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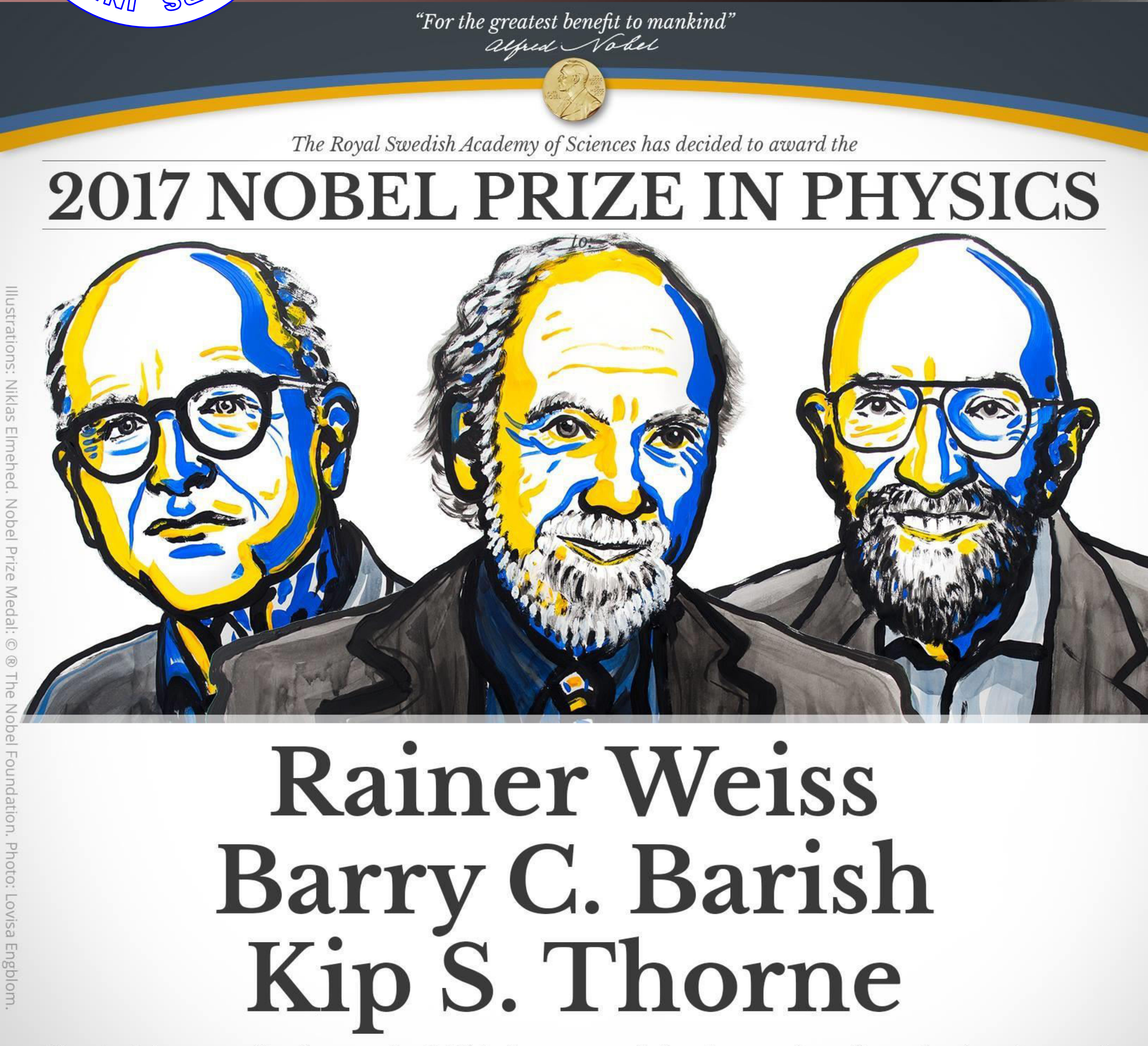

"For the greatest benefit to mankind"
Alfred Nobel

The Royal Swedish Academy of Sciences has decided to award the

2017 NOBEL PRIZE IN PHYSICS

to

Rainer Weiss
Barry C. Barish
Kip S. Thorne

"for decisive contributions to the LIGO detector and the observation of gravitational waves"

Illustrations: Niklas Elmehed. Nobel Prize Medal: © ® The Nobel Foundation. Photo: Lovisa Engblom.

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EDITORIAL

This issue of *Physics Education* comes along at a time when Nobel prizes in physics have been announced. This year's winners, Rainer Weiss, Barry Barish and Kip Thorne were awarded the prize for their decisive contributions that led to the observation of gravitational waves. The observation of gravitational waves last year opened up another window to the universe.

Based on some of the feedback we had received for the redesigned website of *Physics Education*, we understand that there are still few small problems to be ironed out. I assure you that these issues will be sorted out soon.

We are in the midst of festival season in India and elsewhere too. I take this opportunity to convey my festival greetings to all the readers of *Physics Education*.

M. S. Santhanam
Chief Editor
Physics Education

Derivation of Van der Waal's equation of state in microcanonical ensemble formulation

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Abstract

The Van der Waal's equation of state for a (slightly) non-ideal classical gas is usually derived in the context of classical statistical mechanics by using the canonical ensemble. We use the hard sphere potential with no short range interaction and derive Van der Waal's equation of state in microcanonical ensemble formulation.

1 Introduction

The ensemble theory of equilibrium statistical mechanics connects the macroscopic relations of thermodynamic systems and its microscopic constituents [1, 2, 3]. An ensemble of a given thermodynamic system is a set of distinct microstates with appropriately assigned probability for a fixed macrostate [4]. In a macrostate of fixed energy E, volume V and the number of particle N and all its microstates are equiprobable then such an ensemble is called as microcanonical ensemble [5].

The most important concept in statistical mechanics theory is the equivalence of ensemble, that is, the ensemble theory should provide the same macroscopic relations in the thermodynamic limit of infinite size irrespective of the chosen ensemble. This concept of ensemble equivalence has been verified easily by incorporating different ensemble approach to simple system known as ideal gas. Whatever the ensemble one may choose, we can finally obtain the ideal gas equation of state as $PV = nRT$ [2, 5], where P is the pressure, V is the volume, T is the temperature of the system, n is the number of moles and R is the universal gas constant.

An ideal gas is the simplest thermodynamic system in which there is no intermolecular interactions. By considering the intermolecular interactions, Van der Waals proposed the equation of state for a real gas which is given by [6]

$$\left(P+\frac{n^2a}{V^2}\right)(V-nb)=nRT, \tag{1}$$

where a and b are the Van der Waal's constants. The derivation of Van der Waal's equation of state has been found in most of the Statistical Physics books which are in canonical ensemble formulation [7]. To our knowledge, there is no such study available in the literature for any other ensemble formulation, in particular, microcanonical ensemble formulation. In this paper, we use the hard sphere potential approximation and derive the Van der Waal's equation of state in microcanonical ensemble formulation.

2 Hamiltonian for Van der Waal's gas

Consider a monoatomic non ideal gas of N particles having identical mass m in a container of fixed volume V at temperature T. In order to treat the problem in classical statistical mechanics, we assume that the temperature is taken to be sufficiently high and the density $\rho = \frac{N}{V}$ is sufficiently low. The total energy (Hamiltonian) of the system is $H = K + U$, where $K = \frac{1}{2m}\sum_{l=1}^{3N} p_l^2$ is the kinetic energy of the gas of $3N$ degrees of freedom moving with momentum p_l. U is the total potential energy due to the interaction that exists between the molecules. In semi-classical approximation, we consider the molecules to be hard spheres of radius r_0, so that the distance between the two molecules can come close to r_0 [2]. The interaction between a pair of molecules i and j separated by the intermolecular distance r is given by the hard sphere potential with no short range interaction as [7, 8]

$$u(r) \quad = \quad -u_0\left(\frac{r_0}{r}\right)^6 \text{ for } r \geq r_0, \tag{2}$$

where u_0 is the depth of the potential. The total potential energy is given by the sum of interactions between the pair of all molecules as

$$U=\frac{1}{2}\sum_{i=1}^{N} u_i, \tag{3}$$

where u_i is the interaction energy of i^{th} molecule with all other molecules in the specified region given in spherical polar coordinates as

$$u_i=\int_{r_0}^{\infty}\int_0^{2\pi}\int_0^{\pi} \rho u(r)\, r^2 sin\theta \; drd\theta d\phi \tag{4}$$

$$u_i=-4\pi\frac{Nu_0}{V}\int_{r_0}^{\infty}\frac{r_0^6}{r^4}dr=-\frac{4\pi Nu_0r_0^3}{3V}. \tag{5}$$

