

Lattice heat capacity of crystals: A q-oscillator debye model

Rubarani. P. Gangadharan* and S. Sampath Krishnan

**Department of Physics, Rajalakshmi Engineering College, Chennai-602105, TamilNadu, India.
Department of Physics, Sri Venkateswara College of Engg, Sriperumbudur-602105, Tamil Nadu, India*

ABSTRACT

The Debye model for lattice heat capacity is modified retaining all the basic assumptions except that each mode is here treated as a q-deformed quantum harmonic oscillator. The lattice heat capacity C_v is evaluated in the high and low temperature limits. When $T \ll \theta_D$, $C_v \propto T^3$ and when $T \gg \theta_D$, $C_v \propto T^2$. In the case of the alkali elements Rb, Cs and K whose Debye temperature are relatively low, the calculated values agree reasonably well with experimental results over a wide range of temperatures. The lattice heat capacity C_v for semiconducting elements are also studied whose Debye temperature (θ_D) are very large as compared to alkali elements and also studied for rare gases.

Keywords: q-deformed oscillators, Lie algebras, Poisson bracket

INTRODUCTION

Very recently the concept of q-deformed oscillators (Biedenharn 1989, Macfarlane 1989) has attracted the attention of many physicists and the theory of q-deformed oscillators finds applications in many areas of Physics. In the present work, we use this new concept to explain the temperature dependence of lattice heat capacity (C_v) in the high temperature region. The Debye model for lattice heat capacity of solids has been remarkably successful in describing the experimental observations at low temperatures, but it failed to explain the temperature dependence of the lattice heat capacity in the high temperature region. This discrepancy has been explained in the past using anharmonic effects. The q-deformation can take care of anharmonicity effect and we reformulate the Debye theory by treating each mode of vibration of the crystal as an independent q-oscillator. It is found that in the low temperature limit, the q-deformation yields a q-dependent correction to C_v , which is negligible while in the high temperature limit, C_v is found to be proportional to the square of the temperature. The model has been applied to the case of alkali elements Rb, Cs and K and the calculated values compare remarkably well with the experimental data over a wide range of temperatures. The model has also been applied for semiconducting elements and rare earth gases.

HARMONIC OSCILLATOR DEBYE MODEL

The Debye model for lattice heat capacity of solids has been remarkable successful in describing the experimental observations at low temperatures. Alkali elements such as K, Rb and Cs have a low temperature heat capacity

proportional to T^3 (i.e. $C_v = \frac{12}{5} \pi^4 N_0 k \left(\frac{T}{\theta_D} \right)^3$) in accordance with Debye's theory. In the high temperature region

($T \gg \theta_D$), the Debye model leads to the Dulong-Petit law: $C_v = 3R/g$ -atom, a constant for all mono atomic crystals and is independent of temperature. However measurements indicate a temperature dependence in this region.

A q-OSCILLATOR DEBYE MODEL

In this work we reformulate the Debye model treating each as a q-oscillator. In the low temperature limit q-deformed oscillator yields a q-dependent correction for C_v , which is negligible. Thus when $T \ll \theta_D$, the model

effectively coincides with the Debye model . In the high temperature limit ($T \gg \theta_D$), C_v is found to be T^2 dependent, in very good agreement with the experimental results obtained in the cases studied here. When T is large (~ 300 K or more), the variation of C_v with T is seen to be more rapid than predicted.

QUANTUM ALGEBRAS:

It was Dirac who first realized that the Poisson bracket in classical mechanics is a Lie bracket . In setting up his quantum theory, Dirac replaced Poisson bracket by the commutator bracket (divided by $i\hbar$) thus preserving the Lie algebraic structure. Later on it become transparent that quantum mechanics may structurally be viewed as a deformation of classical mechanics with \hbar as the deformation parameter. Inspired by the development of quantum groups and that of non commutative geometry recently a second deformation (called the q -deformation) is being discussed. The quantum algebras can be viewed as deformation of classical Lie algebras.

