

STUDIES IN CONDENSED MATTER PHYSICS USING q-OSCILLATOR ALGEBRA

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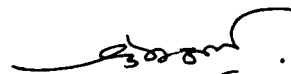
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CERTIFICATE

Certified that the work presented in this thesis is the bonafide work done by Smt. K.K.Leelamma, under my guidance in the Department of Physics, Cochin University of Science and Technology and that this work has not been included in any other thesis submitted previously for the award of any degree.

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PREFACE

The whole history of physics is a story of deformations. In classical mechanics itself, the Lorentz transformation between two inertial frames is a deformation of Galilean transformation with $\beta = \frac{v}{c}$ as the deformation parameter and in the limit $\beta \rightarrow 0$, the original non-relativistic mechanics is regained. Thus special relativity is a deformation of Galilean relativity. Similarly, Quantum Mechanics is a deformation of Classical Mechanics with \hbar as the deformation parameter. In the limit $\hbar \rightarrow 0$, the results of quantum mechanics merge with the classical results.

Quantum groups and quantum algebras are deformations of classical Lie groups and their structure is much more complex than that of Lie groups. They are symmetry groups of non-commutative spaces. Though initially introduced in connection with the quantum inverse scattering theory, they have found applications in many problems of physical and mathematical interest such as conformal field theory, integrable lattice models, knot theory, quantum optics and gauge field theory. However, direct applications of quantum symmetry to real physical systems are limited. There had been a great deal of interest in the study of quantum groups during the last decade.

The representation theory of the quantum algebras has led to the development of q-deformed oscillator algebra. Since then, there has been an increasing interest in the study of physical systems using q-oscillator algebra. It has found applications in several branches of physics such as vibrational spectroscopy, nuclear

physics, many body theory and quantum optics. The work presented in this thesis is also along similar lines. The concept of q -oscillator algebra is applied to some problems in condensed matter physics.

This thesis is organised as follows: It contains five chapters. In the introductory chapter, we present a brief history of the development of the concept of quantum groups and quantum algebras. We review the concept of non-commutative spaces and introduce quantum groups as symmetry groups of non-commutative spaces. The q -deformation of numbers and basics of q -differential calculus are presented. Some simple examples of quantum groups are also illustrated.

In chapter 2, a brief review of the q -harmonic oscillator and the salient features of its energy spectrum are given. The statistical mechanics of slightly deformed oscillator is discussed. It develops the pre-requisites for the investigations reported in the subsequent chapters. A few applications of q -oscillator algebra to real physical systems are also cited.

Chapter 3 deals with the problem of an anharmonic oscillator with quartic interaction. The energy spectrum and the statistical mechanics of q -deformed anharmonic oscillator are discussed.

In chapter 4, the Debye model of lattice heat capacity of crystals is reformulated using q -oscillator algebra, treating the vibrational modes as q -bosons. The theoretical results on lattice heat capacity are compared with experimental data.

Chapter 5 deals with application of q-oscillator algebra to the linear spin wave theory of ferromagnets. The magnons are treated as q-bosons. A comparative study of the theoretical results on spontaneous magnetisation and magnon heat capacity with experimental data is also presented.

A part of these investigations has appeared in the form of the following publications:

- (i). q-Anharmonic oscillator with quartic interaction: V C Kuriakose, K K Leelamma and K Babu Joseph, *Pramana J.Phys*, **39**, 521 (1992).
- (ii). Lattice heat capacity of crystals- a q-oscillator Debye model: K K Leelamma, V C Kuriakose and K Babu Joseph, *Int.J.Mod.Phys. B*, **7**, 2697 (1993)
- (iii). Thermodynamic properties of a q-deformed Heisenberg ferromagnet (communicated to *Phys.Lett. A*.)

SYNOPSIS

The thesis deals with some applications of q -deformation and quantum group ideas to problems in condensed matter physics. They are deformations of classical groups and their structure is much more complex than that of Lie groups. They generalise our familiar concepts of symmetries to the realm of non-commutative geometry.

The q -deformation of numbers was introduced by Heine in 1878. The q -differential calculus which is a generalisation of ordinary differential calculus was also developed in the nineteenth century. Recently, there has been a great deal of interest in the study of quantum groups and quantum algebras. The representation theory of quantum algebras with a single deformation parameter q , has led to the development of the now well-known q -deformed harmonic oscillator algebra. But we know that in real physical systems one cannot dismiss the role of anharmonicity. The fact that the energy levels of the q -oscillator are not equally spaced and the success of the q -oscillator model in accounting for the measurements on the infra-red spectrum of a number of molecules, indicate that q -deformation can take care of anharmonicity effects to some extent.