Here, we assume that the density $(\rho = \frac{N}{V})$ of the gas to be uniform throughout the volume. Thus, the total potential energy is given by

$$U=\frac{1}{2}Nu_i=\frac{-a'N^2}{V}, \tag{6}$$

where $a' = \frac{2\pi u_0 r_0^3}{3}$. Therefore the total Hamiltonian is given by

$$H=\sum_{l=1}^{3N}\frac{p_l^2}{2m}-\frac{a'N^2}{V}\equiv E. \tag{7}$$

3 Microcanonical entropy and equation of state

Because of the hard sphere approximation, there should be a correction in the total volume of the Van der Waal's gas. By considering the molecules as a hard sphere of diameter $2r_0$, the center of each molecules excluded by other molecule by a volume which is equivalent to the volume of sphere of radius $2r_0$ is known as the excluded volume. The excluded volume for the two molecules of radius r_0 is $\frac{4}{3}\pi(2r_0)^3$. Since the system contains N molecules, the excluded volume v for N molecule can be obtained as $v = Nb'$ where $b' = \frac{2\pi(2r_0)^3}{3}$. The corrected volume which is available for the gas molecules in the container is given by

$$V' = V - Nb'. \tag{8}$$

Consider a small volume in phase space, the total number of microstates available for the system in microcanonical ensemble of fixed E, V and N of Eq.(7) is given by [2, 3, 6]

$$\Omega(E,V,N) = \frac{1}{N!h^{3N}}\frac{\partial\omega}{\partial E}, \tag{9}$$

where h is the Planck's constant and the volume integral [5, 6, 9]

$$\omega(E,V,N) = \int\int_{H(q,p)\leqslant E} d^{3N}q\, d^{3N}p. \tag{10}$$

For hard sphere potential, the above integral can be written as

$$\omega(E,V,N) = (V - Nb')^N \int_{H(q,p)\leqslant E} d^{3N}p, \tag{11}$$

where $\int_{H(q,p)\leqslant E} d^{3N}q = (V')^N = (V - Nb')^N$ for Van der Waal's gas and Eq.(7) can be rearranged as

$$\sum_{l=1}^{3N} p_l^2 = 2m\left(E + \frac{a'N^2}{V}\right) \tag{12}$$

The integral in Eq.(11) is just the volume of a $3N$ dimensional sphere of radius $R = \sqrt{2m(E + \frac{a'N^2}{V})}$ which can be obtained as (see appendix) [2, 3]

$$\begin{aligned}\omega(E,V,N) &= \frac{\pi^{3N/2}}{\frac{3N}{2}\Gamma(\frac{3N}{2})}(V - Nb')^N R^{3N} &(13)\\ &= \frac{\pi^{3N/2}}{\frac{3N}{2}\Gamma(\frac{3N}{2})}(V - Nb')^N \left[2m\left(E + \frac{a'N^2}{V}\right)\right]^{3N/2} &(14)\end{aligned}$$

Using the above equation we can calculate the number of microstates as in Eq.(9) for Van der Waal's gas in micro canonical ensemble as

$$\Omega(E,V,N) = \frac{1}{N!h^{3N}}\frac{\pi^{3N/2}}{\Gamma(\frac{3N}{2})}(V - Nb')^N (2m)^{3N/2}\left(E + \frac{a'N^2}{V}\right)^{\frac{3N}{2}-1}. \tag{15}$$

For large N, we can approximate $\frac{3N}{2} - 1 \simeq 3N/2$ and $\Gamma(\frac{3N}{2}) = (\frac{3N}{2} - 1)! \simeq \frac{3N}{2}!$ then

$$\Omega(E,V,N) = \frac{1}{N!h^{3N}} \frac{\pi^{3N/2}}{\frac{3N}{2}!} (V - Nb')^N (2m)^{3N/2} \left(E + \frac{a'N^2}{V}\right)^{\frac{3N}{2}}. \tag{16}$$

The Boltzmann microcanonical entropy of the system is given by [2, 5, 6],

$$S(E,V,N) = k_B \, \ell n \Omega(E,V,N). \tag{17}$$

Using Eq.(16) and applying Stirling approximation $\ell nN! = N \ell nN - N$, we can obtain the microcanonical entropy of Van der Waal's gas is

$$S(E,V,N) = k_B N \left\{ \frac{5}{2} + ln \left\{ \left(\frac{V - Nb'}{N} \right) \left[\frac{4\pi m}{3Nh^2} \left(E + \frac{a'N^2}{V} \right) \right]^{\frac{3}{2}} \right\} \right\}. \tag{18}$$

At constant V and N, from the Maxwell's First thermodynamic relation $dE = TdS - pdV$, we get [1, 5]

$$\frac{\partial S}{\partial E} = \frac{1}{T} \tag{19}$$

$$\frac{\partial S}{\partial V} = \frac{P}{T} \tag{20}$$

Using Eq.(18), we obtain

$$\frac{1}{T} = \frac{3}{2} N k_B \left(E + \frac{a'N^2}{V} \right)^{-1} \tag{21}$$

The above equation can be rearranged in terms of energy as

$$E = \frac{3}{2} N k_B T - \frac{a'N^2}{V} \tag{22}$$

Using Eq.(18) and Eq.(22), one can get

$$\frac{P}{T} = \frac{N k_B}{(V - Nb')} - \frac{a'N^2}{V^2 T}. \tag{23}$$

$$\left(P + \frac{a'N^2}{V^2} \right) (V - Nb') = N k_B T \tag{24}$$

Substitute $N = nN_a$, $a = a'N_a^2$, $b = b'N_a$ and $k_B N_a = R$ in the above equation, we get

$$\left(P + \frac{n^2 a}{V^2} \right) (V - nb) = nRT. \tag{25}$$

where R is gas constant, n is the number of moles and N_a is the Avogadro's number. Thus, we have obtained Van der Waal's equation of state with Van der Waal's constants a and b.

4 conclusion

We used the hard sphere potential and derived Van der Waal's equation of state in microcanonical ensemble formulation. Even though the canonical ensemble is much easier to use in actual application than the microcanonical ensemble, one should not ruled out the various studies of the same system in other ensemble formulation. In this context, our result also verified the equivalence of ensemble for Van der Waal's gas.

Appendix:

The integral in Eq.(11) can be considered as the volume of $3N$ dimensional spheres of radius $R = \sqrt{2m(E + \frac{a'N^2}{V})}$ which is given by [5, 6]

$$\begin{aligned} V_N(R) &= \int_{\sum_{l=1}^{3N} p_l^2 \leqslant R^2} d^{3N}p && (26) \\ &= R^{3N} \int_{\sum_{l=1}^{3N} y_l^2 \leqslant 1} d^{3N}y && (27) \\ &= R^{3N} C_{3N}, && (28) \end{aligned}$$

where $y_l = p_l/R$, $C_{3N} = \int_{\sum_{l=1}^{3N} y_l^2 \leqslant 1} d^{3N}y$ and

$$d^{3N}y = dV_N(R) = 3NC_{3N}R^{3N-1}dR \quad (29)$$

Using the identity $\int_{-\infty}^{+\infty} e^{-y^2}dy = \sqrt{\pi}$ and Eq.(29), we consider the integral

$$\int_{-\infty}^{+\infty} .... \int_{-\infty}^{+\infty} e^{-(y_1^2+y_2^2+.......+y_{3N}^2)} d^{3N}y = \pi^{\frac{3N}{2}} \quad (30)$$

and transform it in to polar coordinates as,

$$3NC_{3N} \int_0^{\infty} R^{3N-1} e^{-R^2} dR = \pi^{\frac{3N}{2}}. \quad (31)$$

Substituting $R^2 = x$, we obtain

$$C_{3N} = \frac{\pi^{3N/2}}{\frac{3N}{2}\Gamma(\frac{3N}{2})} \quad (32)$$

where the Gamma function

$$\Gamma\left(\frac{3N}{2}\right) = \int_0^{\infty} x^{\frac{3N}{2}-1} e^{-x} dx. \quad (33)$$

Therefore, Eq.(11) becomes

$$\begin{aligned} \omega(E, V, N) &= \frac{\pi^{3N/2}}{\frac{3N}{2}\Gamma(\frac{3N}{2})}(V - Nb')^N R^{3N} && (34) \\ &= \frac{\pi^{3N/2}}{\frac{3N}{2}\Gamma(\frac{3N}{2})}(V - Nb')^N \left[2m\left(E + \frac{a'N^2}{V}\right)\right]^{3N/2} && (35) \end{aligned}$$

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Van der Waal's gas equation for an adiabatic process and its Carnot engine efficiency

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Abstract

There has been many studies on gases which obeys Van der Waal's equation of state. However there is no specific and direct studies of Van der Waal's gas which undergoes adiabatic processes are available in the undergraduate text books and also in literature. In an adiabatic process there is no heat energy exchange between the system and its surroundings. In this article, we find that the Van der Waal's equation for the adiabatic process as $\left(P + \frac{n^2a}{V^2}\right)(V - nb)^\Gamma$ = constant, where P is the pressure, V is the volume, n is the number of moles of the Van der Waal's gas, a and b are Van der Waal's constant and Γ is a factor which relates the specific heat at constant pressure and at constant volume. We use this relation explicitly and obtained the efficiency of a Carnot engine whose working substance obeys Van der Waal's equation of state. Our simplest approach may provide clear idea to the undergraduate students that Γ is different from γ of the ideal gas for an adiabatic process. We also shown that the efficiency of the Carnot engine is independent of the working substance.

1 Introduction

In thermodynamics, heat and work are the form of energy transfer across the boundary between the system and its surroundings. If the boundary forbids the flow of heat energy between the system and the surroundings then the thermodynamic process which changes the state of the system is called as adiabatic process. If the energy transfer takes at a fixed system temperature then such a process is called as isothermal process. All heat engines make use of the mechanism of converting heat (Q) in to work (W), without involving any resultant change in the state of the system. It is a series of processes taking place in a cyclic manner in which the engine or system will be returned to its initial state.

