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ORIGINAL ARTICLE

DERIVATION OF STATISTICAL PHYSICAL LAWS FROM QUANTUM MECHANICS

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ABSTRACT

Background: At the end of the nineteenth century, physics consisted essentially of classical mechanics, the theory of electromagnetism, and thermodynamics. Classical mechanics describes the behavior of only few particles; but fails to describe a bulk matter consisting of large number of particles. Statistical mechanics treats matter in bulk. **Objectives:** this work mainly aims to derive Maxwell – Boltzmann distribution, Fermi – Dirac and Bose – Einstein distribution laws depends on the relation between the number of particles and chemical potential beside some thermodynamic relations concerning probability. **Method:** The ordinary quantum mechanical wave function for free particle was differentiated with respect to energy and momentum. **Results:** The derivation of statistical laws from quantum wave function shows the general nature of quantum laws. **Conclusion:** the Maxwell – Boltzmann distribution, Fermi – Dirac and Bose – Einstein distribution are derived.

Key words: *quantum mechanics, wave function, Maxwell – Boltzmann distribution, Fermi – Dirac distribution, Bose – Einstein distribution.*

1. Introduction

Classical mechanics was used to predict the dynamics of material bodies, and Maxwell's electromagnetism provided the proper framework to study radiation; matter and radiation were described in terms of particles and waves, respectively [1]. Most branches of physics like classical mechanics, atomic physics, quantum mechanics, and nuclear physics, deal with one, two, or a few dozen particles. Statistical mechanics deals with, typically, about a mole of particles at one time. A mole is 6.06×10^{23}, considerably larger than a few dozen.

In statistical physics the number of particles are large and their motion is random .this make it difficult to apply Newton's lows to describe their behavior. But fortunately this random behavior can itself be used to formulate a new rule for statistical system. This new role state that the random behavior means that particles can occupy all possible states. Thus, the statistical weight is maximum [2, 3, 4].

Quantum mechanics plays an important role in physics it is now widely used to explain atomic phenomena as well as the behavior of elementary particles [5,6].

The history of quantum mechanics dates from the discovery of plank that light behaves like particles [7]. Later on Debrogglie proposed that particles like electrons behave as waves [8]. This encourages Schrödinger and Heisenberg to formulate a quantum equation that describes atomic world [9]. Heisenberg representation was developed by matrix representation, which represents quantum systems in different space [10].
Many attempts were made by Lutfi and Sugar to use quantum laws in resistive frictional medium and plasma equations to derive statistical laws but their derivation are complex [11,12].

In Schrodinger representation the wave function gives the probability of electrons transition [11,12]. The wave function is used in section 2 to derive Maxwell distribution law .Thermodynamic laws are used to derive the rest of distribution laws. Sections 3 and 4 are devoted for discussion and conclusion.

2. METHODS

To consider the ordinary quantum mechanical wave function free particles, differentiation has been conducted with respect to energy and momentum. This differentiation gives general equation for any quantum system. We used the number of particles that has energy E in terms of the wave function $\Psi(E)$ to find the total energy E_T and the total number of particles N. These assumptions and other physical laws are used to derive Maxwell distribution, Fermi – Dirac and Bose – Einstein distribution.

3. RESULTS

Derivation of Statistical Distribution Laws Using Quantum wave Function

The wave function of free quantum particles is given by:

$$\Psi = A\, e^{\frac{i}{\hbar}(Px-Et)} \qquad (1)$$

Where, p and E standing for momentum and energy respectively .this wave function can split into momentum dependent one $\Psi(P)$ and energy dependent one $\Psi(E)$, i.e:

$$\Psi = Ae^{\frac{i}{\hbar}(px)}.e^{\frac{i}{\hbar}(Et)} = A\Psi(P)\Psi(E) \qquad (2)$$

Differentiating Eq. (2) respect to p yields

$$\frac{d\Psi}{dp} = A\frac{i}{\hbar}xe^{\frac{i}{\hbar}(px)}.e^{\frac{i}{\hbar}(Et)} = A\,\frac{i}{\hbar}x\,\Psi(P)\Psi(E) \qquad (3)$$

$$\frac{d\Psi}{dp} = \frac{i}{\hbar}x\Psi \qquad (4)$$

Similarly, differentiation Eq. (2) respect to E gives:

$$\frac{d\Psi}{dE} = \left(-\frac{i}{\hbar}t\right)Ae^{\frac{i}{\hbar}(px)}.e^{\frac{i}{\hbar}(Et)} = -\frac{i}{\hbar}t\Psi \qquad (5)$$