HEAT CAPACITY OF A SLIGHTLY q -DEFORMED HARMONIC CRYSTAL (q -OSCILLATOR DEBYE MODEL):

The concept of q -deformation is introduced defining the q -creation operator \bar{a}^+ and q -annihilation operator \bar{a} such that

$$[\bar{a}, \bar{a}^+]_q = \bar{a} \bar{a}^+ - q \bar{a}^+ \bar{a} = q^{-\bar{N}}$$

where q is complex and \bar{N} is the number operator satisfying the following relations.

$$[\bar{a}, \bar{N}] = \bar{a}$$

$$[\bar{a}^+, \bar{N}] = -\bar{a}^+, \quad \bar{N} \neq \bar{a}^+ \bar{a}$$

The q -oscillator Hamiltonian then reads

$$\bar{H} = \frac{1}{2} \hbar \omega ([\bar{N} + 1] + [\bar{N}])$$

where $[x] = \frac{q^x - q^{-x}}{q - q^{-1}}$

where $q \rightarrow 1$. Hamiltonian reduces to that of boson oscillator .Introducing a new parameter η such that

$$q = e^{\eta} ; \eta \in \mathbb{R}$$

for sufficiently small values of η \bar{H} becomes

$$\bar{H} = H_0 - \frac{\eta^2}{3!} H_1$$

where $H_0 = \frac{\hbar \omega}{2} (2N+1)$

and $H_1 = \frac{\hbar \omega}{2} ((N+1)^3 + N^3 - (2N+1))$

The partition function Z of a thermodynamic system is given by for slightly deformed oscillator

$$Z_{SDO} = \text{Tr}(e^{-\bar{H}/kT})$$

$$= Z \left(1 - \frac{\eta^2}{3!} \frac{U_1}{kT} \right)$$

and $U_1 = \left(\frac{\hbar \omega}{2} \right) + \frac{\hbar \omega}{e^{\hbar \omega/kT} - 1} - \hbar \omega \sinh \left(\frac{\hbar \omega}{kT} \right) g \left(\frac{\hbar \omega}{kT} \right)$

where $g(x) = \frac{e^{3x} + 4e^{2x} + e^x}{(e^x - 1)^4}$

$$Z = \prod_i z_i = \prod_i z_i \left(1 - \frac{\eta^2 (U_1)_i}{6 kT} \right)$$

The internal energy of the crystal is

$$\bar{U} = kT^2 \frac{\partial}{\partial T} (\ln Z) = U + \frac{\eta^2}{6} \left(U_1 - T \frac{\partial U}{\partial T} \right)$$

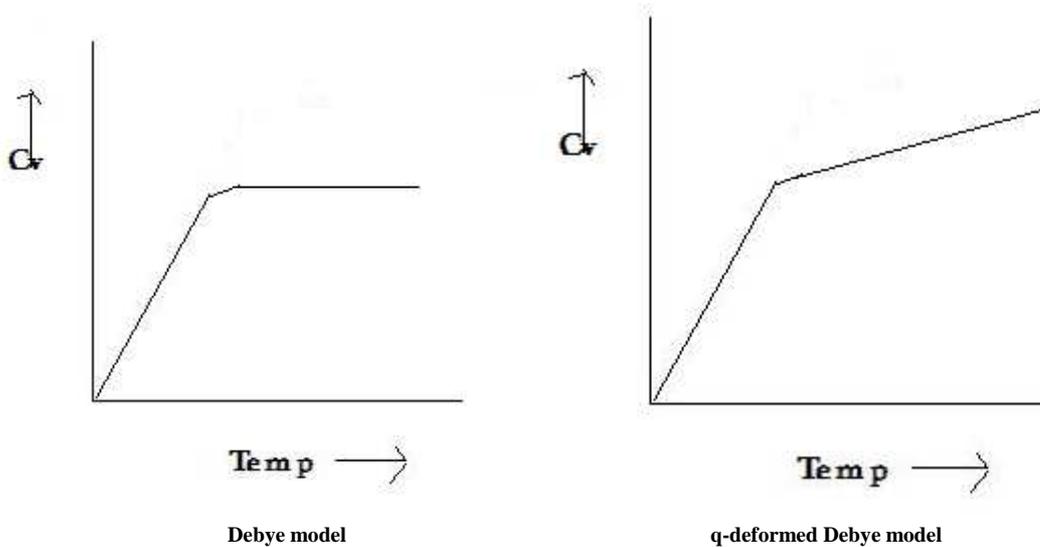
Putting $x_D = \frac{\hbar \omega_D}{kT} = \frac{\theta_D}{T}$