During each of the processes, there may be a heat energy flow between the system and its surroundings. This comprises of a hot reservoir and a cold reservoir, which will be maintained at constant temperatures, and the working substance which exchanges heat. Therefore, the engine is said to operate between these two reservoirs. During a part of cycle performed by the working substance in an engine, some heat Q_H is absorbed from the hotter reservoir and a smaller amount of heat Q_L is rejected to the cooler reservoir during the another part of cycle. In a cyclic process, the system returns to the initial state with no change in internal energy ($\Delta U = 0$). So, from the first law of thermodynamics $Q_{net} - W_{net} = 0$, where $Q_{net} = Q_H - Q_L$ is the net heat exchanged between the system and the surroundings and $W_{net} = Q_{net} = Q_H - Q_L$ is the total or net work performed on the system. The engine efficiency η is defined as [1, 2, 3],

$$\begin{aligned} \eta &= \frac{\text{Net Work}}{\text{Heat absorbed}} \qquad (1) \\ &= \frac{Q_H - Q_L}{Q_H} = 1 - \frac{Q_L}{Q_H}. \end{aligned}$$

1.1 Carnot Cycle

Carnot proposed a thermodynamic cycle called as Carnot cycle which is a set of equilibrium reversible processes any thermodynamic system can perform [1, 2]. Initially the system or working substance in Carnot cycle is imagined to be in thermal equilibrium with a reservoir at lower temperature T_L. Four processes are then performed in the following order:

1. A reversible adiabatic process is performed in such a direction that the temperature rises to that of hotter reservoir temperature T_H. However, no energy in the form of heat flows in to or out of the system.

2. The working substance is maintained in contact with the reservoir at T_H and a reversible isothermal process is performed in such a direction to the extent that Q_H is absorbed from the reservoir. In this case the system is kept at a fixed reservoir temperature.

3. A reversible adiabatic process is performed in a direction opposite to that of the first process with no heat exchange. This is done until the temperature reaches T_L, temperature of the cooler reservoir.

4. A reversible isothermal process opposite to the direction of the second process is performed until the working substance reaches the initial state and Q_L is rejected by the working substance. In this case the system is kept at a fixed reservoir temperature T_L.

Thus an engine in Carnot cycle operates between two reservoirs in a particular simple way. All the absorbed heat enters the system at a constant high temperature, namely that of a hotter reservoir. Also, all the rejected heat leaves the system at a constant low temperature, that of a cooler reservoir. Since all processes are reversible, the Carnot engine is a reversible engine. An engine which operates in this cycle is called as Carnot engine whose efficiency is always greater than any engines operated by the cycle other than Carnot cycle. Any hypothetical engine operated in this cycle is said to be ideal if it gives 100% efficiency. Since it is fact of experience that some heat is always rejected to cooler reservoir, the efficiency of actual engine is always less than the ideal and the Carnot engine [1, 2, 3].

Considering a working substance in a Carnot engine as an ideal gas, with no intermolecular interactions, the gas satisfies the ideal gas equation of state $PV = nRT$. Where P is the pressure, V is the volume, T is the temperature of the system, n is the number of moles and R is the universal gas constant. The thermal efficiency of a Carnot engine whose working substance is an ideal gas is given by [2, 3]

$$\eta = 1 - \frac{T_L}{T_H}. \tag{2}$$

Thus, a Carnot engine absorbing Q_H amount of heat from the reservoir at higher emperature T_H and rejecting Q_L amount of heat to the reservoir at lower temperature T_L has an efficiency that is independent of the nature of the working substance. The above result is obtained by using the ideal gas equation of state for the isothermal process $PV =$ constant and the ideal gas equation for the adiabatic process $PV^\gamma =$ constant. Here, γ is the ratio of the specific heat capacity at constant pressure to the specific heat capacity at constant volume. Further studies using various gas equations [4, 5, 6, 7] also showed that the efficiency of a Carnot cycle is independent of working substance and depends only on temperatures of reservoirs.

1.2 Van der Waal's gas

By considering the intermolecular interactions, Van der Waal proposed the equation of state for a real gas which is given by[2, 3, 5]

$$\left(P + \frac{n^2 a}{V^2}\right)(V - nb) = nRT, \tag{3}$$

where a and b are the Van der Waal's constants. There has been several studies for Van der Waal's equation of state [5, 6]. However, there is no specific and direct studies available in undergraduate text books and also in literature for the equation of Van der Waal's gas subjected to an adiabatic process. In this paper we explicitly find that the Van der Waal's equation for an adiabatic process as

$$\left(P + \frac{n^2 a}{V^2}\right)(V - nb)^\Gamma = \text{constant}, \tag{4}$$

where Γ is a factor which relates the specific heat at constant pressure and at constant volume. We use the above relation and obtained the relation between the specific heat capacity at constant pressure and at constant volume. As similar to ideal gase approach we also used the above relation directly and showed that the efficiency of a Carnot cycle is independent of the working substance and depends only on the temperature of the reservoirs.

2 Van der Waal's gas equation for an Adiabatic process

The entropy of pure substance can be considered as a function of any two variable T and V as

$$\begin{aligned} S &= S(T,V) \qquad (5)\\ dS &= \left(\frac{\partial S}{\partial T}\right)_V dT + \left(\frac{\partial S}{\partial V}\right)_T dV. \end{aligned}$$

Multiply both sides by T we get,

$$TdS = T\left(\frac{\partial S}{\partial T}\right)_V dT + T\left(\frac{\partial S}{\partial V}\right)_T dV. \qquad (6)$$

Since $dQ = nC_V dT$ and $TdS = dQ$ for a reversible isochoric process, from the above equation one can obtain

$$T\left(\frac{\partial S}{\partial T}\right)_V = nC_V, \qquad (7)$$

where C_V is the specific heat capacity at constant volume. According to Maxwell's third thermodynamic relation

$$\left(\frac{\partial S}{\partial V}\right)_T = \left(\frac{\partial P}{\partial T}\right)_V. \qquad (8)$$

Therefore Eq.(6) becomes

$$TdS = nC_V dT + T\left(\frac{\partial P}{\partial T}\right)_V dV. \qquad (9)$$

For an adiabatic process $dQ = TdS = 0$, hence

$$nC_V dT = -T\left(\frac{\partial P}{\partial T}\right)_V dV. \qquad (10)$$

Using Eq.(3), one can obtain

$$\left(\frac{\partial P}{\partial T}\right)_V = \frac{nR}{(V-nb)}. \qquad (11)$$

Therefore Eq.(10) becomes

$$\begin{aligned} nC_V dT &= -T\frac{nR}{(V-nb)}dV \qquad (12)\\ \frac{1}{T}\,dT &= -\frac{R}{C_V}\frac{dV}{(V-nb)}. \end{aligned}$$

Integrating the above equation we get

$$\ell n\ T = -\frac{R}{C_V}\,\ell n\ (V-nb) + \ell n\ z, \qquad (13)$$

where ℓnz is an integrating constant. Rearranging the above equation one can get

$$T(V-nb)^{\frac{R}{C_V}} = z. \qquad (14)$$

Combining Eq.(3) and Eq.(14) one can obtain Van der Waal's gas equation for an adiabatic process as

$$\left(P + \frac{n^2 a}{V^2}\right)(V-nb)^{\Gamma} = K, \qquad (15)$$

where $\Gamma = \frac{R}{C_V} + 1$ and $K = nRz$ = a constant. It should be noted that, for real gas $\Gamma \neq \gamma = \frac{C_P}{C_V}$ of an ideal gas, where C_P is the specific heat capacity at constant pressure. Thus, it would be interesting to obtain the relation between the C_P and C_V of the Van der Waal's gas as follows.

2.1 Relation between C_P and C_V for Van der Waal's gas

The internal energy of a given system can be considered as a function of any two variable

T and V as

$$\begin{aligned} U &= U(T,V) & (16)\\ dU &= \Big(\frac{\partial U}{\partial T}\Big)_V dT + \Big(\frac{\partial U}{\partial V}\Big)_T dV. \end{aligned}$$

Using the above equation, the first law of thermodynamics in an infinitesimal form $dQ = dU + dW$ with $dW = -PdV$, can be written as

$$dQ = \Big(\frac{\partial U}{\partial T}\Big)_V dT + \Big(\frac{\partial U}{\partial V}\Big)_T dV - PdV. \quad (17)$$

In our study we have used the sign convention that the work done on the system is taken as positive and the work done by the system is taken as negative. For constant volume $dV = 0$, the above equation becomes,

$$nC_V = \Big(\frac{\partial U}{\partial T}\Big)_V. \quad (18)$$

Since $dQ/dT = nC_V$ for constant volume and $dQ/dT = nC_P$ for constant pressure, Eq.(17) can be rewritten as

$$dQ = nC_V dT + \Big(\frac{\partial U}{\partial V}\Big)_T dV - PdV \quad (19)$$

$$nC_P dT = nC_V dT + \Big(\frac{\partial U}{\partial V}\Big)_T dV - PdV \quad (20)$$

$$n(C_P - C_V) = \Big\{\Big(\frac{\partial U}{\partial V}\Big)_T - P\Big\}\frac{dV}{dT}. \quad (21)$$

From the first thermodynamic potential $dU = TdS + PdV$ and using Eq.(17) and Eq.(8) at constant temperature one can obtain

$$\begin{aligned} \Big(\frac{\partial U}{\partial V}\Big)_T &= T\Big(\frac{\partial S}{\partial V}\Big)_T + P & (22)\\ &= T\Big(\frac{\partial P}{\partial T}\Big)_V + P. & (23) \end{aligned}$$

Then Eq.(21) becomes

$$n(C_P - C_V) = T\Big(\frac{\partial P}{\partial T}\Big)_V \frac{dV}{dT}. \quad (24)$$

If V is a function of T and P, then change in V for a constant pressure is

$$dV = \Big(\frac{\partial V}{\partial T}\Big)_P dT + \Big(\frac{\partial V}{\partial P}\Big)_T dP. \quad (25)$$

$$\frac{dV}{dT} = \Big(\frac{\partial V}{\partial T}\Big)_P. \quad (26)$$

From Eq.(3) on can obtain

$$\Big(\frac{\partial P}{\partial T}\Big)_V = \frac{nR}{(V - nb)}, \quad (27)$$

$$\Big(\frac{\partial V}{\partial T}\Big)_P = nRV^3(V - nb)G^{-1}, \quad (28)$$

where $G = V^3 nRT - 2n^2 a(V - nb)^2$. Therefore Eq.(24) can be written as

$$C_P - C_V = \frac{R}{f_v}, \quad (29)$$

where

$$f_v = \Big\{1 - \frac{2na}{V^3 RT}(V - nb)^2\Big\}. \quad (30)$$

We have obtained the relation between the C_P and C_V of Van der Waals gas. Divide Eq.(29) throughout by C_V we get

$$\frac{C_P}{C_V} = 1 + \frac{R}{f_v C_V} = 1 + \frac{\Gamma - 1}{f_v}. \quad (31)$$

Thus we have finally obtained the relation between γ of ideal gas and Γ of Van der Waal's gas as

$$\gamma = 1 + \frac{\Gamma - 1}{f_v}. \quad (32)$$

There has been few studies to find out the efficiency of the Carnot cycle whose working substance is different from ideal gases [5, 6, 7]. In what follows, we employ simple approach to find out the efficiency of the Carnot engine whose working substance obeys the Van der Waal's equation of state.

