

Interpretation of the change of Intensity and Spectral line width for Bhutan, Neon, Fluorine, and Chlorine by Using Complex Statistical Distribution and Quantum harmonic Oscillator Model

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Abstract: The determination of atmospheric temperature needs using complex and expensive technology. This requires a new approach for temperatures determination by using simple and cheap technology. To perform this task an attempt was made in this research to relate temperature change to the change of spectra of some gases which are Bhutan (C_4H_{10}), Neon (Ne), Fluorine (F_2) and chlorine (Cl_2). These gas were heated at temperature in the range (300 -337°k.) The spectra of these gas were displayed by USB2000 spectrometer. The result shows appreciable change in the spectral intensity and line width. These changes was shown to be explained theoretically on the basis of non- equilibrium statistical physics by using plasma equation and quantum mechanical laws that relates the photon intensity to atomic and electronic wave functions.

Key words: Intensity, spectra, line width, non-equilibrium, statistical physics, temperature.

I. Introduction

The spectrum of atoms is now widely used in many applications as a finger print characterizing the elements excited in samples.[1] This comes from the fact that each element is characterized by certain specific energy levels. Thus each element emits photons due to transition between these energy levels. The energies and wavelengths of the photons emitted by a certain element is different from that emitted by all other elements [2,3]

Sometimes the wavelength of the emitted photons changes due to some interactions. For example the thermal motion of atoms can produce Doppler shift due to the effect of velocity [4]. Collision of atoms due to thermal vibration can also change the wavelength due to Compton scattering[6,5]. Different attempts were made to accounts for the effect of temperature on atomic spectra. In one of them the spectrum of special fiber Bragg grating (SFBG) shows increase in power and wavelength with temperature[7]. Another work related change of band width to temperature change[8] is also verified experimentally, where line width decreases as temperature increases. Both of them explain their result on the basis of strain change and change of relaxation time. Unfortunately both of them does not use quantum or statistical. Laws which are suitable for spectra of atoms and micro particles

These thermal effects on the spectrum wavelength for some gases is investigated and studied in this work. Section 2 is devoted for the experimental work including devices materials and methods and results. The spectrum of two gases are exhibited here in section 3, Discussion in section 4 and conclusion in section 5.

II. Materials and methods:

The following Apparatus and Instruments and Gases are used in the experiment

2-1 Apparatus and Instruments:

USB2000 Fiber Optic Spectrometer (Ocean Optics), Heater, Thermometer, Laptop, Source of Helium Neon laser -133, Power supply, Connect cable. Test tubes (Borosilicate Glass).

2-2 gases:

Bhutan (C_4H_{10}), Neon (Ne), Fluorine (F_2) and Chlorine (Cl_2).

2-3 Experiment set up:

Glass tube is filled by gases, each gas should be heated in steps about one or two degrees and the spectrum are recorded at each degree by using thermometer. Helium-133 beams is directed to incident on the glass tube, the spectrum of each gas including the intensity and band width is recorded for each temperature by

321	630.8	3515.7	6.51	103.39
322	630.77	2276.22	6.53	103.25
323	630.77	3179.53	6.48	103.4

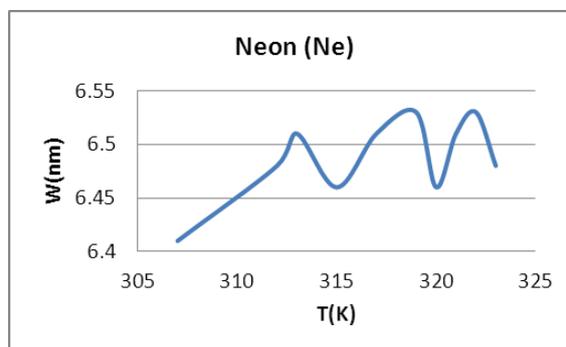
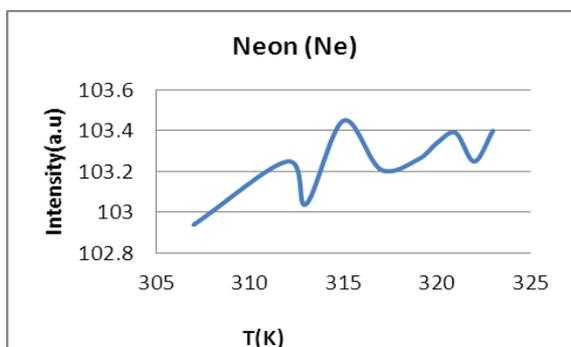


