eigenfunctions and self-adjoint differential equation, should be preferred.

<u>Ordinary Perturbation Theory</u>

$$(H_o+V)\psi = E\psi \tag{14}$$

$$(H_o-E_o)\psi = (E-E_o-V)\psi \tag{14a}$$

$$\left.\begin{aligned} \psi &= \psi_o + \psi_1 + \psi_2 \cdots , \\ E &= E_o + E_1 + E_2 \cdots , \end{aligned}\right\} \tag{14b}$$

$$\begin{aligned}
(H_o-E_o)\psi_o &= 0 , \\
(H_o-E_o)\psi_1 &= (E_1-V)\psi_o , \\
(H_o-E_o)\psi_2 &= (E_1-V)\psi_1 + E_2\psi_o , \\
(H_o-E_o)\psi_3 &= (E_1-V)\psi_2 + E_2\psi_1 + E_3\psi_o , \\
(H_o-E_o)\psi_4 &= (E_1-V)\psi_3 + E_2\psi_2 + E_3\psi_1 + E_4\psi_o , \\
(H_o-E_o)\psi_5 &= (E_1-V)\psi_4 + E_2\psi_3 + E_3\psi_2 + E_4\psi_1 + E_5\psi_o .
\end{aligned} \tag{15}$$

We may take

$$\int \psi_o^2 d\tau = 1 , \quad \int \psi_o\psi_n d\tau = 0 . \tag{16}$$

Hence from the first and (n+1)st equation

$$E_n = \int V\psi_o\psi_{n-1}d\tau \quad . \tag{17}$$

Using various other combinations of the above equations we find

$$\begin{aligned}
E_1 &= \int V\psi_o^{\,2}d\tau \\
E_2 &= \int V\psi_o\psi_1 d\tau \\
E_3 &= \int V\psi_1^{\,2}d\tau - E_1\int\psi_1^{\,2}d\tau \\
E_4 &= \int V\psi_1\psi_2 d\tau - E_1\int\psi_1\psi_2 d\tau - E_2\int\psi_1^{\,2}d\tau \\
E_5 &= \int V\psi_2^{\,2}d\tau - E_1\int\psi_2^{\,2}d\tau - 2E_2\int\psi_1\psi_2 d\tau - E_3\int\psi_1^{\,2}d\tau \quad .
\end{aligned} \tag{18}$$

<u>Application to Laguerre-functions $m = 0$</u>

Looking upon the balance of this theory, considering for simplicity only the ground state with energy

$$E = \tfrac{1}{2}(1+\alpha) \quad , \tag{19}$$

we shall rather have to express it in terms of

$$\epsilon = \frac{\alpha}{2}\left(1+\frac{\alpha}{2}\right) \quad , \tag{19a}$$

with

$$\alpha = \sqrt{1+4\epsilon} - 1 \tag{19b}$$

$$\begin{aligned}
E &= \tfrac{1}{2}\sqrt{1+4\epsilon} = \tfrac{1}{2} + \epsilon - \epsilon^2 + 2\epsilon^3 - 5\epsilon^4 + 14\epsilon^5 - \cdots \\
&= \tfrac{1}{2}\sum_{n=o}^{\infty}\binom{2n}{n}\frac{(-1)^{n-1}\epsilon^n}{2n-1} \quad .
\end{aligned} \tag{20}$$

We now have

$$V = \epsilon x \tag{21}$$

and from

$$xy_n = (2n+1)y_n - (n+1)y_{n+1} - ny_{n-1} \quad ,$$

$$\psi_o = y_o \ , \ \psi_1 = \epsilon y_1 \quad , \tag{21a}$$

we obtain

$$E_o = \tfrac{1}{2} \ , \ E_1 = \epsilon \ , \ E_2 = -\epsilon^2 \ , \ E_3 = 3\epsilon^3 - \epsilon^3 = 2\epsilon^3 \ . \tag{21b}$$

To find E_4 and E_5 we must have $\psi_2(x)$. The right hand side of the third equation (15) is

$$\epsilon^2\Big[(1-x)y_1 - y_o\Big] = \epsilon^2\Big[-2y_1 + 2y_2\Big] \tag{22}$$

from the recurrence formula, and from

$$(H_o-E_o)y_n = ny_n \tag{22a}$$

we find

$$\psi_2 = \epsilon^2\Big[-2y_1 + y_2\Big] \quad . \tag{23}$$

This gives

$$E_4 = -8\epsilon^4 + 2\epsilon^4 + \epsilon^4 = -5\epsilon^4 \quad , \tag{23a}$$

$$E_5 = 25\epsilon^5 - 5\epsilon^5 - 4\epsilon^5 - 2\epsilon^5 = 14\epsilon^5 \quad . \tag{23b}$$