3 Carnot engine efficiency for Van der Waal's gas

Efficiency of the Carnot engine, η, is defined as the ratio of the net work done to the heat absorbed in the Carnot cycle. As discussed earlier, this reversible cycle consist of four processes such as i) adiabatic compression ii) isothermal expansion iii) adiabatic expansion and iv) isothermal compression. In order to find out η, we calculate the total work done during the Carnot cycle as follows.

3.1 Work done in an adiabatic compression

In this process, the volume changes from V_1 to V_2 $(V_1 > V_2)$, the pressure changes from P_1 to P_2 and the temperature from T_L to T_H. There is no heat exchange between the system and the surroundings. The work done during this process W_1 is given by,

$$W_1 = -\int_{V_1}^{V_2} PdV. \qquad (33)$$

The Van der Waal's equation for an adiabatic process obtained in Eq.(15) as

$$\left(P + \frac{n^2 a}{V^2}\right)(V - nb)^{\Gamma} = K. \qquad (34)$$

$$P = \frac{K}{(V - nb)^{\Gamma}} - \frac{n^2 a}{V^2}. \qquad (35)$$

Substitute Eq.(35) in Eq.(33) and integrating, we get

$$W_1 = -\frac{K(V - nb)^{1-\Gamma}}{1 - \Gamma}\Bigg|_{V_1}^{V_2} - \frac{n^2 a}{V}\Bigg|_{V_1}^{V_2},$$

$$\begin{aligned} W_1 &= \frac{K(V_1 - nb)^{1-\Gamma} - K(V_2 - nb)^{1-\Gamma}}{1 - \Gamma} \\ &- \frac{n^2 a}{V_2} + \frac{n^2 a}{V_1}. \end{aligned}$$

The Van der Waal's equation of state for the system in the initial state (P_1, V_1) at T_L is

$$\left(P_1 + \frac{n^2 a}{V_1^2}\right)(V_1 - nb) = nRT_L \qquad (36)$$

and for the system in the final state (P_2, V_2) at T_H as

$$\left(P_2 + \frac{n^2 a}{V_2^2}\right)(V_2 - nb) = nRT_H. \qquad (37)$$

From the Van der Waal's equation (Eq.34) for the adiabatic process, we can relate the system in the initial state (P_1, V_1, T_L) and final state (P_2, V_2, T_H) as

$$\frac{\left(P_1 + \frac{n^2 a}{V_1^2}\right)}{\left(P_2 + \frac{n^2 a}{V_2^2}\right)} = \frac{(V_2 - nb)^{\Gamma}}{(V_1 - nb)^{\Gamma}} \qquad (38)$$

Substitute Eq.(36) and Eq.(37) in the above equation, we get

$$\frac{nRT_L}{(V_1 - nb)^{1-\Gamma}} = \frac{nRT_H}{(V_2 - nb)^{1-\Gamma}} \equiv K. \qquad (39)$$

Therefore,

$$K(V_1 - nb)^{1-\Gamma} = nRT_L \qquad (40)$$

$$K(V_2 - nb)^{1-\Gamma} = nRT_H \qquad (41)$$

and hence the work done in an adiabatic compression becomes

$$W_1 = \frac{nR(T_L - T_H)}{1-\Gamma} - \frac{n^2a}{V_2} + \frac{n^2a}{V_1}. \qquad (42)$$

3.2 Work done in an isothermal expansion

In this process, the system undergoes volume expansion V_2 to V_3 and the pressure change from P_2 to P_3, while the temperature remains constant at T_H. During this process the system absorbs Q_H amount of heat energy from the hot reservoir, then the work done,

$$W_2 = -\int_{V_2}^{V3} PdV. \qquad (43)$$

For a reservoir temperature T_H, Eq.(3) can be written as,

$$P = \frac{nRT_H}{V-nb} - \frac{n^2a}{V^2} \qquad (44)$$

Substitute the above equation in Eq.(43) and integrating, we get

$$W_2 = nRT_H \ell n \left(\frac{V_2 - nb}{V_3 - nb}\right) - \frac{n^2a}{V_3} + \frac{n^2a}{V_2}. (45)$$

From the Van der Waal's equation of state (Eq.3), we can relate the system in the initial state (P_2, V_2) and final state (P_3, V_3) at a fixed temperature T_H as

$$\frac{\left(P_2 + \frac{n^2a}{V_2^2}\right)}{\left(P_3 + \frac{n^2a}{V_3^2}\right)} = \frac{(V_3 - nb)}{(V_2 - nb)}. \qquad (46)$$

Substitute Eq.(46) in Eq.(38), then

$$\frac{P_1 + \frac{n^2a}{V_1^2}}{P_3 + \frac{n^2a}{V_3^2}} = \frac{(V_3 - nb)(V_1 - nb)^{-\Gamma}}{(V_2 - nb)^{1-\Gamma}}. \qquad (47)$$

3.3 Work done in an adiabatic expansion

As similar to adiabatic compression, the heat exchange in an adiabatic expansion is zero. As the system expands from V_3 to V_4, the pressure changes from P_3 to P_4, and the temperature changes from T_H to T_L, then the work done W_3 during this process is given by,

$$W_3 = -\int_{V_3}^{V_4} PdV. \qquad (48)$$

Substitute Eq.(35) for an adiabatic process in the above equation, we get

$$\begin{aligned} W_3 \;=\; & \frac{K(V_3 - nb)^{1-\Gamma} - K(V_4 - nb)^{1-\Gamma}}{1-\Gamma} \\ & - \frac{n^2a}{V_4} + \frac{n^2a}{V_3}. \end{aligned}$$

The Van der Waal's equation of state for the system in the initial state (P_3, V_3) at T_H is

$$\left(P_3 + \frac{n^2a}{V_3^2}\right)(V_3 - nb) = nRT_H \qquad (49)$$

and for the system in the final state (P_4, V_4) at T_L as

$$\left(P_4 + \frac{n^2a}{V_4^2}\right)(V_4 - nb) = nRT_L. \qquad (50)$$

From the Van der Waal's equation (Eq.34) for the adiabatic process, we can relate the system in the initial state (P_3, V_3, T_H) and final state (P_4, V_4, T_L) as

$$\frac{\left(P_3 + \frac{n^2a}{V_3^2}\right)}{\left(P_4 + \frac{n^2a}{V_4^2}\right)} = \frac{(V_4 - nb)^{\Gamma}}{(V_3 - nb)^{\Gamma}}. \qquad (51)$$

Substitute Eq.(49) and Eq.(50) in the above equation, we get

$$\frac{nRT_H}{(V_3-nb)^{1-\Gamma}} = \frac{nRT_L}{(V_4-nb)^{1-\Gamma}} \equiv K. \quad (52)$$

Therefore,

$$K(V_3-nb)^{1-\Gamma} = nRT_H \quad (53)$$

$$K(V_4-nb)^{1-\Gamma} = nRT_L \quad (54)$$

and hence the work done in an adiabatic expansion becomes

$$W_3 = \frac{nR(T_H-T_L)}{1-\Gamma} - \frac{n^2a}{V_4} + \frac{n^2a}{V_3}. \quad (55)$$

3.4 Work done in an isothermal compression

In this process, the pressure changes from P_4 to P_1, the volume changes from V_4 to V_1 and Q_L amount of heat energy rejected to a cold reservoir at constant temperature T_L. Work done during this process W_4 is given by

$$W_4 = -\int_{V_4}^{V1} PdV. \quad (56)$$

For a reservoir temperature T_L, Eq.(3) can be written as,

$$P = \frac{nRT_L}{V-nb} - \frac{n^2a}{V^2} \quad (57)$$

Substitute the above in equation in Eq.(56) and integrating, we get

$$W_4 = nRT_L\ell n\left(\frac{V_4-nb}{V_1-nb}\right) - \frac{n^2a}{V_1} + \frac{n^2a}{V_4}. \quad (58)$$

From the Van der Waal's equation of state (Eq.3), we can relate the system in the initial state (P_4, V_4) and final state (P_1, V_1) at a fixed temperature T_L as

$$\frac{\left(P_4+\frac{n^2a}{V_4^2}\right)}{\left(P_1+\frac{n^2a}{V_1^2}\right)} = \frac{(V_1-nb)}{(V_4-nb)}. \quad (59)$$