Fig (2-4-2-1) Relation between Intensity and temperature

Fig(2-4-2-2) relationship between line width and temperature

Table (2-4-3): spectrum of Fluorine(F₂)at different temperatures

T(K)	λ (nm)	A(m ²)	W(nm)	I(a.u)
304	631.02	6337.97	7.04	100.25
305	630.81	5964.04	6.44	98.63
307	630.9	5565.97	7.11	102.13
309	630.01	4442.99	7.16	102
311	631.01	5302.56	7.23	101.88
312	630.98	5332.11	7.25	101.52
314	631.06	4669.27	7.23	101.95
316	631.05	5193.09	7.16	101.82
317	631.08	5193.92	7.19	101.37
319	631.04	4549.7	7.2	101.66
321	631.11	3541.63	7.21	102.04
323	631.07	3351.55	7.13	102.3
325	631.08	4702.13	7.18	102.5

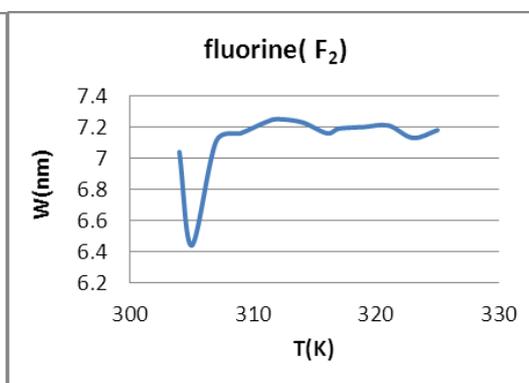
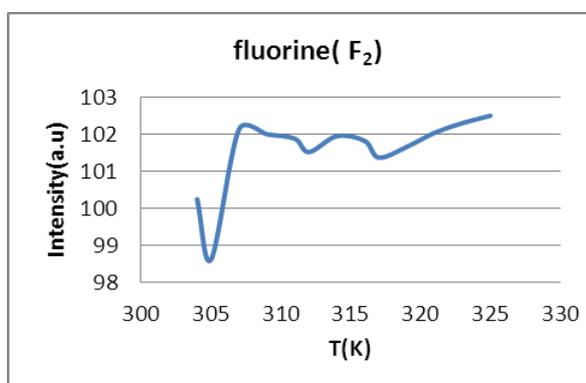


Fig (2-4-3-1) Relation between Intensity and temperature

Fig(2-4-3-2) relationship between line width and temperature

Table (2-4-4): spectrum of Chlorine (CL₂) at different temperatures

T(K)	λ (nm)	A(m ²)	W(nm)	I(a.u)
301	630.86	15934.5	6.92	122.23
303	630.83	7706.45	7.03	130.73
306	630.96	7478.8	7	124.24
308	630.95	8890.52	7.01	124.92
311	630.88	5738.32	7.08	126.31
313	630.94	5137.66	7.11	127.67
315	630.87	4995.6	7.01	127.81
317	630.88	4764.68	7.11	128.59
319	630.85	6501.06	7.006	129.27
321	630.93	4897.88	7.09	130.43
323	630.72	7777.74	6.88	131.22
325	630.77	6840.38	7.012	132.51
327	630.75	4907.18	6.92	134.15
329	630.75	5803.33	7.001	135.56
330	630.77	2866.74	7.05	137.006
331	630.83	2045.54	7.09	137.77

