NOTE

The Harmonic Oscillator – A Simplified Approach

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Abstract Among the early problems in quantum chemistry, the one dimensional harmonic oscillator problem is an important one, providing a valuable exercise in the study of quantum mechanical methods. There are several approaches to this problem, the time honoured infinite series method, the ladder operator method *etc.* A method which is much shorter, mathematically simpler is presented here.

Keywords: Schrödinger equation, Hermite's equation and polynomials.

The Schrödinger equation for the one dimensional harmonic oscillator¹, viz.,

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} \left(E - \frac{kx^2}{2} \right) \psi = 0$$

can be reduced to the form

$$\frac{d^2\psi}{d\xi^2} = (\xi^2 - \lambda) \psi \text{ by the substitution,}$$

$$x = \alpha \xi$$

$$\frac{2mE\alpha^2}{\hbar^2} = \lambda$$

$$\text{and } \frac{mk\alpha^4}{\hbar^2} = 1 = \left(\frac{m^2\omega^2\alpha^4}{\hbar^2} \right)$$

In what follows, we shall use the notation (') and (') to denote single and double differentiation with respect to ξ .

Thus the Schrödinger equation has the form $\frac{\psi''}{\psi} = \xi^2 - \lambda$.

By direct differentiation of $\left(\frac{\psi'}{\psi} \right)$, we have $\left(\frac{\psi'}{\psi} \right)' = \frac{\psi''}{\psi} - \left(\frac{\psi'}{\psi} \right)^2$

$$i.e., \frac{\Psi''}{\Psi} = \left(\frac{\Psi'}{\Psi}\right)^2 + \left(\frac{\Psi'}{\Psi}\right)'.$$

Comparison with $\frac{\Psi''}{\Psi} = (\xi^2 - \lambda)$ shows that

$$\frac{\Psi'}{\Psi} = \pm \xi \text{ and } \left(\frac{\Psi'}{\Psi}\right)' = -\lambda.$$

Since λ is non-negative*, it follows that $\frac{\Psi'}{\Psi} = -\xi$ and not $+\xi$ and thus

$$\left(\frac{\Psi'}{\Psi}\right)' = -1. \text{ This shows that } \lambda = 1.$$

From $E = \frac{\lambda \hbar^2}{2m\alpha^2}$ and $\alpha^2 = \frac{\hbar}{m\omega}$, we get $E = \frac{1}{2} \hbar\omega$

We can show that this is the lowest energy level as follows:

Let us substitute for $\left(\frac{\Psi'}{\Psi}\right)$, the expression

$$\left(\frac{f'}{f}\right) - \xi. \text{ By differentiating, } \frac{\Psi''}{\Psi} - \left(\frac{\Psi'}{\Psi}\right)^2 = \left(\frac{f''}{f}\right) - \left(\frac{f'}{f}\right)^2 - 1.$$

$$\text{Substitute: } \frac{\Psi''}{\Psi} = (\xi^2 - \lambda) \text{ and } \left(\frac{\Psi'}{\Psi}\right) = \left(\frac{f'}{f} - \xi\right)$$

In this, we easily get $f'' - 2\xi f' + (\lambda - 1)f = 0$

This is Hermite's differential equation²⁻⁴.

Suppose it has a solution, 'f', for some value of λ , then by direct differentiation, one gets

$$f''' - 2\xi f'' + (\lambda - 3)f' = 0.$$

If we put $f' = g$ and $(\lambda - 2) = \lambda'$. We obtain $g'' - 2\xi g' + (\lambda' - 1)g = 0$, which shows that g is a solution of the equation.

Thus starting from any solution of the equation, f , we obtain another by differentiating f . The new solution g , corresponds to a value of λ . two units lower than the value of λ for f . This process can obviously be continued. But we know that $\lambda = 1$ is one of the values of λ . A value two units lower will yield $\lambda = -1$, which is impossible, since $\lambda > 0$. Thus $\lambda = 1$ and $E = \frac{1}{2} \hbar\omega$ are the lowest possible values. Successive values of λ should differ by two units.

Thus the only possible values of λ are $1, 3, 5, \dots (2n - 1)$. This shows that the only possible values of energy are $\left(n + \frac{1}{2}\right) \hbar\omega$

$\Psi = (Ae^{-\xi^2/2}) \times f$, which shows that $f = \text{constant}$

for $\lambda = 1$. The next value viz., $\lambda = 3$ should correspond to $f = a\xi + b$ since by differentiating it we get a constant for $\lambda = 1$.

By similar reasoning $\lambda = 5, 7 \dots$ should correspond to a quadratic, a cubic-expression in ξ .

This shows that f is a polynomial. It is named Hermite polynomial.

*The energy E is non-negative and thus also λ

Finally the operator $\left[\frac{d^2}{d\xi^2} - 2\xi \frac{d}{d\xi} + (\lambda - 1) \right]$ is inversion symmetric. It follows that the functions, f , can be chosen to be either symmetric or antisymmetric for inversion. Hence, f contains either only even powers of ξ or only odd powers of ξ . The polynomials, f are easily constructed as follows. One may assume that $f_0 = 1$ for $\lambda = 1$ without any loss of generality. Integrating, $f_1 = \xi$ for $\lambda = 3$. The arbitrary constant has been omitted since f_1 is an odd degree polynomial antisymmetric for inversion. This is quite general: no odd degree polynomial has any constant term in it.

$$f_2 = \left(\frac{\xi^2}{2} + a \right) \text{ for } \lambda = 5.$$

Substituting in Hermite's equation,

$$f_2'' - 2\xi f_2' + (5-1)f_2 = 0. \text{ Putting } f_0 = 1, f_1 = \xi \text{ and } f_2' = \frac{\xi^2}{2} + a,$$

One easily gets $a = -\frac{1}{4}$.

Quite generally the equation $f_n'' - 2\xi f_n' + (2n+1)f_n = 0$, fixes the form of f_{n+2} from those of f_n and f_{n+1} .

The above method described is neither the usual infinite series method, nor the ladder operator approach. From the point of view of chemists, not too familiar with concepts of convergence of infinite series or the technique of raising and lowering operator, the above method is not only shorter but mathematically easier.

References

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