Substitute Eq.(59) in Eq.(51), then

$$\frac{P_3+\frac{n^2a}{V_3^2}}{P_1+\frac{n^2a}{V_1^2}} = \frac{(V_1-nb)(V_3-nb)^{-\Gamma}}{(V_4-nb)^{1-\Gamma}}. \quad (60)$$

3.5 Efficiency of the engine

The net work done W_{net} for one complete cycle is $W_{net} = W_1+W_2+W_3+W_4$. Therefore, the total work done for the Carnot cycle is given by

$$W_{net} = w_H + w_L, \quad (61)$$

where

$$w_H = nRT_H\ell n\left(\frac{V_2-nb}{V_3-nb}\right) \quad (62)$$

$$w_L = nRT_L\ell n\left(\frac{V_4-nb}{V_1-nb}\right). \quad (63)$$

According to the first law of thermodynamics $Q_{net} - W_{net} = \Delta U$, where $Q_{net} = Q_H - Q_L$ is the net heat energy exchange between the system and the reservoir and ΔU is the change in the internal energy. Here we have used the sign convention that the heat energy flow in to the system is taken as positive and the heat energy flow out of the system is taken as negative. For a cyclic process, the change in internal energy ΔU is zero. Therefore, the net heat energy exchange between the system and the reservoir in a given cycle is completely converted in to net work done which is given by

$$W_{net} \quad = \quad Q_H - Q_L. \tag{64}$$

In the Carnot cycle, all the absorbed heat Q_H enters the system at a constant high temperature T_H and all the rejected heat Q_L leaves the system at a constant low temperature T_L. Hence, comparing Eq.(61) and Eq.(64), one can identify

$$Q_H = \left|w_H\right| = \left| nRT_H \ell n \left(\frac{V_2 - nb}{V_3 - nb}\right) \right| \tag{65}$$

$$-Q_L = \left|w_L\right| = \left| nRT_L \ell n \left(\frac{V_4 - nb}{V_1 - nb}\right) \right|. \tag{66}$$

It should be noted that Q can also be obtained from other approaches. Using Eq.(23) and Eq.(27) for an isothermal process, Eq.(17) becomes

$$dQ = T\Big(\frac{\partial P}{\partial T}\Big)_V dV = \frac{nRT}{(V - nb)} dV.$$

Integrating the above equation from the initial volume V_i to the final volume V_f, one can obtain the amount of heat transferred between the system and the sorrounding as

$$Q = nRT \ell n (V - nb)\Big|_{V_i}^{V_f}.$$

The efficiency of the engine obtained from Eq.(2) as

$$\eta = 1 - \frac{Q_L}{Q_H} = 1 + \frac{T_L \ \ell n \left(\frac{V_4 - nb}{V_1 - nb}\right)}{T_H \ \ell n \left(\frac{V_2 - nb}{V_3 - nb}\right)}.$$

The above equation can be rewritten as

$$\eta \quad = \quad 1 - \frac{T_L \ \ell n \left(\frac{V_4 - nb}{V_1 - nb}\right)}{T_H \ \ell n \left(\frac{V_3 - nb}{V_2 - nb}\right)}. \tag{67}$$

In order to simply the above equation, substitute Eq.(60) in Eq.(47) and rearranging, we get

$$\left(\frac{V_3 - nb}{V_2 - nb}\right)^{1-\Gamma} = \left(\frac{V_4 - nb}{V_1 - nb}\right)^{1-\Gamma}.$$

So,

$$\left(\frac{V_3 - nb}{V_2 - nb}\right) = \left(\frac{V_4 - nb}{V_1 - nb}\right) \tag{68}$$

Therefore, Eq.(67) reduces to

$$\eta = 1 - \frac{T_L}{T_H}. \tag{69}$$

Thus, we used Van der Waal's gas as a working substance and obtained the efficiency of the Carnot engine which is independent of the working substance.

4 Conclusion

In summary, we have obtained the Van der Waal's equation for the adiabatic process as $\left(P + \frac{n^2 a}{V^2}\right)(V - nb)^{\Gamma}$ = constant. Our result explicitly shows that Γ of the Van der Waal's gas is different from γ of ideal gas for adiabatic process. This equation has been used directly in Carnot cycle for the adiabatic process and shown that the efficiency of the Carnot engine is independent of the working substance. For this calculation we have used the simple approach as similar to the ideal gas usually found in the undergraduate text books. With this we find out the efficiency of the Carnot engine whose working substance obeys Van der Waal's equation of state $\left(P + \frac{n^2 a}{V^2}\right)(V - nb) = nRT$. Using the above two equations, we have also shown that the alternative Van der Waal's equation for an adiabatic process is $T(V - nb)^{\Gamma-1} =$ constant. We can also write the above relation as $\left(P + \frac{n^2a}{V^2}\right) T^{\frac{\Gamma}{1-\Gamma}} =$ constant.

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Restoring Force for a Slinky's Fundamental Oscillation

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Abstract

A Slinky's fundamental oscillation is the lowest order standing longitudinal wave the Slinky supports. The frequency is determined by solving a transcendental equation obtained from a wave equation solution. To evaluate the frequency a so-called "Slinky effective mass" is employed in contrast of the fact a Slinky has a well defined mass. The solution's mathematical complexity obscures a significant Slinky physical property to find the fundamental frequency: The Slinky's center-of-mass restoring force is produced by only the coils between the support and the center of mass. Experimental evidence is presented to verify the aforementioned property.

1. Introduction

In previous works dealing with Slinky oscillation frequencies, the Slinky is modeled as a continuous mass distribution undergoing longitudinal wave motion [1-8]. In general, the model does not incorporate some of the Slinky's obvious features such as the number of coils, the fact their separation decreases with increasing displacement from the support, and the fact the mass per unit length is not constant [2] . In addition, a so-called effective mass is introduced despite the fact the Slinky mass is well defined. For these reasons, a Slinky center-of-mass model (hereafter COM) is adopted as a series configuration of equivalent single coil springs. The model takes into account the number of coils, their variable separations and the Slinky's distinct mass. The first four sections discuss the specifics of the Slinky used for the experimental data, the physical rational for the COM model and its properties. The remaining sections discuss the experimental procedures and their results and the conclusion.

The major physical conclusion from the experimental evidence here is to determine a constraint or physical justification for neglecting the spring's mass in simple harmonic motion analysis. In general, the analysis is of a two-body problem with two equations of motion for the simultaneous motion of both the spring and the attached mass. Introduction of the massless spring approximation reduces the analysis to a simple one-body equation of motion for the attached. However there is no discussion of any physical constraints or restrictions in order for the approximate solution to be valid. The conclusion here is a physical criterion for the validity of the approximation: The system's COM must be at or below the spring's bottom coil.

2. The Slinky

The Slinky is a Poof-Slinky (www.poof-slinky.com) of 206 grams with 84 coils. Each coil has a thickness of 0.7 mm and a mass of 2.45 grams. Two coils are clipped together for support at each end. The two top coils do not participate in the oscillatory motion, they are used to support the hanging Slinky. The two coils at the bottom are included in the attached mass. Close inspection of all the Slinky coils indicate they are members of one of two groups [9]. The $N_f$free coils of the top group are visually separated whereas the lower group of N_a coilsare not. The physical reason for the two groups is that near the spring's bottom the mass of the lower coils is not sufficient to produce a visible separation. These few coils move in tandem during the oscillation. They behave as a single mass attached to the end of the free coils. Hence, the lower group is referred to as the attached Na coils. Their group integrity (hereafter the attached mass) is maintained by placing two small zip-ties around them. The set of $N_f$free coils and the set of N_a bound or attached coils are referred to as the Slinky. In the event the attached mass is not a set of bound coils, N_a is the equivalent number of coils given by $N_a = M_a/m_c$, where M_a is the attached mass and m_c is the mass of one coil. Only the free coils, all or inpart, contribute to the restoring force. However all the coils, both free and attached, contribute to the oscillating Slinky's mass.

3. Rational for the Center of Mass Model

The classic solution of an oscillating mass attached to a spring is an oversimplification of the physical arrangement because both the spring and attached mass oscillate. In format terms, it is a two-body problem. The classic solution assumes the spring is massless which simplifies it into a one-body problem. One approach to the two-body problem is to consider only the fundamental oscillation of both the spring and the mass. In this particular case, all coils oscillate in phase; hence, the coils and the Slinky's COM oscillate with the same frequency. Both are taken into consideration by focusing our attention on only the COM oscillation. Of principle interest is the restoring force acting upon the COM which accounts for both the motion of the attached mass and the spring.

The present analysis begins with the physical interpretation of ω^2 expressed by Crawford[10] which is

$$\omega^2 = F / x M \qquad (1)$$

In the present case, F is COM restoring force, x is the COM displacement from equilibrium. And oscillating mass M is the sum of the masses of the free (N_f) and attached coils (N_a).

4. Center of Mass Model's Properties.

We adopt the scheme initially put forth by Sawicki[11] to model the Slinkyas a configuration of identical Hooke's Law coils, where each coil supports the weight of all the coils below it. Figure 1 illustrates the Slinky segments described below. Hooke's Law applied to the i-th free coil yields.

$$k_c S_i = m_c \, g \, (N_f - i) + N_a m_c g \, , \qquad (2)$$

Where k_c and m_c are the spring constant and mass of one coil. S_i is the separation between the i-th coil's top and bottom. The displacement D_j to the bottom of the j-th free coil from the top support is obtained by summing S_i from i=1 to i=j. Using the integer summation identity$\sum_1^j i$ = (j/2) (j+1), the result is

$$D_j = \Sigma_1^j S_i = (g/\omega_c^2)((N_f + N_a)j - (j/2)(j+1)) \quad (3)$$

where$\omega^2 = k_c/m_c$, and ω^2 is the angular frequency of one coil. The factor g/ω^2has units of length and is therefore taken as a Slinky natural length and is set equal to the parameter δ.

