

1995/110572

N95-22989

N95- 22989

A METHOD OF SOLVING SIMPLE HARMONIC OSCILLATOR SCHRÖDINGER EQUATION.

Juan Carlos Maury F.
Departamento de Física, Universidad Nacional.
Heredia, Costa Rica.

Abstract

A usual step in solving totally Schrödinger equation is to try first the case when dimensionless position independent variable w is large. In this case the Harmonic Oscillator equation takes the form $(d^2/dw^2 - w^2)F = 0$, and following *W.K.B.* method, it gives the intermediate corresponding solution $F = \exp(-w^2/2)$, which actually satisfies exactly another equation, $(d^2/dw^2 + 1 - w^2)F = 0$.

We apply a different method, useful in anharmonic oscillator equations, similar to that of Rampal and Datta [1], and although it is slightly more complicated however it is also more general and systematic.

After some arrangements Schrödinger equation for a simple harmonic oscillator is set as in (1):

$$(d^2/du^2 + c_0 - c_2u^2)N(u) = 0 \quad (1)$$

$$\hbar^2c_0 = 2mE \quad \hbar^2c_2 = (m\omega_0)^2 \quad (2)$$

where c_0 and c_2 are the parameters of the differential equation, $u = x - a$ is the distance from the particle to the point where potential energy is a minimum, ω_0 is the classical angular frequency of the movement, E is the total energy and N is the probability amplitude for the particle to be found at u . In a very common procedure, (1) is first transformed to equation (3), in which w is a dimensionless independent variable, obtained by the mathematical manipulation (4):

$$(d^2/dw^2 + b - w^2)f(w) = 0 \quad (3)$$

$$w^2\hbar = m\omega_0u^2 \quad \hbar\omega_0b = 2E \quad (4)$$

Some authors [2] get the solution of (3) for large w as a decaying exponential function of $w/2$, by means of the *W.K.B.* method, which is a factor in the total wave function.

But others [3] simply propose the change of dependent variable (5) without mentioning the *W.K.B.* method:

$$f = \exp(-w^2/2)P(w) \quad (5)$$

And a few ones [4] consider that the dominant term, when w is large, is w^2 and they write (6) with $b = 0$ as an approximation of (3); and assert that (7) are its solutions:

$$(d^2/dw^2 - w^2)F = 0 \quad (6)$$

$$F = \exp(\pm w^2/2) \quad (7)$$

But after choosing the negative sign in (7), for the good behaviour of F , it is easy to demonstrate that (7) does not satisfy (6), and rather satisfies (3) when $b = 1$. We will use a method whose intermediate steps at all stages are correct.

Starting with (1), the Ansatz (8) is composed of two factors: P that gives information of the zeros of N , and G :

$$N = \exp(-G)P \quad (8)$$

Non linear equation (9) is obtained from (8) and (1), with unknowns P and G :

$$[P'' - 2P'G'] + [(G')^2 - G'']P = [-c_0 + c_2u^2]P \quad (9)$$

$$[(G')^2 - G''] = -c_0(0) + c_2u^2 \quad (10)$$

(' means derivative with respect to u).

If P is an n degree polynomial P_n , then for $n = 0$, P_0 is a constant, and (10) is a non-linear equation with only one unknown. By watching (10) it is noticed that (11) is the solution of (10) if constraints (12) hold:

$$G = \beta u^2 \quad (11)$$

$$4\beta^2 = c_2 \quad 2\beta = c_0(0) \quad (12)$$

The first eigenvalue $E(0)$ can be obtained from (2) and (12). Consequently, (13) is the solution of the Schrödinger equation for $n = 0$; βu^2 as the argument of the exponential function must be dimensionless:

$$N = f_0 = P_0 \exp(-\beta u^2) \quad (13)$$

Therefore w becomes a dimensionless variable and (1) is transformed into (7), and taking into account (12):

$$w^2 = \alpha \beta u^2 \quad (14)$$

$$[d^2/dw^2 + c_0(n)/\alpha\beta - 4w^2/\alpha^2]f_n(w) = 0 \quad (15)$$

(15) is precisely (3), with $b(n) = c_0(n)/\alpha\beta$, and $b(0) = c_0(o)/\alpha\beta = 2/\alpha$. (16) is the correct solution of (15) and (17) is the differential equation of the polynomial P_n :

$$N_n = P_n \exp(-w^2/2) \quad (16)$$

$$[d^2/dw^2 - (4w/\alpha)d/dw + 2(b-1)/\alpha]P_n = 0 \quad (17)$$

For $\alpha = 2$ and $b(n) = 2n + 1$, (17) is the equation of Hermite, and $P_n = H_n$ are Hermite's polynomials. The energy eigenvalues can easily be obtained.

The Simple Harmonic Oscillator Schrödinger equation is perhaps the known differential equation with the most accurate solution. It would not be worthy to obtain that solution again, if methodological aspects are not taken into account. If a physicist plans to work in problems related to differential equations, it is useful to give her (him) general and powerful methods. As the Simple Harmonic Oscillator is the first approximation to many physical models, and one of the first problems with which the students are put into contact, it is good to take advantage of methods that can be used in better approximations to more complex physical models, and more exact formulations, as relativistic ones for instance. The author has made a review of the relativistic and non-relativistic isotropic harmonic oscillators, and uniform magnetic fields [5], using this method. With polar coordinates and centrifugal potentials, other polynomials depending on two quantum numbers, and one extra factor are the solutions of the radial equations. First the author had used the method in solving anharmonic rectilinear oscillators, and anharmonic isotropic oscillator equations [6], and continues working further these topics. In all those cases mentioned, and here, we consider that writing equations (9) and (10), is the most important step that permits to find the solution for large w , and the independent dimensionless variable.

References

- [1] A. Rampal and K. Datta, *J.Math.Phys.* **24**, 860 (1983).
- [2] D. Bohm, *Quantum Theory*(Prentice-Hall, 1961)
- [3] E. Merzbacher, *Quantum Mechanics* (John Wiley and Sons, 1970)
- [4] E. Anderson, *Modern Physics and Quantum Mechanics* (W.B. Saunders Co., 1971)
- [5] J. Maury, Comparación Sistemática de Ecuaciones Diferenciales de Osciladores Armónicos y Acoples Mínimos. (To be sent for publication).
- [6] J. Maury and J. Páez, *Sobre Algunas Ecuaciones Para Osciladores Cuánticos*(Memorias del Tercer Congreso Nacional de Matemáticas, Costa Rica, Editor Angel Ruiz, 1990)