θ_D being the Debye temperature we find

$$\bar{U} = 9N_0 kT \left(\frac{T}{\theta_D} \right)^3 \left[\int_0^{x_D} \frac{x^3 dx}{e^x - 1} + \frac{\eta^2}{2} \int_0^{x_D} \left[\frac{x^4 e^x + x^3 e^x + 4x^4 e^{2x} + x^4 e^{3x} - x^3 e^{3x}}{(e^x - 1)^4} \right] dx \right]$$

where N_0 = number of atoms in the specimen.

The lattice heat capacity of the q-deformed crystal can now be evaluated as $\frac{\partial U}{\partial T}$.



We compute this quantity in two limiting cases

1) $T \ll \theta_D$. In this case

$$C_v = \frac{12\pi^4}{5} N_0 k \left(\frac{T}{\theta_D} \right)^3 \left(1 + \eta^2 \frac{45}{2\pi^2} \right)$$

Here we note that q-deformation brings in a q-dependent correction which is negligible. Thus the proposal model coincides with the Debye model in the low temperature limit.

2) $T \gg \theta_D$. In this case

$$C_v = 3N_0k \left(1 + \eta^2 \frac{18T^2}{\theta_D^2 V} \right)$$

In the high temperature limit, in contrast to the Debye theory this expression exhibits at T^2 dependence. Though η^2 is small, the correction term as a whole is not negligible.

MATERIALS AND METHODS

The present work comprises of calculating the lattice heat capacity per g-atom for three alkali elements namely potassium, rubidium and caesium for which the Debye temperatures (θ_D) are relatively low. η is assigned values $\sim 10^{-5}$. The lattice heat capacity for different elements are calculated using C program.

RESULTS AND DISCUSSION

The lattice heat capacity per g-atom for three alkali elements namely potassium, rubidium and caesium for which the Debye temperature (θ_D) are relatively low are calculated. η is assigned values $\sim 10^{-5}$. The results are shown in table 2. Experimental values are also given for comparison. The results are plotted for the range 100-300K along with the experimental curves in figure.2. It is observed that there is a very good agreement for not too high values of T (100-250K). As the temperature becomes higher, discrepancies arise; the heat capacity increases much more than predicted by the theory.

The lattice heat capacity per g-atom for two semiconducting elements namely germanium and silicon are also studied. But as the Debye temperature (θ_D) are very large i.e., $\theta_D = 363$ K for germanium and $\theta_D = 636$ K for silicon, C_v can be calculated above 400 K for germanium and above 700K for silicon. Table 3 shows the results for germanium in the range 600K-1500K and for silicon in the range 1000K-1500K. The results are plotted in figure 3.

The lattice heat capacity C_v is also studied for rare gases such as neon, argon, krypton and xenon but there is not much variation in C_v as in the case of alkali metals.