The value of δ is determined by recognizing the Slinky's hanging length from the support to the bottom of the free coils $L_f$is the displacement to the N_f free coil. We solve for δ which satisfies

$$L_f = \delta \, ((N_f + N_a) \, N_f - (N_f/2)(N_f+1)), \qquad (4)$$

Where, N_f = 70, N_a = 10, and L_f = 1.27 m we obtain δ =0.40 mm. By way of observation δ appears to be about one-half with thickness of a Slinky coil.

The angular frequency ω for one coil is 155 rad/sec or 24.7 Hz. The corresponding single coil spring constant k_c is equal to 59 N/m as determined from the single coil mass of 2.45 grams.

The expression for the Slinky's COM, D_{com} is obtained in a straight forward fashion using the expression for the COM of the free coilsD_{Nf}, the COM of the attached coilsD_a, and isexpressed by

$$D_{com} = (D_{Nf} N_f + N_a D_a)/(N_f + N_a) . \qquad (5)$$

The expression for D_{Nf} is evaluated using the definition of the COM and summation identity

$$\sum_1^j i^2 = \text{(j/6)(j+1)(2j+1)}.$$

The result is

$$D_{Nf} = \delta((N_f+1)/2)\ (2/3)((N_f-1)+\text{Na}) \qquad (6)$$

The displacement of the COM of the attached coils is expressed by

$$D_a = L_f + (\text{cw}/2)\ N_a, \qquad (7)$$

Where cw is the coil thickness of 0.7 mm.

5. The Experimental Procedure

The COM Slinky model is a series configuration of individual identical coils each with spring constant k_c , mass m_c with a corresponding single coil oscillation frequency ω^2 . The series spring constant K_j for a configuration of j free coils is expressed as [12]

$$K_j = k_c/j \qquad (8)$$

For data taking purposes, the Slinky is partitioned into five different configurations corresponding to 20,30,40,50, and 60 free coils and in each configuration N_a =10 coils. The remaining coils were tied together above the free coils using zip-ties. For each configuration the fundamental frequency ω_j is measured and recorded in Table 1.

An experimental value for the series spring constant of j free coils ,K_j^* is obtained from Eq.(1). Hence, the expression for the experimental spring constant is given by

$$K_j^* = \omega_j^2 M_j = \omega_j^2\ ((N_f + N_a)\ m_c) \qquad (9)$$

Where the last factor $((N_f + N_a)\ m_c)$ is the well defined oscillating mass and ω is the observed oscillation frequency. The experimental values are shown in column three of Table 1.

At specific issue here is how many individual coils J^* in series are responsible for the experimental series spring constant K_j^* ? The number of coils J^* is obtained from Eq.(8) which yields,

$$J^* = k_c\ /\ K_j^* \qquad (10)$$

The corresponding J^* values are shown in column four of Table 1.

The important question is: Which of the given N_f free coils correspond to the J^* coils providing the restoring force?

6. Results and Discussion.

For a given configuration in the COM model, only two forces act upon the COM, the restoring force responsible for the oscillation and the weight. The weight is a constant force and has no influence upon the oscillation frequency. From a simple physical point of view we assume the only coils producing the restoring force are those between the COM and the support. To investigate the assumption two quantities are needed for each configuration of N_f coils. First, is the displacement D_{com} from the COM to the support obtained from Eq.(5). Second is the displacement D_j^* of the corresponding J^* coils from the support point obtained from Eq.(3). Both are evaluated and presented in the fifth and sixth columns in Table 1.

7. Conclusion.

Table 1 displays for each free coil configuration N_f the two corresponding displacements D_{com} and D_j. The average percentage error between the two values is about 5% which is taken to be in good agreement with the assumption only the coils between the COM and the support provide the restoring force. This conclusion provides the physical constraint for the validity of the massless spring approximation. Namely it is valid only so long as the system's COM is at or below the spring's bottom coil.

TABLE 1. The first column displays the number of free coils N_f. The attachedcoils N_a is 10 for all cases. The second column displays the observed fundamental frequency ω_j.Using Eq.(3), the third column contains the corresponding experimental series spring constant K_j^*.Equation (10) is used to determine for the fourth column the number of coils J^* necessary to produce the corresponding spring constant K_j^*. Column five displays$D_j^*$the displacement of the J^* coils from the support to the COM found from Eq.(3). Column six displays the Slinky's COM displacement D_{com} from the support using Eq.(5).

N_f	ω_j	K_j^*	J^*	D_j^*	D_{com}
Coils	**(rad/sec)**	**(N/m)**	**Coils**	**(m)**	**(m)**
20	8.29	5.05	11.7	0.11	0.12
30	6.15	3.71	15.9	0.21	0.20
40	4.96	3.03	19.6	0.31	0.34
50	4.14	2.52	23.4	0.46	0.47
60	3.58	2.20	26.8	0.62	0.61

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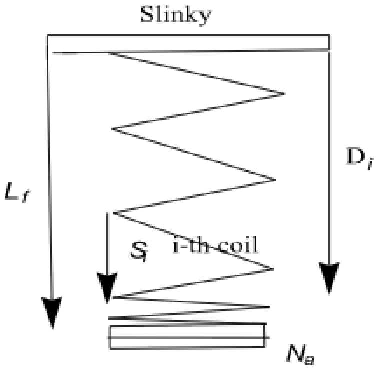

Figure 1. Diagram of a Slinky where the hanging length is measured from the support to the top of the attached mass (with coils), the i-th coil separation is from its top to the bottom, and the i-th coil displacement is from the support to the bottom of the i-th coil.

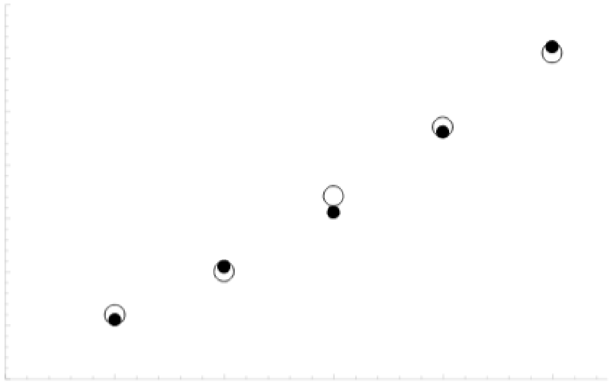

Figure 2. A plot of the displacements, (filled circles) and (open circles) vs the number of free coils producing the Slinky’s oscillations. Both circles have been enlarged for visibility.

Stacking 2-D Lattices to Construct 3-D Bravais Lattices

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Abstract

In this paper, an activity has been proposed to construct 3-Dimensional(3-D) Bravais lattices, based on the idea of stacking 2-D Bravais lattices. AA and AB stacking of 2-D square lattices result in simple cubic and body-centered cubic structures respectively. Extending these stacking ideas to other 2-D Bravais lattices results in the construction of all 3-D Bravais lattices. While AA stacking of oblique, square and regular centered hexagonal lattices results in monoclinic, cubic and hexagonal lattices respectively, AA stacking of rectangular lattice gives rise to the formation of orthorhombic and tetragonal lattices and that of centered rectangular yields side-centered orthorhombic. Similarly, AB stacking of oblique and square lattices gives body-centered monoclinic and body-centered cubic lattice and that of rectangular gives body centered orthorhombic and body centered tetragonal lattices. Moreover, AB stacking of centered rectangular lattice results in face-centered orthorhombic, and that of square lattice with special conditions imposed on the height of stacking yields face-centered cubic lattice. In addition to these, ABC stacking of centered regular hexagonal lattice gives rise to trigonal lattice with rhombohedral primitive unit cell.

1 Introduction

One of the major challenges faced by students is to learn the art of abstraction. An activity has been proposed previously by us [1], for arriving at the five 2-D Bravais lattices based on the seven types of triangles. In this paper, we extend the activity to construct the 3-D Bravais lattices by stacking the 2-D Bravais lattices, taking inspiration from graphene [2](that has been peeled out layer by layer from graphite).

3-D Bravais lattices play an important role in understanding about crystal structure. Even though many of these 14 Bravais lattices are non-primitive, they are the preferred unit cells for description of crystal structure for two reasons. Firstly, they are easier to visualize as compared to the primitive cells associated with them. Secondly, most of them allow easy tessellation along three specific directions, resulting in expression of the inherent translational symmetry using simple mathematical formula[3, 4].

Since the discovery of fourteen Bravais lattices, physicists have been trying to propose various methods to realize these in physical form. Based on the previous work of Langmuir & Nelson[5], Patterson[6] has probed the results of close packing of spheres, which the former authors have proposed to achieve through boxes with plane walls. It has been deduced, that there exist fifteen possible arrangements, classified on the basis of either symmetries or on the basis of the contacts made by the spheres with their neighbors. Ten 3-D Bravais lattices have been obtained through these fifteen arrangements. In the book, *Crystallography: An Introduction*[7], an attempt has been made to stack the 2-D Bravais lattice planes, but the effort has been limited to constructing primitive unit cells. Moreover, point group symmetries have been employed to attain the remaining cells. Similar endeavor has been taken up by Muecklich [8], but once again point group symmetries have been used. Here, we intend to utilize simple physical considerations while stacking the planes without too much emphasis on point group symmetries.

In the next section we deliberate on the thought process, that has evolved into developing the idea of stacking 2-D planes.