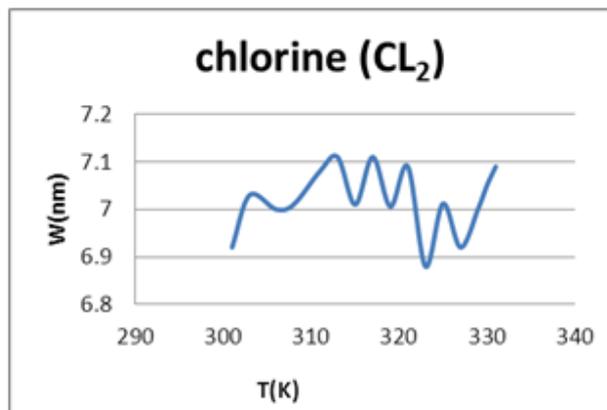
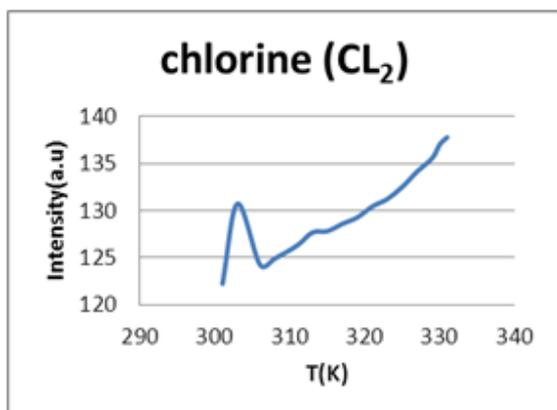


Fig (2-4-4-1) Relation between Intensity and temperature

Fig(2-4-4-2) relationship between line width and temperature

III. Theoretical Interpretation

Three scenarios are proposed to explain the temperature effect on the atomic spectra

(3-1)Complex Energy statistical Distribution

Heat energy results from collision of particles which lead to loss of energy that appears as heat thermal energy. In some theories, like optical theorem the energy is written as a summation of real and imaginary part. The real part stands for the particle energy, while the imaginary part represents the energy lost by the particle due to its interaction with the surrounding medium.

$$E = E_1 + iE_2 \tag{3-1-1}$$

If the uniform back ground is the attractive gas ions potential. Then

$$\bar{E} = -V_m \tag{3-1-2}$$

According to Shair .S model for non-equilibrium is given by sestem ,the distribution

$$n = n_0 e^{-\frac{E}{\bar{E}}}$$

Where E represents the non-uniform particle energy, where as \bar{E} stands for uniform particle energy thus substituting this in the equation

$$n = n_0 e^{\frac{E_1 + iE_2}{V_m}}$$

$$n = n_0 e^{\frac{E_1}{V_m}} e^{\frac{iE_2}{V_m}}$$

$$n = n_0 e^{\left(\frac{E_1}{V_m}\right)} \left[\cos \frac{E_2}{V_m} + i \sin \frac{E_2}{V_m} \right] \tag{3-1-3}$$

Considering the complex term standing for thermal energy

$$n = n_0 e^{\left(\frac{E_1}{V_m}\right)} \left[\sin \frac{E_2}{V_m} \right] \tag{3-1-4}$$

In view of equations (3-1-4)

$$I = I_0 e^{\left(\frac{E_1}{V_m}\right)} \left[\sin \frac{E_2}{V_m} \right] \tag{3-1-5}$$

Assuming E_1 to be kinetic thermal energy of the particle and E_2 be the lost thermal energy such that

$$E_2 = C_0 E_1 = C_0 kT \tag{3-1-6}$$

$$V_m = k \tag{3-1-7}$$

It follows that

$$I = I_0 e^T \sin C_0 T \tag{3-1-8}$$

$$C_0 = \pi$$

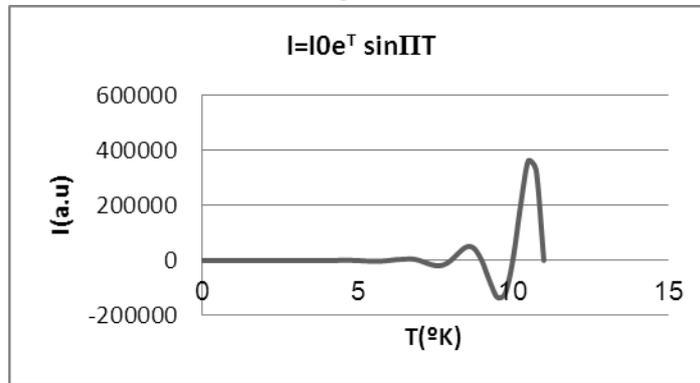


Fig (3-1-1)