Table-1: Experimental and theoretically predicted values of lattice heat capacity (C_v) of alkali metals Cs, Rb and K

T(K)	Caesium $\theta_D = 38.4K$ $\eta = 8.5 \times 10^{-5}$		Rubidium $\theta_D = 55.6K$ $\eta = 9.0 \times 10^{-5}$		Potassium $\theta_D = 90.6K$ $\eta = 10^{-4}$	
	C_v (cal/g-atom/K)		C_v (cal/g-atom/K)		C_v (cal/g-atom/K)	
	Theoretical	Experimental	Theoretical	Experimental	Theoretical	Experimental
100	6.034	6	6.01		5.988	
110	6.049	6.01	6.02		5.994	
120	6.067	6.04	6.032		6	
130	6.085	6.08	6.045		6.01	
140	6.105	6.13	6.058	6.02	6.016	
150	6.126	6.16	6.073	6.04	6.024	
160	6.15	6.17	6.088	6.07	6.033	
170	6.174	6.18	6.105	6.09	6.043	
180	6.2	6.2	6.123	6.11	6.053	5.983
190	6.227	6.22	6.141	6.13	6.063	6.005
200	6.256	6.26	6.16	6.14	6.074	6.03
210	6.286	6.6	6.181	6.17	6.086	6.057
220	6.318	6.33	6.203	6.19	6.099	6.085
230	6.351	6.35	6.226	6.22	6.112	6.117
240	6.386	6.38	6.249	6.26	6.125	6.15
250	6.422	6.46	6.274	6.3	6.14	6.183
260	6.46	6.55	6.3	6.35	6.154	6.219
270	6.5	6.61	6.326	6.4	6.17	6.263
273.15	6.512	6.64	6.335	6.42	6.174	6.278
280	6.54	6.71	6.354	6.47	6.185	6.317
290	6.582	6.84	6.383	6.56	6.201	6.379
298.15	6.617	6.97	6.407	6.67	6.215	6.439
300	6.625	7	6.412	6.69	6.218	6.454

