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Quantizing Simple Periodic Systems Using Bohr's Rule and its Modification

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Abstract. Here we present some new applications of the well-known Bohr's quantisation rule along with its modifications to deduce quantised energy levels of some simple systems. The values agree quite well with those derived from proper quantum mechanics. The article has a pedagogical value.

KEY WORDS: Bound states, Bohr's quantisation rule, Periodic systems.

1 Introduction

It is well-known how Niels Bohr in 1913 applied his, the then revolutionary quantum rule $(mvr = n\hbar)$ to deduce the energy levels of the Hydrogen atom [1]. Bohr's rule was later modified by Arnold Sommerfeld for elliptical orbits etc. Since then Bohr's rule apparently has not been applied to other systems as it was superseded by proper quantum mechanics developed by Schrödinger, Bohr and Heisenberg around 192 6 [2, 3]. In this article we have applied Bohr's quantisation rule as well as it's suitable modifications to several periodic systems. We are able to deduce quantised energy levels in a remarkably simple way. The method presented has a pedagogical value too.

2 Simple Harmonic Oscillator

This is a system having Hamiltonian

$$H = \frac{p^2}{2m} + \frac{1}{2}Kx^2 \,. \tag{1}$$

We can think about the linear motion as a projection of a uniform circular motion on one axis-say the x-axis. Thus, we can write

$$x = R\cos\omega t\,, \tag{2}$$

where R is the amplitude and $\omega = \sqrt{K/m}$ being the uniform angular frequency [5]. Balancing the forces on m that is moving in a circular orbit of radius R, we have

$$m\omega^2 R = KR\,. \tag{3}$$

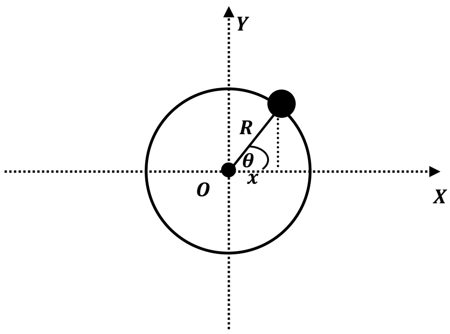

Figure 1. Projection of uniform circular motion on x axis.

Introducing Bohr's idea of quantisation for angular momentum, we can write

$$mvR = m\omega R^2 = n\hbar\,. \tag{4}$$

As $\omega^2 = K/m$, we get

$$R^2 = \frac{n\hbar}{\sqrt{Km}}\,. \tag{5}$$

Therefore, kinetic energy of the particle executing simple harmonic motion is

$$T = \frac{1}{2}mv^2 = \frac{1}{2}m\omega^2 R^2 = \frac{1}{2}n\hbar\omega$$

and the corresponding potential energy is

$$V = \frac{1}{2}KR^2 = \frac{1}{2}K\frac{n\hbar}{\sqrt{Km}} = \frac{1}{2}n\hbar\omega\,.$$

Thus, the total energy is

$$E = T + V = n\hbar\omega\,. \tag{6}$$

The exact value of energy of the simple harmonic oscillator obtained by solving Schrödinger equation is [4]

$$E = T + V = \left(n + \frac{1}{2}\right)\hbar\omega\,. \tag{7}$$

Replacing n by $\left(n+\frac{1}{2}\right)$ in equation (6) as one does in going from old quantum theory to modern quantum mechanics, Bohr's quantisation rule is able to give the exact values without solving Schrödinger's equation.

3 Charged Particle in a Uniform Magnetic Field

Let the axial magnetic field vary as

$$B = B_0\,.$$

Hence, we get a uniform circular motion of a particular radius R that is given by the equation

$$\frac{mv^2}{R} = qvB_0\,. \tag{8}$$

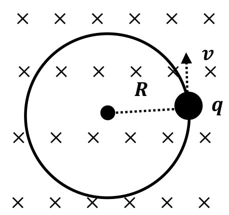

Figure 2. Charged particle in a uniform magnetic field

This has to be combined with the Bohr's rule

$$mvR = n\hbar\,.$$

We can write for the kinetic energy of the particle

$$T = \frac{1}{2}mv^2 = \frac{1}{2}qB\left(\frac{n\hbar}{m}\right) = \frac{1}{2}\hbar\omega_c\,. \tag{9}$$

Once again, this is a stationary system, i.e., a system in equilibrium. Hence, using equipartition theorem for equilibrium situations [7], where we should get on the average $T = V$.

$$\therefore E = T + V = 2T = n\hbar\omega_c\,, \tag{10}$$

where $\omega_c = \frac{qB}{m}$ is the cyclotron frequency [8].