The energy series is easily continued into

$$E = \tfrac{1}{2} + \epsilon - \epsilon^2 + 2\epsilon^3 - 5\epsilon^4 + 14\epsilon^5 - 42\epsilon^6 + 132\epsilon^7 - \cdots \qquad (24)$$

according to the general expression (20). Similarly the wave function is, because of

$$\frac{\alpha}{2+\alpha} = \frac{\sqrt{1+4\epsilon}-1}{\sqrt{1+4\epsilon}+1} = \frac{2+4\epsilon-2\sqrt{1+4\epsilon}}{4\epsilon}$$

$$= \frac{1}{\epsilon}\left[\tfrac{1}{2} + \epsilon - \tfrac{1}{2}\sqrt{1+4\epsilon}\right] = \epsilon - 2\epsilon^2 + 5\epsilon^3 - 14\epsilon^4 + 42\epsilon^5 - \cdots \qquad (25)$$

and from (12), putting $\ell = 0$,

$$\psi = \sum_{n=o}^{\infty} \left(\frac{\alpha}{2+\alpha}\right)^n y_n = y_o + (\epsilon - 2\epsilon^2 + 5\epsilon^3 - 14\epsilon^4)y_1$$

$$+ (\epsilon^2 - 4\epsilon^3 + 14\epsilon^4)y_2 + (\epsilon^3 - 6\epsilon^4)y_3 + \epsilon^4 y_4 + \cdots \quad . \qquad (25a)$$

From this is seen that the successive approximations of the wave function according to the above method are

$$\begin{aligned}
\psi_o &= y_o \quad , \\
\psi_1 &= \epsilon y_1 \quad , \\
\psi_2 &= \epsilon^2\left[-2y_1 + y_2\right] \quad , \\
\psi_3 &= \epsilon^3\left[5y_1 - 4y_2 + y_3\right] \quad , \\
\psi_4 &= \epsilon^4\left[-14y_1 + 14y_2 - 6y_3 + y_4\right] \quad .
\end{aligned} \qquad (25b)$$

The series can be easily continued.

Finally it may be nice to see that the series

$$\psi = \sum_{n=o}^{\infty} \left(\frac{\alpha}{2+\alpha}\right)^n y_n \tag{26}$$

really gives the correct normalization integral and the correct energy

$$\int_0^{\infty} \psi^2 d\tau = \sum_{n=o}^{\infty} \left(\frac{\alpha}{2+\alpha}\right)^{2n} = \frac{(2+\alpha)^2}{(2+\alpha)^2 - \alpha^2} = \frac{(1+\frac{\alpha}{2})^2}{1+\alpha} \tag{26a}$$

as it should be.

On the other hand, we find

$$\int \psi H \psi d\tau = \sum_{n=o}^{\infty} \left(\frac{\alpha}{2+\alpha}\right)^n \left[(n+\tfrac{1}{2})(1+\alpha) + (2n+1)\left(\frac{\alpha}{2}\right)^2 - (2n+2)\left(\frac{\alpha}{2}\right)^2\right]$$

$$= \frac{(1+\frac{\alpha}{2})^2}{1+\alpha} \left[\tfrac{1}{2}(1+\alpha) - \left(\frac{\alpha}{2}\right)^2\right] + (1+\alpha)\sum_{n=o}^{\infty} n\left(\frac{\alpha}{2+\alpha}\right)^n \tag{26b}$$

$$= \frac{(1+\frac{\alpha}{2})^2}{1+\alpha} \left[\tfrac{1}{2}(1+\alpha) - \left(\frac{\alpha}{2}\right)^2 + \left(\frac{\alpha}{2}\right)^2\right] = \tfrac{1}{2}(1+\alpha)\frac{(1+\frac{\alpha}{2})^2}{1+\alpha}$$

Hence,

$$E = \tfrac{1}{2}(1+\alpha) \tag{27}$$

APPENDIX

Additional Considerations Concerning Laguerre Functions

Consider the two-dimensional wave equation

$$\left\{\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+E+\frac{Z}{r}\right\}\psi = 0 \ , \quad r = \sqrt{x^2+y^2} \ , \tag{A1}$$

in polar coordinates

$$\left\{\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2}+E+\frac{Z}{r}\right\}\psi = 0 \quad . \tag{A2}$$

Make the substitution

$$\psi = y(r)e^{im\varphi} \tag{A3}$$

to obtain the radial equation

$$\left\{\frac{d^2}{dr^2}+\frac{1}{r}\frac{d}{dr}-\frac{m^2}{r^2}+E+\frac{Z}{r}\right\}y(r) = 0 \quad . \tag{A4}$$