2 Rationale for Stacking

The main conceptual idea behind construction of a lattice is to identify the points in space in such a way that by standing at any one of the arbitrary points belonging to it, one would always see the same environment all around. Such a structure requires to have an inbuilt order and symmetry. In general, we look for translational symmetry so that it is easy to express such a structure using mathematical formulas.

2.1 Covering 2-D space

To obtain the set of lattices in 2-D, we look for the smallest unit that can be enclosed by a set of points which covers an area (or 2-D space) and then tessellate the figure obtained (by connecting the points by straight lines) along two directions to cover a 2-D planar surface. Even though only 3 non-collinear points in the form of a triangle are enough to enclose such an area, a triangle cannot be simply tessellated along 2-D to cover a plane as a triangle would need to be reflected or rotated for this task. Hence, we have constructed different quadrilaterals using the seven classes of triangles and arrived at the five unique units that can be easily tessellated to cover a 2-D space[1]. These have been referred to as 2-D Bravais lattices.

2.2 Covering 3-D space

Using a similar argument, the smallest 3-D space can be enclosed by using only 4 points (3 non-collinear points in a plane and one point chosen anywhere out of the plane) that forms a pyramidal structure. Once again, it is neither easy to visualize pyramidal stacking, nor is it possible to tessellate these structures conveniently in 3 directions to obtain a lattice structure in 3-D space that would have the required translational symmetry.

Another option is to try and construct parallelepipeds by appropriate rotation and reflection of various available pyramidal structures as was done in 2-D case. However we are not utilizing the effort put into obtaining the 2-D lattices that allowed us to tessellate in 2-directions. So for easy tessellation in 3 specific directions to cover a 3-D space, one must chose two or more planes associated with one of the five 2-D Bravais lattices, and stack them one over the other to obtain parallelepipeds/cuboids wherever possible.

In standard texts,[3, 4] to understand fcc and hcp closed packed structures, we assume that the spheres of equal sizes are placed adjacent to each other such that they touch one another in a plane. Then more balls are placed either on the existing balls or in the gaps resulting in various stacking methods AA, ABAB or ABCABC. This model has the disadvantage of creating only sc, bcc, fcc and hcp structures. This is so, because of the assumption that the spheres have to touch one another. This automatically limits the stacking to two types:

- AA and AB stacking of square lattices, which results in sc and bcc structures respectively.
- ABAB and ABCABC stacking of rhombic (type-2 [1]) lattices, that gives rise to hcp and fcc structures respectively.

This concept of AA and AB stacking has been extended to all five 2-D Bravais lattices in order to construct twelve 3-D Bravais lattices. ABC stacking of equilateral triangular lattices (subset of regular centered hexagonal lattice) results in trigonal lattice.

3 Constructing 3-D Bravais Lattices

One of the simplest and straight forward ways is to stack the most general 2-D Bravais lattice, the oblique plane lattice with no specific conditions imposed. This results in most general space lattice, which can be tessellated in order to generate a 3-D periodic array of points. This primitive unit cell in Fig. 1 corresponds to the 3-D Bravais lattice known as **triclinic**, and includes all remaining lattices as its special cases. Boric acid powder, which is used on carrom boards, and copper sulphate which is used for dying purposes, are common day to-day examples which exist in this structure.

The formation of the remaining lattices by AA and AB stacking is discussed subsequently and the resulting lattices are presented in Table 1.

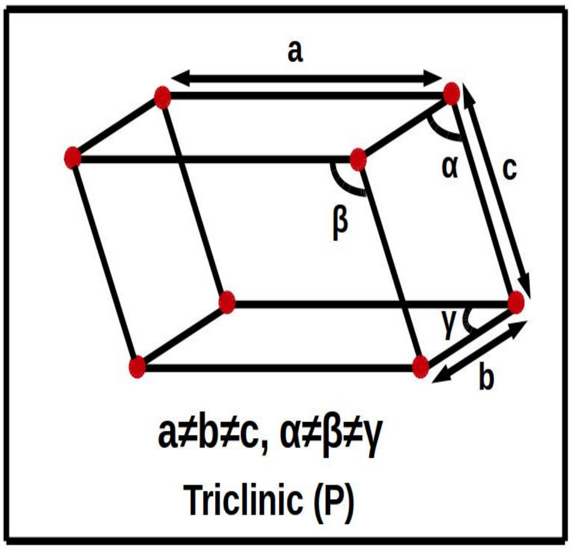

Figure 1: Random Stacking of Oblique Plane Lattices

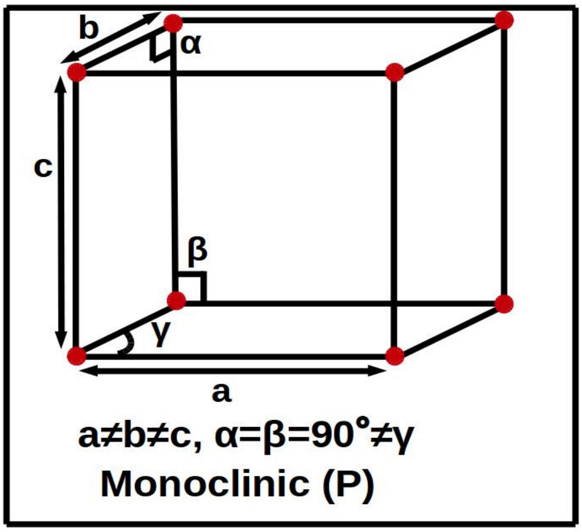

Figure 2: AA Stacking

3.1 AA Stacking: Primitive Crystal lattices

Figure 2 shows A-A stacking of two Oblique plane lattices, exactly one over the other as this would yield a primitive unit cell which has the advantage of being tessellated in two perpendicular directions. The cell and its parameters correspond to **monoclinic (primitive)** Bravais lattice in 3-D. Here, 'c' is the perpendicular distance between the two planes, while 'α' and 'β' are the angles between sides 'b' and 'c', and sides 'c' and 'a' respectively. It is important to note that distance 'c' may or may not be equal to any one of the sides of the base plane, but the resultant cell would be monoclinic in both cases. Sugar, most commonly used sweetener, crystallizes in the form of anhydrous prisms on oblique axes, is in monoclinic structure.

The following is a listing of AA stacking of the five 2-D Bravais lattices resulting in 5 primitive unit cells. The numbers in the parenthesis next to a resultant lattice, are given to keep track of the total expected 14 Bravais lattices.

- Oblique lattice for both cases of height 'c' gives monoclinic primitive unit cell(2)

- Rectangular lattice with 'c' unequal to either sides of the base plane gives orthorhombic primitive unit cell(3), and same lattice with 'c' equal to either sides of the base plane gives tetragonal primitive unit cell (4).

- Square lattice with 'c' unequal to either sides of the base plane gives tetragonal primitive unit cell (4) and with 'c' equal to either sides of the base plane gives cubic primitive unit cell (5)

- Regular centered hexagonal with 'c' unequal or equal to either sides of the base plane gives hexagonal primitive unit cell (6)

While crystal form of Sulphur is an example corresponding to orthorhombic structure, Zircon crystal possesses tetragonal structure. Interestingly, Polonium happens to be only monoatomic simple cubic crystal in the entire periodic table. Cesium chloride (CsCl), which is used for cancer therapy, is an example of diatomic simple cubic structure. In this, there are two interpenetrating simple cubic lattices, of cesium and chlorine (with Cs at (0,0,0) and Cl at $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$). The non-primitive unit cell for this could be visualized as a bcc with cesium ions at the corners and the chlorine ion at the body-center or vice-versa. Gems like ruby, emerald and sapphire are all having simple hexagonal structure with eight surfaces.

AA stacking of centered rectangular lattice, with either c≠a and c≠b or c=a (or c=b), would lead to orthorhombic side centered or orthorhombic C-centered lattice (8).

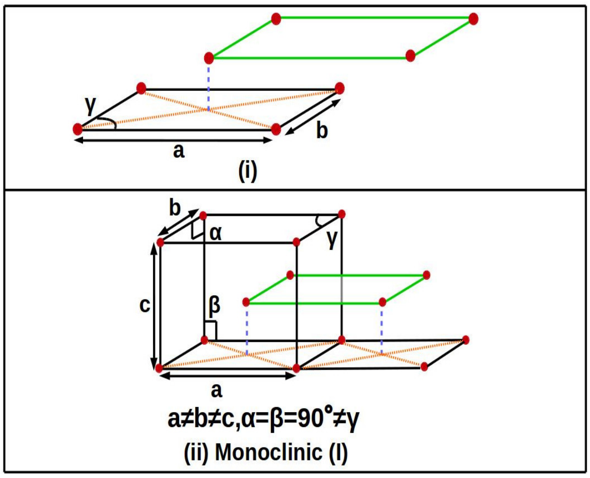

Figure 3: (i)AB Stacking & (ii)Extending AB Stacking

3.2 AB Stacking: Body Centered Lattices

In the second method of stacking, the planes are placed over each other in such a way that the lattice points of the second (or upper) plane would be centered to those of the first plane below. In Fig. 3(i) A-B stacking has been shown, where the placement of second oblique plane over the first one is such that the vertex of the upper plane lies exactly over the point of intersection of the two diagonals of the lower plane. The resulting parallelepiped is a primitive unit cell that has the disadvantage of not being able to tessellate in three orthogonal directions. To overcome this, we extend the stacking by placing a third oblique plane using the same technique. This would result in third plane being parallel to the base plane.

Figure 3(ii) shows the extension of this stacking by placing a third oblique plane exactly parallel to the first one. The resultant unit cell would comprise of a lattice point at the center of the body of the cell besides those at the corners, a non-primitive unit cell, named as body-centered monoclinic lattice and referred as **monoclinic (I)** in literature[9]. 'c' here is the distance between two consecutive coincident parallel planes and might or might not be equal to any one of the sides of the base plane.