However if the uniform background is the negative repulsive electron gas .In this case

$$\bar{E} = V_m \tag{3-1-9}$$

Thus equation (3-1-7) and (3-1-8) reduces to

$$n = n_0 e^{\left(\frac{-E_1}{V_m}\right)} \left[\cos \frac{E_2}{V_m} - i \sin \frac{E_2}{V_m} \right] \tag{3-1-10}$$

$$I = I_0 e^{\left(\frac{-E_1}{V_m}\right)} \left[\sin \frac{E_2}{V_m} \right] \tag{3-1-11}$$

In view of equations (3-1-8) and(3-1-7)

$$I = I_0 e^{-T} \sin C_0 T \tag{3-1-12}$$

$$C_0 = \pi$$

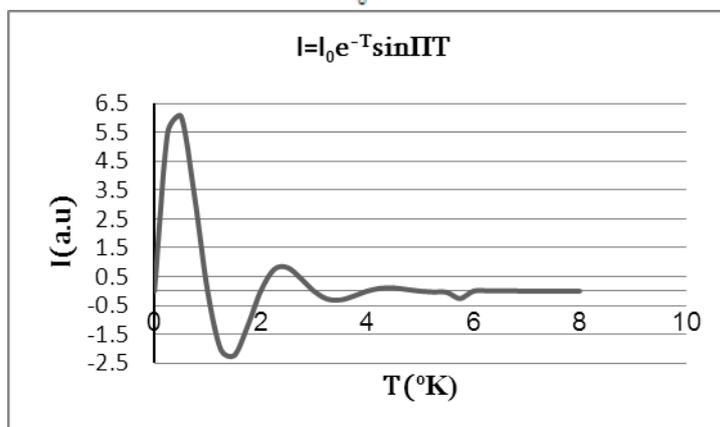


Fig (3-1-2)

Using Maxwell _Boltzmann disturbuation for electron

$$n_e = g e^{-\alpha} e^{-\beta(E_1+iE_2)} \quad (3-1-13)$$

The imaginary part stands for absorption from medium or emission to the medium

$$E_e = E_1 + i E_2 \quad (3-1-14)$$

For photon the number of photons is given by

$$n_p = e^{-\beta(E_3+iE_4)} \quad (3-1-15)$$

$$E_p = E_3 + i E_4$$

The for composite system medium which consists of electrons emitting photons, the energy is given by

$$E = E_e + E_p \quad (3-1-16)$$

Where E is the energy of the electron in excited state, E_e is the electron energy in the ground state, while E_p is the photon energy Thus the number of photon which is equal to the number of excited electrons is given by

$$n = e^{-\beta(E)} = e^{-\beta(E_e+E_p)} \quad (3-1-17)$$

For electron and photons colliding with particles medium, the energy lost appears as an imaginary part. Thus

$$n = e^{-\beta(E_1+E_2)} e^{-j\beta(E_2)} e^{-j\beta(E_4)}$$

For

$$E_1 \rightarrow 0 \quad E_3 \rightarrow 0$$

$$n = e^{-j\beta(E_2)} e^{-j\beta(E_4)} \quad (3-1-18)$$

$$= (\cos\beta E_2 - i \sin \beta E_2) (\cos\beta E_4 + i \sin \beta E_4) \quad (3-1-19)$$

Taking real part yields

$$n = \cos\beta E_2 \cos\beta E_4 \quad (3-1-20)$$

$$n = \cos \theta_2 \cos \theta_4 \quad (3-1-21)$$

$$I = \cos \theta_2 \cos \theta_4$$

If one assumes energy lost by the electron is 10 times that lost by the photon, it follows that