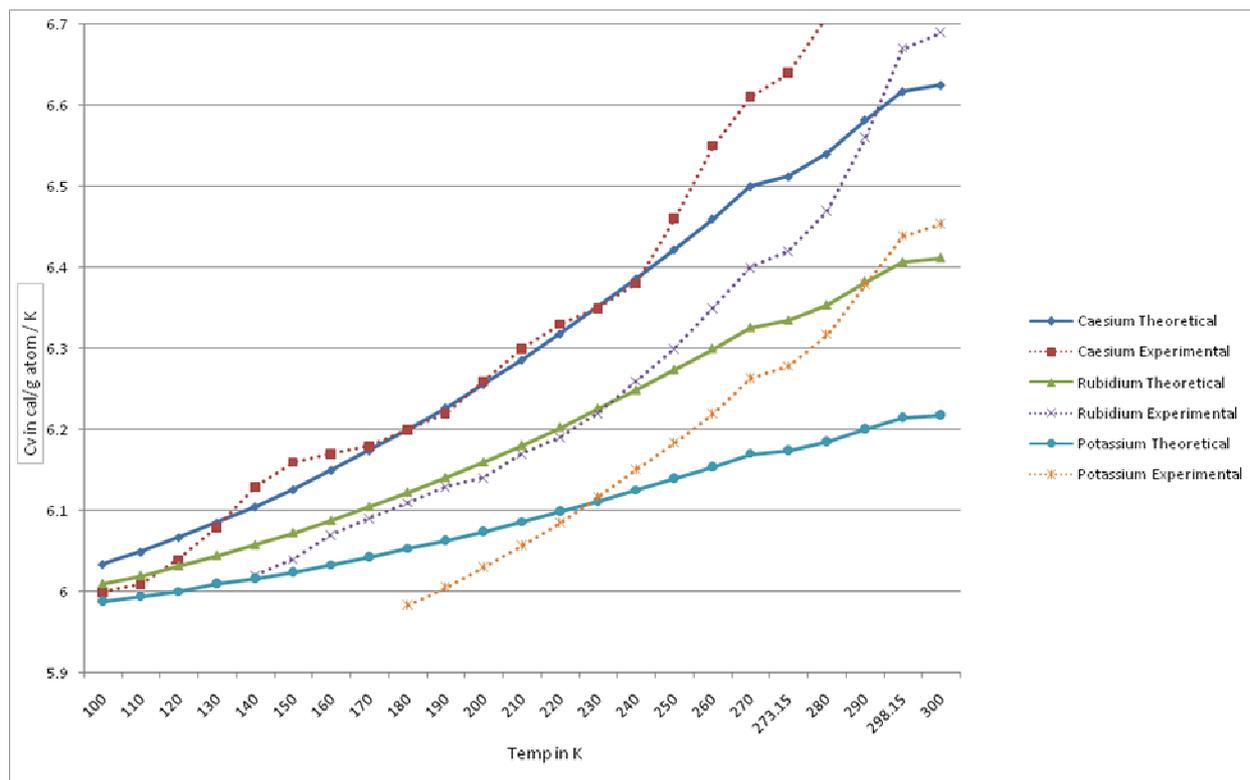


Figure:1 Experimentally and theoretically predicted values of lattice heat capacity(C_v) of alkali metals

Table 2: Theoretically predicted values of lattice heat capacity(C_v) of semiconducting elements Germanium and Silicon

T(K)	Germanium $\theta_D = 363K$ $\eta = 1 \times 10^{-4}$	Silicon $\theta_D = 636K$ $\eta = 1.5 \times 10^{-4}$
	C_v (cal/g-atom/K)	C_v (cal/g-atom/K)
600	6.178	
650	6.216	
700	6.257	
750	6.3	
800	6.347	
850	6.397	
900	6.45	
950	6.506	
1000	6.565	6.448
1050	6.627	6.498
1100	6.693	6.551
1150	6.76	6.606
1200	6.832	6.663
1250	6.906	6.723
1300	6.983	6.785
1350	7.064	6.85
1400	7.147	6.917
1450	7.233	6.987
1500	7.323	7.059