If we replace n by $\left(n+\frac{1}{2}\right)$ and allow n to range over $0, 1, 2, \cdots$, Bohr's quantisation rule is able to reproduce the well-known Landau levels without the Schrödinger equation.

4 Charged Particle in a Non-Uniform Magnetic Field

Let us say the magnetic field is varying along its transverse direction as

$$B\left(R\right) = B_0 R^{\alpha} \,. \tag{11}$$

Once again, a charged particle of mass m and charge q with a velocity $\vec{v}$ transverse to the magnetic field would describe a circular orbit with a particular radius R, balancing the magnetic force with the centrifugal force gives the equation

$$\frac{mv^2}{R} = qvB_0 R^{\alpha} \,. \tag{12}$$

Applying Bohr's quantisation rule $mvR = n\hbar$, we get from equation (11)

$$mv = qB_0 \left(\frac{n\hbar}{mv}\right)^{1+\alpha} \,. \tag{13}$$

Therefore,

$$\left(mv\right)^{2+\alpha} = qB_0 \left(n\hbar\right)^{1+\alpha} \,.$$

We can write for the kinetic energy of the particle

$$T = \frac{1}{2m}\left(mv\right)^2 = \frac{1}{2m}\left[qB_0\left(n\hbar\right)^{1+\alpha}\right]^{\frac{2}{2+\alpha}} \,.$$

Simplifying

$$T = \frac{1}{2m}\left(qB_0\right)^{\frac{2}{2+\alpha}}\left(n\hbar\right)^{\frac{2+2\alpha}{2+\alpha}} \,. \tag{14}$$

Again applying the equipartition theorem, we equate the potential energy (V) to the kinetic energy in this stationary (stable) state. Hence the total energy can be written as

$$E = 2T = \frac{1}{m}\left(qB_0\right)^{\frac{2}{2+\alpha}}\left(n\hbar\right)^{\frac{2+2\alpha}{2+\alpha}} \,. \tag{15}$$

We are able to obtain the quantised energy values without solving Schrödinger equation.

To get correct quantum mechanical expression, we replace n by $\left(n+\frac{1}{2}\right)$ to get:

$$E_n = \frac{1}{m}\left(qB_0\right)^{\frac{2}{2+\alpha}}\left[\left(n+\frac{1}{2}\right)\hbar\right]^{\frac{2+2\alpha}{2+\alpha}} \,. \tag{16}$$

Unfortunately, there does not seem to be a quantum mechanical calculation for a non-uniform magnetic field for us to make a comparison.

5 Simple Harmonic Oscillator with a Modified Method

We have the Hamiltonian

$$H = \frac{p^2}{2m} + \frac{1}{2}Kx^2 \,.$$

Now for this one dimensional periodic system we modify the Bohr's rule to read

$$px = n\hbar, \tag{17}$$

and then find the stationary values of H to deduce the energy levels. Hence,

$$H = \frac{1}{2m}\left(\frac{n\hbar}{x}\right)^2 + \frac{1}{2}Kx^2 \,. \tag{18}$$

Stationary state energies can be obtained by finding that x_0 for which

$$\left(\frac{dH}{dx}\right)_{x_0} = 0 \,.$$

Thus we get

$$x_0^2 = \frac{n\hbar}{\sqrt{Km}} \,. \tag{19}$$

Putting the value of x_0 in equation (18), we get

$$H = \frac{1}{2}n\hbar\omega + \frac{1}{2}n\hbar\omega = n\hbar\omega \,. \tag{20}$$

These are the well-known harmonic oscillator energy levels [6], but for n in the place $\left(n + \frac{1}{2}\right)$ just as we have discussed earlier to pass from the old quantum theory to quantum mechanics.