$$I = \cos 10\theta_4 \cos \theta_4 \quad \theta_2 = 10\theta_4$$

$$I = \cos 10T \cos T$$

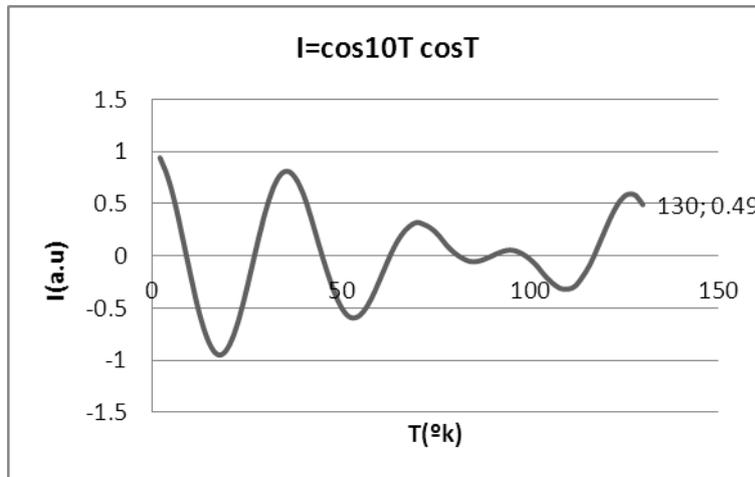


Fig (3-1-3)

(3-2)Quantum Mechanical approach

According to the laws of quantum mechanics, the density and number of particles n are related to the wave function Ψ according to the relation

$$n = |\Psi|^2 \quad (3-2-1)$$

But the intensities of radiation I is related to the total number of excited electrons per unit volume n

$$I = C n_p = C C_0 n \quad (3-2-2)$$

But the number of electrons n is given by

$n =$ number of atoms excited per second X number of electrons excited per second

$$n = \frac{dn_a}{dt} \times \frac{dn_e}{dt} = \left(\frac{d|\Psi_a|^2}{dt} \right) \left(\frac{d|\Psi_e|^2}{dt} \right) \quad (3-2-3)$$

Now consider simple case of free particles. In this case such equation. Reads

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} = E\Psi \quad (3-2-4)$$

The solution will be

$$\Psi = A \sin \alpha x, \Psi = -\alpha^2 \Psi \tag{3-2-5}$$

$$\frac{\hbar^2}{2m} \alpha^2 \Psi = E \Psi, \alpha^2 = \frac{2mE}{\hbar^2} \tag{3-2-6}$$

The probability current density is given by equation to be

$$S = \frac{\hbar^2}{m} [\Psi^* \nabla \Psi] = A^2 \frac{\hbar^2}{m} [\alpha \sin \alpha x \cos \alpha x]$$

$$\frac{dm}{dt} = s = \frac{A^2 \alpha \hbar^2}{2m} \sin 2 \alpha x = c_0 \sin 2 \alpha x \tag{3-2-7}$$

But since

$$v = 0$$

$$E = \frac{mv^2}{2} = \frac{p^2}{2m}$$

$$2mE = p^2 = \hbar^2 k^2 \tag{3-2-8}$$

From (3-2-6)

$$\alpha^2 = k^2$$

$$\alpha = k = \frac{2\pi}{\lambda} = \frac{2\pi f}{\lambda f} = \frac{\omega}{v}$$

$$\alpha = \frac{\hbar \omega}{\hbar v} \tag{3-2-9}$$

If one heat particles are harmonic oscillator, thus according to equation (3-2-8) the kinetic thermal energy becomes

$$KT = E = \hbar \omega \tag{3-2-10}$$

$$\alpha = \frac{KT}{\hbar v} \tag{3-2-11}$$

Thus for atoms and electrons see equation (3-2-7)

$$\frac{dn_a}{dt} = c_a \sin 2 \frac{KT}{\hbar v_a} x \tag{3-2-12}$$

$$\frac{dn_e}{dt} = c_e \sin 2 \frac{KT}{\hbar v_e} x \tag{3-2-13}$$

In view of equation (3-2-2)

$$I = C C_0 n = C C_0 C_a C_e \sin 2 \frac{KT x}{\hbar v_a} \sin 2 \frac{KT x}{\hbar v_e} \tag{3-2-14}$$

t a certain position x_0

$$I = C_a C_e \sin 2 \frac{KT x_0}{\hbar v_a} \sin 2 \frac{KT x_0}{\hbar v_e} \tag{3-2-15}$$

$$I = C_T \sin 2 \frac{KT x_0}{\hbar v_a} \sin 2 \frac{KT x_0}{\hbar v_e} \tag{3-2-16}$$