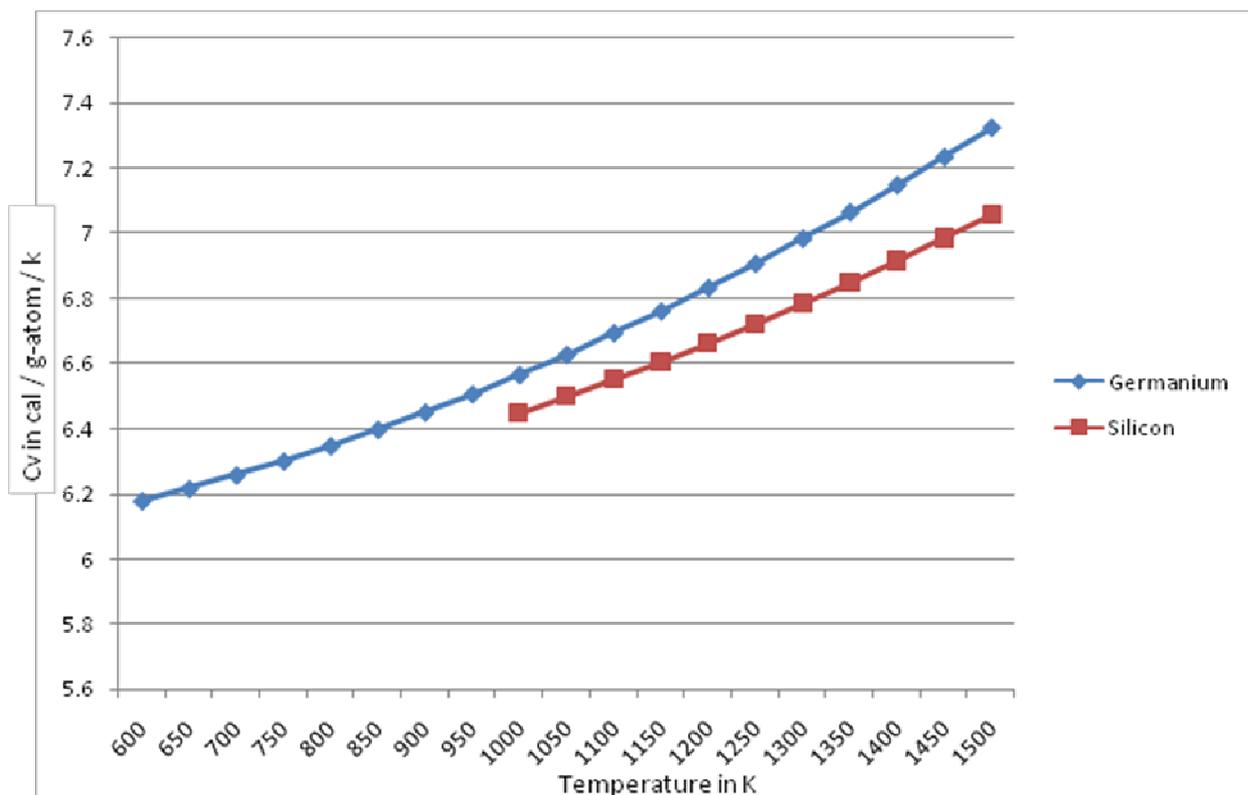


Figure 2: Theoretical values of Cv for Germanium and Silicon

Table 3: Theoretically predicted values of lattice heat capacity (Cv) of rare gases

T(K)	Xenon $\theta_D = 64K$ $\eta = 9.0 \times 10^{-5}$	Krypton $\theta_D = 72K$ $\eta = 1 \times 10^{-4}$	Argon $\theta_D = 92K$ $\eta = 1.5 \times 10^{-4}$	Neon $\theta_D = 75K$ $\eta = 2.0 \times 10^{-4}$
	Cv(cal/g-atom/K)			
100	5.96	5.96	5.9601	5.9603
110	5.9601	5.9601	5.9601	5.9603
120	5.9601	5.9601	5.9601	5.9604
130	5.9601	5.9601	5.9602	5.9605
140	5.9601	5.9601	5.9602	5.9606
150	5.9602	5.9601	5.9602	5.9607
160	5.9602	5.9602	5.9603	5.9609
170	5.9602	5.9602	5.9603	5.9609
180	5.9602	5.9602	5.9603	5.961
190	5.9603	5.9603	5.9604	5.9611
200	5.9603	5.9603	5.9604	5.9612
210	5.9603	5.9603	5.9605	5.9613
220	5.9604	5.9604	5.9605	5.9615
230	5.9604	5.9604	5.9606	5.9616
240	5.9605	5.9604	5.9606	5.9618
250	5.9605	5.9605	5.9607	5.9619
260	5.9606	5.9605	5.9608	5.9621
270	5.9606	5.9606	5.9608	5.9623
273.15	5.9606	5.9606	5.9608	5.9624
280	5.9606	5.9606	5.9609	5.9625
290	5.9607	5.9607	5.9609	5.9626
298.15	5.9607	5.9607	5.961	5.9628
300	5.9608	5.9607	5.961	5.9628