6 Energy Levels of Quarkonium

Quarkonium is a bound system formed by quark and an anti-quark. Here, the force law is

$$f\left(r\right) = -gr \,, \tag{21}$$

where g is strong coupling constant.

Therefore, the Hamiltonian of the system is

$$H = \frac{p^2}{2m} + \frac{l^2}{2mr^2} + \frac{1}{2}gr^2 \,. \tag{22}$$

Using Bohr's quantisation rule, taking $l = n\hbar$ and minimising the value of H in equation (22) w.r.t $r = r_0$, such that

$$\left(\frac{dH}{dr}\right)_{r=r_0} = 0 \,.$$

Hence, we get

$$r_0^2 = \left[\frac{2n^2\hbar^2}{mg}\right]^{\frac{1}{2}}. \tag{23}$$

Putting equation (23) in equation (22), we get

$$E_n = \left(\sqrt{\frac{2g}{m}}\right) n\hbar\,. \tag{24}$$

Once again, replacing n by $\left(n+\frac{1}{2}\right)$, we get

$$E_n = \left(\sqrt{\frac{2g}{m}}\right)\left(n+\frac{1}{2}\right)\hbar\,. \tag{25}$$

Equation (25) can be easily compared with eigenenergies obtained by solving complex equations [9].

7 Particle in a Constant Magnetic Field by Modified Method

The energy of a charged particle placed in an electromagnetic field is

$$E = \frac{p_1^2}{2m} + e\phi\,, \tag{26}$$

where $\vec{p}_1 = \vec{p} - \frac{e\vec{A}}{c}$ by using the minimal coupling rule. But

$$\left(\vec{p} - \frac{e\vec{A}}{c}\right)^2 = p^2 - \frac{e}{c}\left(\vec{p}\cdot\vec{A}\right) - \frac{e}{c}\left(\vec{A}\cdot\vec{p}\right) + \frac{e^2}{c^2}A^2\,.$$

For a static magnetic field $\mathrm{div}\vec{A} = 0$.

$$E = \left[\frac{p^2}{2m} - \frac{e}{mc}\left(\vec{A}\cdot\vec{p}\right) + \frac{e^2}{c^2}A^2 + e\phi\right]. \tag{27}$$

For uniform magnetic field (only H) along $z-$axis, we put $\phi = 0$, $H_x = H_y = 0$, $H_z = H$, we have the components of the vector potential

$$A_x = -\frac{yH}{2}, \quad A_y = \frac{xH}{2}, \quad A_z = 0, \tag{28}$$

$$\therefore \quad \frac{e}{mc}\left(\vec{A}\cdot\vec{p}\right) = \frac{eH}{2mc}\frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = -\frac{eH}{2mc}L_z.$$

Putting these in equation (27),

$$E = \left[\frac{p^2}{2m} + \frac{e^2H^2}{8mc^2}\left(x^2+y^2\right) + \frac{eH}{2mc}L_z\right]. \tag{29}$$

Now by using the modified Bohr's quantisation rule: $pr = n\hbar$ and putting $L_z = n\hbar$, we get

$$E = \left[\frac{n^2\hbar^2}{2mr^2} + \frac{e^2H^2}{8mc^2}r^2 + \frac{eH}{2mc}(n\hbar) \right] . \tag{30}$$

Now we minimise E in equation (30) w.r.t 'r'. Let at $r = r_0$, $\left(\frac{dE}{dr}\right)_{r=r_0} = 0$, we get

$$r_0^2 = \frac{2n\hbar c}{eH} . \tag{31}$$

Putting equation (31) in equation (30), we get

$$E = \frac{eH}{mc}(n\hbar) .$$

Taking $\Omega = \frac{eH}{mc}$, the cyclotron frequency

$$E = n\hbar\Omega . \tag{32}$$

Once again, replacing n by $\left(n + \frac{1}{2}\right)$,

$$E = \left(n + \frac{1}{2}\right)\hbar\Omega . \tag{33}$$

The eigenenergies thus obtained are exactly same as well-known Landau levels obtained by solving the Schrödinger equation [10].