For Simi plicate let

$$20Kx_0 = \hbar v_0 \tag{3-2-17}$$

$$\frac{2Kx_0}{\hbar} = \frac{v_0}{10} \tag{3-2-18}$$

Thus

$$I = C_T \sin \frac{TV_0}{10v_a} \sin \frac{TV_0}{10v_e} \tag{3-2-19}$$

Let also

$$v_a = \frac{1}{3} v_e = \frac{1}{3} v_0$$

$$I = C_T \sin 3T \sin T = C_T \sin T \sin 3T \tag{3-2-20}$$

$$C_T = 10$$

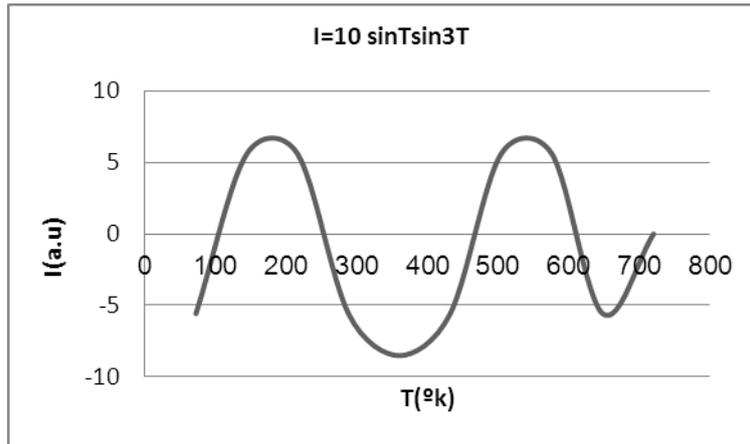


Fig (3-2-1)

(3-3)Semi Classical Harmonic Oscillator Mod

Consider on electric field that causes oscillation of atoms and electrons to emit radiation. The equation of motion of the oscillating particle is given by

$$ma = -F \tag{3-3-1}$$

The force acting on the electron or atom is the electric field. Thus

$$F = eE \tag{3-3-2}$$

The displacement is given by

$$x = x_0 e^{-i\omega_0 t}$$

Hence, the speed and acceleration are given by

$$v = \dot{x} = -i\omega_0 x, a = \ddot{x} = -\omega_0^2 x \tag{3-3-3}$$

Inserting (3-3-3) and (3-3-2) in (3-3-1)

$$-m\omega_0^2 x = -eE \tag{3-3-4}$$

If resistive force for a medium of particles density n is the form

$$F_r = \frac{-nmv}{\tau} = \frac{nim}{\tau} \omega x \tag{3-3-5}$$

The frequency change from ω_0 to ω , thus the equation of motion becomes

$$ma = -eE - F_r \tag{3-3-6}$$

With

$$x = x_0 e^{-i\omega t}$$

$$v = \dot{x} = -i\omega x, a = \ddot{x} = -\omega^2 x \tag{3-3-7}$$

Therefore, inserting (3-3-4),(3-3-5) and(3-3-7) in(3-3-6)yields

$$\begin{aligned} -m\omega^2 x &= -m\omega_0^2 x + \frac{inm\omega x}{\tau} \\ \omega_0^2 - \omega^2 &= \frac{i n \omega}{\tau} \\ (\omega + \omega_0)(\omega_0 - \omega) &= \frac{i n \omega}{\tau} \end{aligned} \tag{3-3-8}$$

If

$$\omega \approx \omega_0, \omega + \omega_0 \approx 2\omega, \omega_0 - \omega = \Delta\omega \tag{3-3-9}$$

Thus

$$\begin{aligned} (2\omega)(\Delta\omega) &= \frac{i n \omega}{\tau} \\ (\Delta\omega) &= \frac{i n}{2\tau} \end{aligned} \tag{3-3-10}$$

According to quantum harmonic oscillator model, if one treat the electrons and atoms as harmonic oscillators, their energy is given by

$$E_0 = \hbar\omega_0 \quad E = \hbar\omega \quad (3-3-11)$$

The energy difference due to friction is thus given by

$$\Delta E = E_0 - E = \hbar(\omega_0 - \omega) = \hbar\Delta\omega = \frac{\hbar n}{2\tau} \quad (3-3-12)$$

The imaginary term is not surprising as far as the inelastic scattering is described by imaginary potential. This is known as optical theorem, in which inelastic scattering, where particles lose energy by collision, is described by a complex potential.