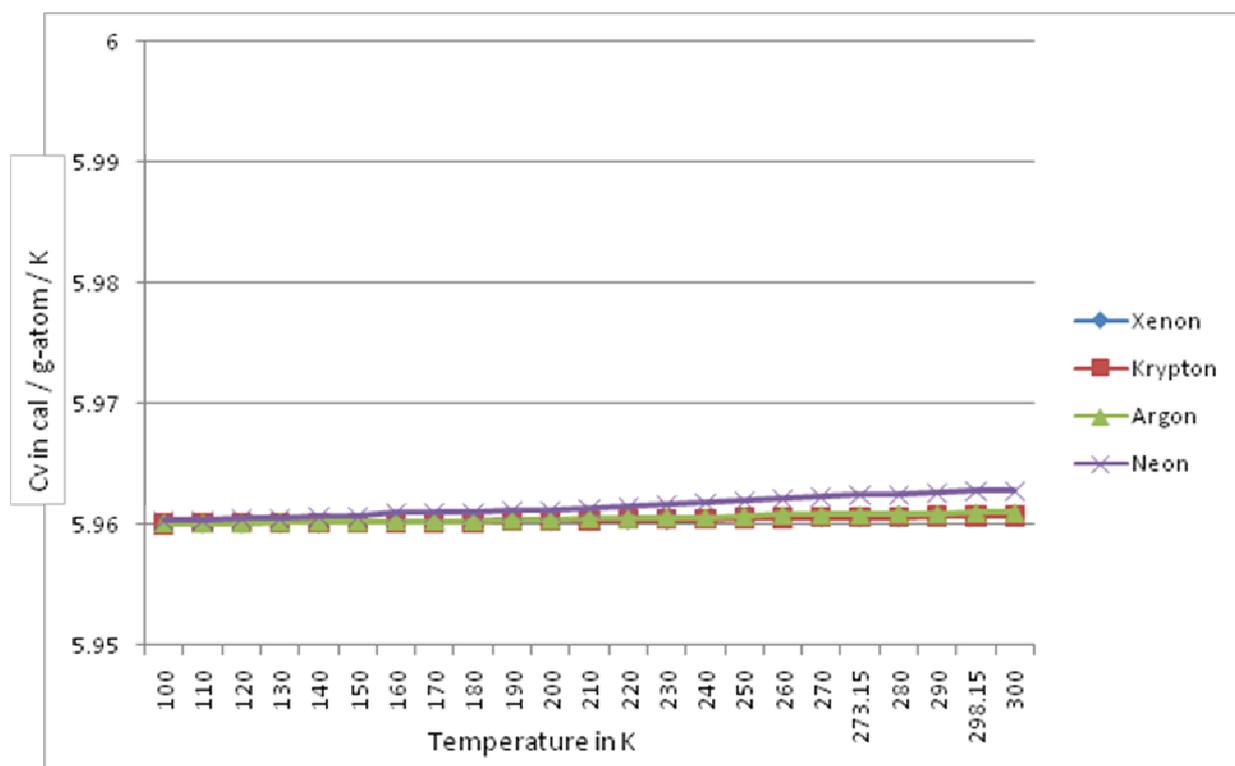


Figure 3: Theoretically values for rare gases

CONCLUSION

From q-oscillator Debye model it is observed that there is a very good agreement for not too high values of T(100-250 K) for alkali metals. As the temperature becomes higher, discrepancies arise; the heat capacity increases much more rapidly than predicted by theory. It has been discussed as a q-deformed quantized oscillator version of the old Debye model of lattice heat capacity and shown that it rectifies the weakness of the original model in the high temperature regime. The deformation though marginal ($\eta \sim 10^{-5}$ - 10^{-4}) produces excellent agreement in the three alkali cases studied over a wide range of temperatures. The investigations tend support to the view that phonons in crystals may be q-quantised excitations. Such phonons may be termed as q-phonons.

REFERENCES

- [1] K.K.Leelamma, V.C.Kuriakose and K.Babu Joseph, *International Journal of Mod.Phy.B*, 7 No.14(1993)2697-2706.
- [2] A.K.Ghatak and L.S.Kothari, *An introduction to Lattice Dynamics* (Addison Wesley, London, 1972), pp.132-142.
- [3] L.C.Biedenharn, *J.Phys.* **A22**(1989)L873-L878.
- [4] A.J.Macfarlane, *J.Phys.* **A22**,4589(1989).
- [5] C.Kittel, *Introduction to Solid State Physics*, 4th Ed. John Wiley, New York, 1971.
- [6] A.J.Dekker, *Solid State Physics*, Macmillan India Ltd., 1993.
- [7] A.P.Polychronakos, *Mod.Phys.Lett.* **A5**,2325(1990).
- [8] E.G.Floratos, *J.Phys.* **A24**,4739(1991).