8 Application of Modified Method for Anharmonic Oscillators

For pure anharmonic oscillators, the total energy takes the form

$$E = \frac{p^2}{2m} + \lambda x^{2\alpha} , \tag{34}$$

where λ is anharmonicity coupling parameter, $\alpha = 2, 3, 4 \cdots$ correspond to quartic, sextic, octic anharmonic oscillators.

8.1 Pure quartic oscillator

For a pure quartic oscillator $\alpha = 2$,

$$E = \frac{p^2}{2m} + \lambda x^4 . \tag{35}$$

Now imposing modified Bohr's quantisation condition $px = n\hbar$ in E. Then, we get

$$E = \frac{n^2\hbar^2}{2mx^2} + \lambda x^4 . \tag{36}$$

Now we minimise E in equation (36) w.r.t x. Let the minimum occur at $x = x_0$, such that $\left(\frac{dE}{dx}\right)_{x=x_0} = 0$, we get

$$x_0^2 = \left[\frac{n^2\hbar^2}{4m\lambda}\right]^{\frac{1}{3}} . \tag{37}$$

Putting equation (37) in equation (36),

$$E_n = \frac{\hbar^{\frac{4}{3}}\lambda^{\frac{1}{3}}}{m^{\frac{2}{3}}}\left[\left(\frac{1}{2}\right)^{\frac{1}{3}} + \left(\frac{1}{4}\right)^{\frac{2}{3}}\right] n^{\frac{4}{3}} . \tag{38}$$

In order to compare this with the results obtained by other methods, we put $m = \frac{1}{2}, \lambda = \hbar = 1$ and we replace n by $n + \frac{1}{2}$. Thus, we get

$$E_n = 2.45047\left(n + \frac{1}{2}\right)^{\frac{4}{3}} , \tag{39}$$

which is in very good agreement with the value obtained by Kagali et al., by phase-space integration method [11], according to which the energy eigenvalues of quartic oscillator is given by

$$E_n = 2.185\left(n + \frac{1}{2}\right)^{\frac{4}{3}} . \tag{40}$$

8.2 Pure sextic oscillator

For a pure quartic oscillator $\alpha = 2$,

$$E = \frac{p^2}{2m} + \lambda x^6 . \tag{41}$$

Imposing Bohr's quantisation condition $px = n\hbar$, we get

$$E = \frac{n^2\hbar^2}{2mx^2} + \lambda x^6 . \tag{42}$$

Now we minimise E in equation (42) w.r.t 'r'. Let at $r = r_0$, $\left(\frac{dE}{dr}\right)_{r=r_0} = 0$, we get

$$x_0 = \left[\frac{n^2\hbar^2}{6m\lambda}\right]^{\frac{1}{8}} . \tag{43}$$

Putting equation (43) in equation (42),

$$E_n = 1.0433\frac{\lambda^{\frac{1}{4}}\hbar^{\frac{3}{2}}n^{\frac{3}{2}}}{m^{\frac{3}{4}}} . \tag{44}$$

Once again to compare this with the results obtained by other methods, we put $m = \frac{1}{2}$, $\lambda = \hbar = 1$ and we replace n by $n + \frac{1}{2}$. Thus, we get

$$E_n = 1.75476 \left(n + \frac{1}{2}\right)^{\frac{3}{2}} , \tag{45}$$

which is again comparable with the value obtained by Kagali et al., by phase-space integration method [11], according to which the energy eigenvalue of sextic oscillator is given by

$$E_n = 2.2622 \left(n + \frac{1}{2}\right)^{\frac{3}{2}} . \tag{46}$$

Similar calculations can be done to verify the validity of the modified method for other higher order anharmonic oscillators.

9 Results and Discussion

Bohr's quantisation rule and its modification that is suggested here can be employed to deduce quantised energy levels of simple periodic physical systems without going through the elaborate steps of the standard quantum mechanics. The method suggested here can be used as a first step to get the energy levels quickly prior to solving the appropriate Schrödinger equation. We wish to apply the new method to more complicated systems to test its range and strength. The method apparently has a good pedagogical value in understanding quantum systems.

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