Putting

$$\psi = \sum_{v=o}^{n} c_v \, r^{\frac{m}{2}+v} \, e^{-\sqrt{-E}\,r} \tag{A5}$$

it is found on requiring the series terminating on n that

$$Z = \sqrt{-E}\,(2n+m+1) \tag{A6}$$

or

$$E = -\frac{Z^2}{4(n+\frac{m+1}{2})^2} \quad . \tag{A7}$$

Therefore, making the transformation

$$r = 2\sqrt{-E}\,x \ , \quad x = r/2\sqrt{-E} \tag{A8}$$

we may write

$$\left\{ \frac{d^2}{dx^2} + \frac{1}{x}\frac{d}{dx} - \frac{m^2}{x^2} - \frac{1}{4} + \frac{n+\frac{m+1}{2}}{x} \right\} y = 0 \quad , \tag{A9}$$

which for integral n has the solutions

$$y = e^{-\frac{x}{2}} x^{\frac{m}{2}} L^m_{n+m}(x) \quad , \tag{A10}$$

the L^m_{n+m} being the well-known generalized Laguerre polynomials of degree n.

The ordinary Laguerre polynomials $L_n(x)$ obey the equation

$$\left\{ x\frac{d^2}{dx^2} + (1-x)\frac{d}{dx} + n \right\} L_n = 0 \quad , \tag{A11}$$

or

$$\left\{ x\frac{d^2}{dx^2} + (1-x)\frac{d}{dx} + n+m \right\} L_{n+m} = 0 \quad . \tag{A11a}$$

On differentiating m times the latter equation we obtain

$$\left\{ x\frac{d^2}{dx^2} + (m+1-x)\frac{d}{dx} + n \right\} L^{(m)}_{n+m}(x) = 0 \quad . \tag{A11b}$$

Substituting (A10) into (A9), we have

$$\left\{ x\frac{d^2}{dx^2} + (m+1-x)\frac{d}{dx} + n \right\} L^m_{n+m}(x) = 0 \quad , \tag{A11c}$$

the same equation if $L^m_{n+m}(x) = \frac{d^m}{dx^m} L_{n+m}(x)$.

The polynomial may be defined as

$$L^m_{n+m}(x) = x^{-m} e^x \frac{1}{n!} \frac{d^n}{dx^n} x^{n+m} e^{-x} \tag{A12}$$

from which their explicit expressions

$$L^m_{n+m}(x) = \sum_{k=o}^{n} \binom{n+m}{n-k} \frac{(-x)^k}{k!} \tag{A12a}$$

as well as their differential equation (A11) are easily obtained. Another equivalent and often useful definition is

$$\psi(x,t) = \frac{e^{-\frac{xt}{1-t}}}{(1-t)^{m+1}} = \sum_{n=0}^{\infty} L_{n+m}^{m}(x)\, t^{n} \quad . \tag{A12b}$$

It should be observed, however, that by this definition

$$L_{n+m}^{m}(x) = (-1)^{m} L_{n+m}^{m}(x) \tag{A12c}$$

for integral m . For non-integral m , we must stick to the above direct definition.

Example:

$$L_5(x) = 1 - 5x + 10\,\frac{x^2}{2} - 10\,\frac{x^3}{3!} + 5\,\frac{x^4}{4!} - \frac{x^5}{5!} \quad ,$$

$$L_5^{(3)}(x) = -10 + 5x - \frac{x^2}{2!} = (-1)^3 L_{2+3}^{3}(x) \quad . \tag{A13}$$

If in (A9) we make only the substitution

$$y = x^{\frac{m}{2}} Y \tag{A14}$$

we find the equation

$$\left\{ x\,\frac{d^2}{dx^2} + (m+1-x)\,\frac{d}{dx} - \frac{x}{4} + n + \frac{m+1}{2} \right\} Y = 0 \tag{A14a}$$

referred to in the former Eqs. (2) and (3).

If in the function Y we replace the argument x by $x(1+\alpha)$

$$Y((1+\alpha)x) = Z(x) \quad , \tag{A15}$$

we, of course, obtain the equation

$$\left\{ x\,\frac{d^2}{dx^2} + (m+1-x)\,\frac{d}{dx} - (1+\alpha)^2\,\frac{x}{4} + \left(n+\frac{m+1}{2}\right)(1+\alpha) \right\} Z = 0 \tag{A15a}$$

The normalization factors

$$\int_0^\infty e^{-x} L^m_{n+m}(x) L^m_{n+m}(x) x^m dx = \frac{(n+m)!}{n!} \tag{A16}$$

are most easily found from the integral

$$\int_0^\infty x^m e^{-x} \psi(x,s)\psi(x,t)dx = \int_0^\infty \frac{e^{-x \frac{1-st}{(1-s)(1-t)}}}{(1-s)^{m+1}(1-t)^{m+1}} x^m dx = \frac{m!}{(1-st)^{m+1}}$$

$$= \sum_{n=0}^\infty \frac{(n+m)!}{n!} s^n t^n \quad . \tag{A16a}$$