Using Eq. (2) in Eq. (4) gives

$$A\Psi(\mathrm{E})\frac{d\Psi(\mathrm{P})}{dP} = \mathrm{A}\frac{i}{\hbar}x\Psi(E)\Psi(P)$$

Therefore,

$$\frac{d\Psi(\mathrm{P})}{dP} = \frac{i}{\hbar}x\Psi(P) \qquad (6)$$

In view of Eqs. (2) and (5) one finds:

$$\Psi(\mathrm{P})\frac{d\Psi(\mathrm{E})}{dE} = -\frac{i}{\hbar}t\Psi(P)\Psi(E)$$

$$\frac{d\Psi(\mathrm{E})}{dE} = -\frac{i}{\hbar}t\,\Psi(E) \qquad (7)$$

One can rewrite Eqs. (6) And (7) as functions of P and E and the left hand side as functions of x and t on the right hand side, i.e.:

$$\frac{1}{\Psi(\mathrm{P})}\frac{d\Psi(\mathrm{P})}{dP} = \frac{i}{\hbar}x \qquad (8)$$

$$\frac{d\Psi(\mathrm{E})}{\Psi(E)dE} = -\frac{i}{\hbar}t \qquad (9)$$

Bearing in mind that the momentum P is given in terms of m, v, x and t as :

$$\mathrm{p} = mv = m\frac{x}{t}, \qquad v = \frac{x}{t} \qquad (10)$$

Therefore Eqs. (8), (9) and (10) give:

$$\frac{\frac{d\Psi(\mathrm{P})}{\Psi(p)dP}}{\frac{d\Psi(\mathrm{E})}{\Psi(E)dE}} = -\frac{x}{t} = -v = -\frac{mv}{m} = -\frac{p}{m} \qquad (11)$$

Assume now that Eq. (11) is general for any quantum system, thus:

$$\frac{d\Psi(\mathrm{P})}{\Psi(p)dP} = -\frac{p}{m}\frac{d\Psi(\mathrm{E})}{\Psi(E)dE} \qquad (12)$$

Rearranging Eq. (12) by making the P dependent terms on the left hand side and the E dependent one on the right hand side, one gets:

$$\frac{2md\Psi(\mathrm{P})}{2\mathrm{p}\Psi(p)dP} = -\frac{d\Psi(\mathrm{E})}{\Psi(E)dE} = c \qquad (13)$$

Where c is a constant parameter:

But since

$$dp^2 = 2pdp \qquad (14)$$

It follows that:

$$\frac{2m}{\Psi(P)}\frac{d\Psi(\mathrm{P})}{dP^2} = -\frac{d\Psi(\mathrm{E})}{\Psi(E)dE} = c \qquad (15)$$

Let $p^2 = y$ (16)

Thus, Eq. (15) becomes:

$$\frac{d\Psi(\mathrm{E})}{\Psi(E)dE} = -c \qquad (17)$$

$$\frac{2md\Psi(\mathrm{y})}{\Psi(y)dy} = c \qquad (18)$$

It one split Ψ on the left hand side and E on the right hand side, and integrate both sides, we can get:

$$\int \frac{d\Psi(\mathrm{E})}{\Psi(E)} = -C\int dE = -CE + C_1 \qquad (19)$$

Therefore

$$ln\Psi(\mathrm{E}) = -CE + C_1 \qquad (20)$$

Hence

$$\Psi(\mathrm{E}) = e^{-CE+C_1} = e^{c_1}e^{-cE} = A_1 e^{-CE} \qquad (21)$$

Similarly splitting Ψdependence on one side and y dependence on the other side yourself:

$$\frac{d\Psi(y)}{\Psi(y)} = \frac{c}{2m}dy \qquad (22)$$

Integrating both sides gives:

$$\int \frac{d\Psi(y)}{\Psi(y)} = \frac{c}{2m}\int dy \qquad (23)$$

$$ln\Psi(\mathrm{y}) = \frac{c}{2m}y + c_2 \qquad (24)$$

$$\Psi(\mathrm{y}) = e^{(\frac{c}{2m}y+c_2)} = e^{\frac{c}{2m}y}e^{c_2} = A_2 e^{\frac{c}{2m}y} \qquad (25)$$