In atomic spectra thus thermal energy leads to loss or gain of energy by collision leading numerically to the change of frequency in the form

$$\Delta f = \frac{\Delta\omega}{2\pi} = \frac{n}{4\pi\tau} \quad (3-3-13)$$

The corresponding change of length takes the form

$$\begin{aligned} \Delta f &= f_0 - f = \frac{c}{\lambda_0} - \frac{c}{\lambda} = \frac{c(\lambda - \lambda_0)}{\lambda\lambda_0} \\ &= \frac{c\Delta\lambda}{\lambda^2} = \frac{c^2}{c\lambda^2} \Delta\lambda = \frac{f^2}{c} \Delta\lambda \end{aligned} \quad (3-3-14)$$

Where

$$\lambda \approx \lambda_0 \quad \Delta\lambda = \lambda - \lambda_0 \quad (3-3-15)$$

Thus, in view of (3-3-15), equation (3-3-13) gives

$$\Delta\lambda = \frac{nc}{4\pi f^2\tau} = \frac{\pi n c}{\omega^2\tau} \quad (3-3-16)$$

But since the number density is related to the wave function according to the relation $n = |\Psi|^2$

Thus

$$\Delta\lambda = \frac{\pi c |\Psi|^2}{\omega^2\tau} \quad (3-3-17)$$

Using the complex energy statistical distribution in equation

$$n = n_0 e^{E_1/V_m} \sin \frac{E_2}{V_m} \quad (3-3-18)$$

Following the same procedures in equation from (3-1-6) to (3-1-12) one gets the line width in the form

$$w \sim \Delta\lambda \sim e^{-T} \sin \pi T \quad (3-3-19)$$

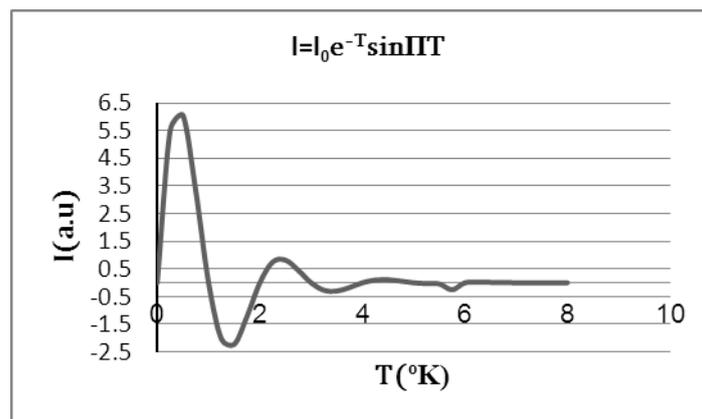


Fig (3-3-1)

If one uses the expression for the total number of electrons resulting from multiplying the number of electrons in each atom by the number of atoms, one gets

$$\begin{aligned} w \sim \Delta\lambda &\sim \cos\beta E_2 \cos\beta E_4 \\ &\sim \cos 10T \cos T \end{aligned} \quad (3-3-20)$$

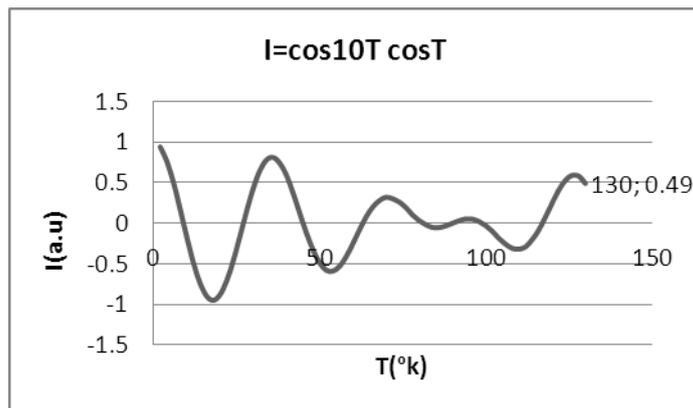


Fig (3-3-2)