Now, we discuss the various cases of AB stacking:

- Oblique lattice for both cases of height c, gives rise to monoclinic (I)(9).
- While the 2-D rectangular lattice gives rise to orthorhombic (I)(10) in case of c≠a and b, tetragonal (I)(11) is obtained when c=a or c=b.
- The 2-D Square lattice with third plane stacked at a height unequal to the sides of the base plane result in tetragonal(I), at a height equal to the sides, cubic (I)(12) is obtained. Sodium, the softest metal, exists in body centered cubic structure.
- Regular centered hexagonal, on AB stacking results in hexagonal(P) itself.

3.3 AB Stacking Special Cases: Face Centered Lattices

3.3.1 Square Lattice

Common salt or sodium chloride (NaCl), available in every kitchen, happens to have a face-centered cubic structure which is extremely difficult to visualize. We have also found in our endeavor that it is one of the most intriguing structures to construct. After much deliberation, we have come up with the following process of obtaining this structure.

AB stacking of square lattice, when the height of second plane is $\frac{a}{\sqrt{2}}$ would result in face centered cubic(13) structure with each side of length $\sqrt{2}$a. To view this structure, we need to rotate the whole structure by an angle of 45^o.

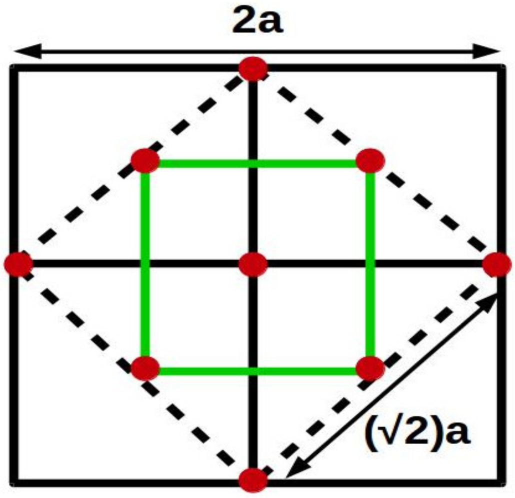

Figure 4: *Formation of Face Centered Cubic*

For constructing this structure, choose four square lattices to form a big square lattice of side 2a. But, we can also observe a square of side $\sqrt{2}$a, which is formed by the diagonals of the smaller square as shown in Fig. 4, embedded in the bigger square. Now, the second plane would have one square with its vertices at the center of each of the

Table 1: Stacking of 2-D Bravais lattices to obtain 3-D Bravais lattices.P: Primitive; I: Body Centered; F: Face Centered; C: Side Centered

2-D Bravais lattice	AA Stacking		AB Stacking	
	'c' not equal to either of the sides	'c' equal to either one or both of the sides	'c' not equal to either of the sides	'c' equal to either one or both of the sides
Oblique lattice, a$\neq$b, $\gamma \neq 90^o$	$c\neq a\neq b$ or $c=a\neq b$, $\alpha=\beta=90^o, \gamma \neq 90^o$, **Mono.(P)**		$c\neq a\neq b$ or $c=a\neq b$, $\alpha=\beta=90^o, \gamma \neq 90^o$, **Mono.(I)**	
Rectangular lattice, a$\neq$b, $\gamma = 90^o$	$c\neq a\neq b$, $\alpha=\beta=\gamma=90^o$ **Ortho.(P)**	$c=a\neq b$, $\alpha=\beta=\gamma=90^o$ **Tetra.(P)**	$c\neq a\neq b$, $\alpha=\beta=\gamma=90^o$ **Ortho.(I)**	$c=a\neq b$, $\alpha=\beta=\gamma=90^o$ **Tetra.(I)**
Square lattice, a=b, $\gamma = 90^o$	$c\neq a=b$, $\alpha=\beta=\gamma=90^o$ **Tetra.(P)**	$c=a=b$, $\alpha=\beta=\gamma=90^o$ **Cubic(P)**	$c\neq a=b$, $\alpha=\beta=\gamma=90^o$ **Tetra.(I)**	$c=a=b$, $\alpha=\beta=\gamma=90^o$ **Cubic(I)**
Centered Rectangular lattice, a$\neq$b, $\gamma = 90^o$	$c\neq a\neq b$ or $c=a\neq b$, $\alpha=\beta = \gamma = 90^o$, **Ortho.(C)**			
Regular Centered Hexagonal lattice, a=b, $\gamma = 60^o/120^o$	$c\neq a\neq b$ or $c=a\neq b$, $\alpha=\beta=90^o$, $\gamma = 60^o/120^o$, **Hex.(P)**			

small squares of side a, at a height of $\frac{a}{\sqrt{2}}$. Then, the third plane would be coincident with the base plane and shall be at a height of $\sqrt{2}$a from it. Thus, we obtain a face centered cubic lattice of side $\sqrt{2}$a starting with square lattices of side a. One should remember that this same lattice structure can also be viewed as tetragonal(I) lattice with sides a=b and height c=$\sqrt{2}$a.

Now, we explore if there would be any further possibilities of centered stacking which can be achieved using the fundamental rhombus type-1 and rhombus type-2 lattices, corresponding to the centered rectangular and centered regular hexagonal 2-D Bravais lattices [1].

3.3.2 Rhombus Type-1

AB stacking of rhombus type-1 lattices would result in face centered orthorhombic(14), which again needs careful visualization. Figure 5 gives the idea, wherein centering of the rhombuses result in the desired 3-D lattice. Similarly, AB stacking of rhombus type-2 lattices would result in monoclinic(I) with a special condition of a=b in the base plane.

Thus random stacking, AA and AB stacking of the five 2-D Bravais lattices in two different ways has produced thirteen of the fourteen 3-D Bravais lattice structures except the trigonal lattice which needs special discussion.

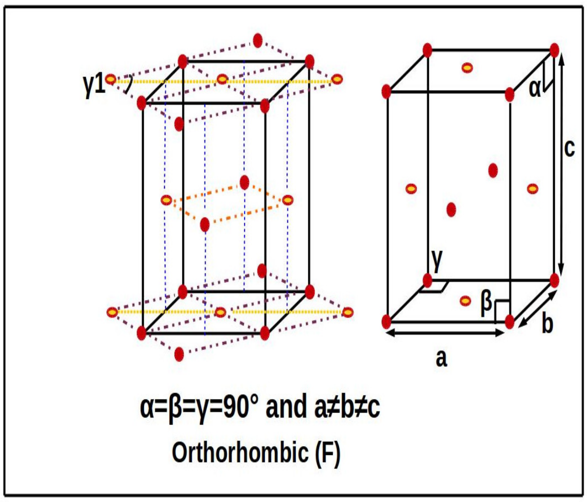

Figure 5: ***Formation of Face Centered Orthorhombic***

4 ABC Stacking: Trigonal (Rhombohedral) Lattice

Here, on considering the alternative possibilities of centering rhombus type-2 lattice, we would see that the answer lies in realizing an important aspect, which is, the diagonal of this rhombus is equal to its side length and it is in fact an equilateral triangle with perfect symmetry, the only triangle with possibility of centering. The solution is to center stack the centered Hexagonal lattices at the centroid of the equilateral triangle. At once we realize that fourth plane instead of third, would match its vertices with the first base plane. Hence, extended stacking has four planes (A-B-C-A), instead of three to obtain a non-primitive cell. The stacking is illustrated in *Crystallography: An Introduction*[7] and is reproduced here for completeness in Fig. 6. It results in two distinct unit cells. This is the reason for it being a separate class in seven crystal systems.

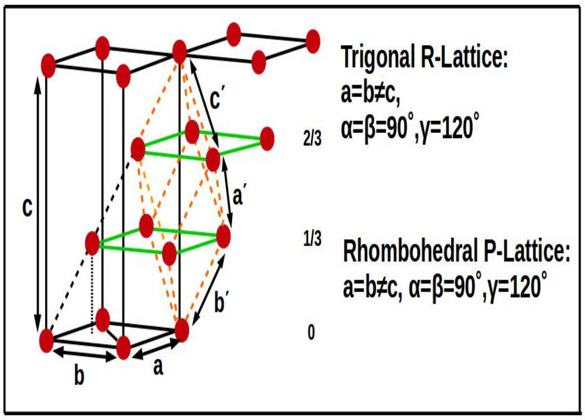

Figure 6: ***Formation of Trigonal and Rhombohedral Unit cell***

Dolomite crystal, which is widely used as a healing stone, has rhombohedral structure.

5 Conclusion

We have proposed two types of stacking of 2-D planes, A-A stacking and A-B stacking. Using AA stacking, we have demonstrated the construction of five primitive unit cells and the lone side centered orthorhombic lattice. The AB stacking along with extension to a third plane allowed us to visualize the four body centered crystal structures. While the face centered cubic Bravais lattice is constructed by using AB stacking of square lattice with the height between the first and third plane being $\sqrt{2}a$, to obtain face centered orthorhombic, rhombus type-1 lattice has been centered instead of centered rectangular lattice.

All these 12 lattices are the special cases of the most general 3-D crystal system obtained by randomly stacking the 2-D oblique lattices, which is called the triclinic primitive unit cell.

The trigonal system which encompasses the rhombohedral primitive lattice is a special crystal structure that could be constructed by AB stacking of equilateral triangular 2-D lattices with a total of 4 planes.

The proposed methodology to arrive at the 14 Bravais lattices could be converted into an interesting classroom/lab activity which could be assessed for its effectiveness using Physics Education Research strategies.

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