In view of Eq. (16), Eq. (25) become:

$$\Psi(\mathrm{p}) = A_2 e^{\frac{c}{2m}} = A_2 e^{\frac{cp^2}{2m}} \tag{26}$$

According to Eq. (21) the number of particles that have energy E is given in terms of the wave function $\Psi(\mathrm{E})$ to be

$$\boldsymbol{n(E) = n = \Psi(\mathrm{E})\overline{\Psi(\mathrm{E})} = |A_1|^2 e^{-2cE} = B_1 e^{-2cE}} \tag{27}$$

Thus, the total energy E_T is given by:

$$E_T = \int_0^\infty E\, \boldsymbol{e}^{-2cE} dE \tag{28}$$

Using Eq. (27), one gets

$$E_T = B_1 \int_0^\infty E\, \boldsymbol{e}^{-2cE} dE \tag{28}$$

Also, from Eq. (27) the total number of particles is given by

$$N = \int \overline{\Psi}(E)\, \Psi(E) dE = \int A_1 e^{-cE}.A_1 e^{-cE} = A_1^2 \int e^{-2cE} dE$$

$$= B_1 \int_0^\infty e^{-2cE} dE \tag{29}$$

From Eq. (29), N is given by

$$N = A_1^2 \left[-\frac{1}{2C} e^{-2cE}\right]_0^\infty = -\frac{B_1}{2C}[e^{-\infty} - e^{-0}] = \frac{B_1}{2c} \tag{30}$$

The average energy $\bar{E}$ is given by:

$$< E > = \bar{E} = \frac{\sum En(E)}{\sum n(E)} = \frac{\int \overline{\Psi}(E)\mathrm{E}\Psi(E)dE}{\int \overline{\Psi}(E)\mathrm{E}\Psi(E)dE} \tag{31}$$

This is also given by:

$$\bar{E} = \frac{E_T}{N} \tag{32}$$

The total energy in Eq. (28) can be found by using partial differentiation:

$$E_T = B_1 \int_0^\infty E e^{-2cE} dE = \int_0^\infty udv = [uv]_0^\infty - \int_0^\infty vdu \tag{33}$$

Where,

$$u = E \quad , dv = e^{-2cE} dE \ , v = \frac{e^{-2cE}}{-2c} \tag{34}$$

Thus:

$$E_T = \mathrm{B}_1[uv - \int vdu] = \mathrm{B}_1 \left\{\left[E \frac{e^{-2CE}}{2C}\right]_0^\infty - \int_0^\infty \frac{e^{-2CE}}{2C} dE\right\}$$

$$= \mathrm{B}_1 \left\{[E e^{-\infty} - 0e^{-0}] - \frac{1}{4c^2}[e^{-2cE}]_0^\infty\right\}$$

$$E_T = -\frac{B_1}{4c^2}\{[e^{-\infty} - e^{-0}]\} = \frac{B_1}{4c^2} \tag{35}$$

Thus from Esq. (30) and (35) the average energy is given by:

$$< E >= \bar{E} = \frac{E_T}{N} = \frac{(B_1/4c^2)}{(B_1/2c)} = \frac{1}{2c} \tag{36}$$

There fore

$$2c = \frac{1}{\bar{E}} \tag{37}$$

Thus a direct substitution of Eq. (37) in Eq. (27) gives the number of particles n, in the energy state E, as follow:

$$n = n(E) = B_1 e^{-\frac{E}{\bar{E}}} \tag{38}$$

Similarly Eq. (26) can also be used to find the average energy for free particles, where:

$$E = \frac{P^2}{2m} \tag{39}$$

Thus Eq. (26) gives

$$n = \Psi(\mathrm{E})\overline{\Psi(\mathrm{E})} = A_2^2\, e^{2CE} = B_2 e^{2cE} \tag{40}$$