Where one follows the same procedures used for the intensity expression derived for complex energy by using Maxwell's distribution. (see equation)(3-1-20)

The use of quantum expression in equations (3-2-20) together with equation (3-3-17) leads to

$$W \sim \Delta\lambda \sim \sin T \sin 3T \quad (3 - 3 - 21)$$

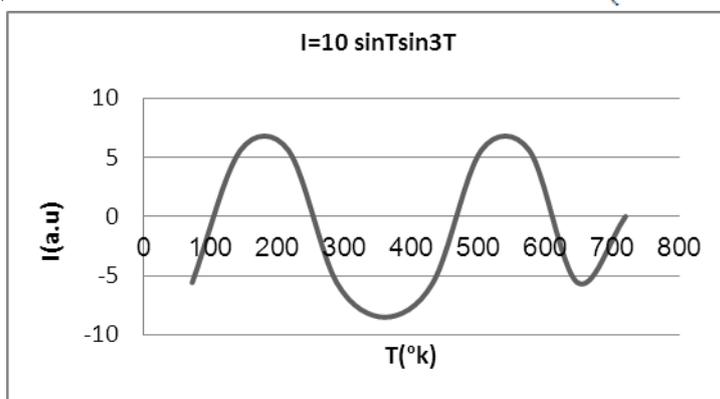


Fig (3-3-3)

IV. Discussion

The relation between Intensity and temperature for Neon (Ne) see fig. (2-4-2-1) resembles that obtained theoretically in equations (3-1-5) and (3-1-8) ,for the case when the temperature is non-uniform[see fig (3-1-1)].Thus

$$E_1, E_2 \sim kT$$

And the electric static potential is assumed to be uniform. This agrees with the fact that the gas is heated at the bottom, where it is very hot, while its temperature at the top is less. The same empirical relation for Ne can be explained by using quantum mechanics model in Fig (3-2-1) .

The model based on semi classical harmonic oscillator and quantum mechanics explains the effect of temperatures on the line width of the spectrum for the gases Bhutan (C_4H_{10}) , Neon (Ne), Fluorine(F2) and chlorine (CL2).

The comparison of Figs (2-4-1-2) with Fig (3-3-2), (2-4-2-2) with Fig (3-3-3) , (2-4-4-2) with Fig (3-3-2) and (2-4-3-2) with Fig (3-1-2) shows that the theoretical relations of line width with temperatures resembles the corresponding empirical relation .

V. Conclusion

The effect of temperature on spectra of gases can be explained by using non equilibrium statistical laws derived from plasma equation as well as a quantum and semi classical models for harmonic oscillator.

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References:

- [1]. John Morrison, Modern Physics: for Scientists and Engineers, (California, Academic Press, 2009).
- [2]. Raymond Serway& Clement Moses& Curt Moyer& Modern Physics (United State of America ,Cengage Learning, 2004).
- [3]. J .Michael Holles , Modern Spectroscopy ,(University of reading ,New Delhi ,2010).
- [4]. A . Beiser . concept of modern Physics ,(Mc Hill company ,New York ,1990) .
- [5]. A . N .Matreev ,Optics ,(Mir publishers ,Moscow , 1988) .
- [6]. ward T.Peltzer & Peter G.Brewer, Natural gas Hydrate in Oceanic and Permafrost Environments,M. D.MaxedKluwer, (Academic Publishers,Netherlands,2000).
- [7]. S.W.James,M.L.Dockney,& R.P.Tatam, Simultaneous independent Temperature and strain measurement using in-fiber Bragg grating sensors Electron,(Lett,vol.32, no .12,pp.1133-1134 ,1996)
- [8]. Hassan .M.Ahmed, Mcs Thesis,Measurement of Temperature Using Line width Broadening,2009.