Therefore, the total number of particles is given by:

$$N = B_2 \int_0^{\infty} e^{2cE}\, dE \tag{41}$$

$$N = \frac{B_2}{2c}[e^{2cE}]_0^{\infty} \tag{42}$$

If c= +

The integration became infinite which is in conflict with the fact that N is finite. The only way to makes N Finite is to assume that:

c=- co (43)

Thus

$$N = \frac{B_2}{-2co}[e^{-2coE}]_0^{\infty} = \frac{B_2}{-2co}[e^{-\infty} - e^{-0}] = \frac{B_2}{2co} \tag{44}$$

The total energy is also given by:

$$E_T = \int_0^{\infty} En(E)dE = B_2 \int_0^{\infty} Ee^{-2cE}\, dE = \int udv = uv - \int vdu \tag{45}$$

With

$$u = B_2 E \qquad , dv = e^{-2cE} dE \quad , \quad du = B_2 dE$$

$$v = \int dv = \int e^{-2c0E}\, dE = \frac{e^{-2coE}}{-2co} \tag{46}$$

Thus

$$E_T = B_2 E \left[\frac{e^{-2COE}}{-2co}\right]_0^{\infty} + \frac{B_2}{2co}\int_0^{\infty} e^{-2coE}\, dE = B_2 \frac{[0 - e^{-\infty}]}{-2co} - \frac{B_2}{4co^2}[e^{-2co}]_0^{\infty} = 0 + \frac{B_2}{4co^2}$$

$$E_T = \frac{B_2}{4co^2} \tag{47}$$

Thus the average energy is given by:

$$\bar{E} = \frac{E_T}{N} = \frac{B_2/4co^2}{B_2/2co} = \frac{1}{2co}$$

$$\bar{E} = \frac{1}{2co} \tag{48}$$

Inserting Eq. (48) in Eq. (40) and using the assumption (43) yields:

$$n = B_2 e^{-\frac{E}{\bar{E}}} \quad (49)$$

Which rambles Eq. (38) for:

$$B_2 = ge^{-\alpha} \quad , \quad \bar{E} = KT \quad (50)$$

From which one gets Maxwell distribution:

$$n = ge^{-\alpha} = e^{-\frac{E}{KT}} \quad (51)$$

Fermi – Dirac and Bose – Einstein distribution can also be found by using entropy approach.

The entropy S is related to the distribution function W according to the relation:

$$S = KLnw = k\sigma \quad (52)$$

$$\sigma = Lnw \quad (53)$$

The probability that one can find a particle in the energy state n is related to σ according to the relation:

$$\sigma = -Ln\Gamma_n \quad (54)$$

Thus from Eq. (52) and Eq. (54) one gets:

$$S = -kLn\,\Gamma_n \quad (55)$$

Where this probability is given according to Eq. (38) by:

$$\Gamma_n = Ae^{-\frac{E_n}{KT}} \quad (56)$$

Where one substitutes $B_1 = A \;\; , \bar{E} = kT$ (57)

Taking the Ln of both sides of Eq. (56) yields:

$$\mathrm{Ln}\Gamma_n = LnA - \frac{En}{kT} \quad (58)$$

Thus according to Eq. (55), one gets:

$$S = -kLn\,A + \frac{E_n}{T} \quad (59)$$

$$kLnA = \frac{E_n - Ts}{T} \quad (60)$$

But from thermo dynamites laws:

$$F = E - Ts = E_n - Ts \quad (61)$$

Therefore Eq. (60) gives:

$$kLnA = \frac{F}{T} \quad (62)$$

Hence

$$A = e^{F/kT} \quad (63)$$

Inserting Eq. (63) in Eq. (56) yields $\Gamma_n = e^{(F-E_n)/kT}$ (64)

One can generalized Eq. (55) to get include chemical potential to become:

$$S = -\mathrm{kLn}\Gamma_n = -kLnA - \frac{mN}{T} + \frac{E}{T} \qquad (65)$$

Rearranging Eq. (65) yields:

$$kTLnA = E - Ts - mN = F - mN = F - G = \Omega \qquad (66)$$

Where

$$G = mN \qquad (67)$$

Therefore, Eq. (64) becomes:

$$\Gamma_n = e^{\frac{\Omega}{Kt}} e^{\frac{(\mu N - E_n)}{Kt}} \qquad (68)$$

But since the total probability is equal to one this means that:

$$\Gamma_n = 1 = e^{\Omega/kT} \sum_{ni} e^{\frac{(\mu N - E_n)}{KT}} \qquad (69)$$

Where

$$E_n = \sum n_i E_i \qquad (70)$$

Thus, one can write:

$$\Omega_i = -kTLn \sum_{n_i} e^{\frac{(\mu - E_i)n_i}{KT}} \qquad (71)$$

For this case when:

$$dE = dU = dQ + PdV \qquad (72)$$

$$\Omega = F = -PV \qquad (73)$$

Fermi-Dirac distribution law requires the number of particles to be zero or 1 in each cell, thus Eq. (71) gives:

$$\Omega_i = -kTLn \sum_{n_i=0}^{1} e^{\frac{(\mu - E_i)n_i}{KT}} = -kTLn \sum_{n_i=0}^{1} \left[e^{\frac{(\mu - E_i)n_i}{KT}}\right]^{n_i} = -kTLn\left[1 + e^{\frac{(\mu - E_i)}{KT}}\right] \qquad (74)$$

Using the definition of the number of particles in state i, one gets:

$$n_i = \frac{-\partial \Omega i}{\partial \mu} = \frac{1}{e^{\frac{(E_i - \mu)}{KT}} + 1} \qquad (75)$$

This is Fermi_Dirac distribution law.

Bose – Einstein distribution can also be found by using the same argument, where the number of particles ranges from 0 to ∞ thus,

$$\Omega_i = -kTLn \sum_{n_i=0}^{\infty} \left[e^{\frac{(\mu - E_i)}{KT}}\right]^{n_i} \qquad (76)$$

This is a sum of geometric series as the form:

$$\sum_{i=0}^{n} r_i = \frac{r^n - 1}{r - 1} \qquad (77)$$

Since:

$$\mu - E_i < 0 \tag{78}$$

$$e^{\frac{(\mu - E_i)}{KT}} < 1 \tag{79}$$

But

$$r = e^{\frac{(\mu - E_i)}{KT}} \tag{80}$$

$$r < 1 \tag{81}$$

For $n \to \infty$

Becomes the geometric series:

$$\sum_{i=0}^{\infty} \mathrm{r}_i = -\frac{1}{r-1} = \frac{1}{1-r} = (1-r)^{-1} \tag{82}$$

Thus

$$\Omega_i = -kTLn\left[1 - e^{\frac{(\mu - E_i)}{KT}}\right] \tag{83}$$

Hence

$$\mathrm{n}_i = \frac{-\partial \Omega_i}{\partial \mu} = \frac{e^{\frac{(\mu - E_i)}{KT}}}{1 - e^{\frac{(\mu - E_i)}{KT}}}$$

$$\mathrm{n}_i = \frac{1}{e^{\frac{(\mu - E_i)}{KT}} - 1} \tag{84}$$

The Eq. (84) is the ordinary Bose – Einstein distribution.

4. DISCUSSION

The wave function in the energy and momentum space are differentiated with respect to energy and momentum in equations (4) and (7) and then divided to be expressed in terms of momentum in Eq.(11). The energy and momentum parts are separated in Eq. (13) and the energy one is found to be similar to Maxwell distribution. The momentum part also is integrated to find another expression similar to Maxwell distribution as shown by Eq. (26). The number of particles in terms of the energy wave function in the energy space was found in Eq. (27). To find the unknown Parameter c the expression of the average energy in Eq. (31) is used to find c in Eq. (37). This enable finding generalized Maxwell distribution in Eq. (38).The expression of momentum in Eq. (26) is also used to find average energy. Then again Maxwell distribution was obtained in equations (49) and (51).

Using some thermo dynamical relations related to the probability and the relation of chemical potential for the number of particles see equations (52,...,61) Fermi-Dirac distribution and Bose-Einstein one were found as shown by Eqs. (75) and (84) respectively. The theoretical results found in this work fully concur with the author theoretical results [13, 14, 15, 16, 17], but in present work we use simple models to derive these laws.

5. CONCLUSION

The derivation of statistical laws from quantum wave function shows the general nature of quantum laws. It also shows the close relation between the probabilistic nature in both quantum laws and statistical laws.

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