Motivated by these considerations, we have studied the problem of q -deformations of an anharmonic oscillator with quartic interaction and obtained the energy spectrum. The energy values are found to depend on the deformation parameter q . We have also evaluated various thermodynamic quantities such as

partition function, entropy and internal energy. Such studies are expected to be relevant in the context of lattice dynamics.

The Debye model of lattice heat capacity of solids has been remarkably successful in describing the experimental observations at low temperatures in many pure crystalline solids. Alkali elements such as potassium, rubidium and caesium have a low temperature heat capacity proportional to T^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. However, measurements in this region indicate deviations from the predictions of Debye model.

Debye's theory is based on the harmonic approximation. Real crystals do exhibit anharmonic effects such as thermal expansion. We have reformulated the Debye theory, taking each mode as a q-oscillator. In the low-temperature limit, the q-deformed model yields a q-dependent correction for C_v which is negligible and thus when $T \ll \Theta_D$, the model effectively coincides with the Debye model. In the high temperature limit, C_v is found to be T -dependent, in very good agreement with the experimental results obtained in the three cases studied. The investigations lend support to the view that phonons in crystals may be q-quantised excitations. Such phonons may be termed q-phonons. When T is very large ($\sim 300\text{K}$ or more), the variation of C_v with T is found to be more rapid than predicted. The deviation may perhaps be taken care of by q-anharmonic model incorporating interactions.

The concept of q-deformation is also applied to investigate the

magnetic properties of ferromagnets. The agreement between the linear spin wave theory of ferromagnetism and experimental observations on ferromagnets is not satisfactory. The q-deformed Holstein-Primakoff transformation is used to describe the spin variables of a Heisenberg ferromagnet and the magnons are treated as q-bosons. The exchange Hamiltonian in the nearest neighbour approximation is obtained for small values of the deformation parameter when the excitation is low. The thermodynamic quantities in the low temperature region are also evaluated. It is found that the spontaneous magnetisation and magnetic contribution to the heat capacity have q-dependent $T^{\frac{1}{2}}$ terms in addition to the well known Bloch $T^{\frac{3}{2}}$ term. Calculations are done for the cases of EuO and EuS, the simplest Heisenberg ferromagnets known. A comparison of the theoretical results and experimental values indicates that our model is an improvement over the linear spin wave theory. The general pattern of temperature dependence of magnon heat capacity and spontaneous magnetisation is predicted by the model.

Chapter 1

INTRODUCTION

Symmetry plays an important role in physics. Progress in modern physics has been intimately related to the study of symmetry. Applications of symmetry principles and conservation laws have paved a novel way of understanding physical systems. Gauge symmetry has led to the standard model in high energy physics. Crystallographic space symmetry is fundamental to solid state physics and conformal symmetry plays an important role in string theory and critical phenomena. The mathematical tool for studying the symmetry of a system is group theory.

Quantum groups and quantum algebras have attracted much attention of physicists and mathematicians during the last eight years [1]. There had been a great deal of interest in this field, especially after the introduction of the q -deformed harmonic oscillator [2&3]. Quantum groups and quantum algebras have found unexpected applications in theoretical physics.

Historically quantum groups first appeared as a deformation of the

universal enveloping algebra of a Lie algebra in the study of integrable quantum systems. In the beginning of the 1980s, there was much progress made in the field of quantum integrable field theories. One of the most important studies is the development of a quantum mechanical version of the well-known inverse scattering method used in the theory of integrable nonlinear evolution equations like the Korteweg de Vries (KdV) equation. This method was developed by Faddeev, Sklyanin and Takhtajan [4-6] in formulating a quantum theory of solitons. Kulish and Reshetikhin [7] showed that the quantum linear problem of the quantum sine-Gordon equation was not associated with the Lie algebra $sl(2)$ as in the classical case, but with a deformation of this algebra. Sklyanin showed that [8&9] deformations of Lie algebraic structures were not special to the quantum sine-Gordon equation and that it seemed to be part of a general theory. It was Drinfel'd who showed that a suitable quantisation of Poisson Lie groups reproduced exactly the same deformed algebraic structures encountered in the theory of quantum inverse scattering [10-12]. Almost at the same time, Jimbo arrived at the same result [13&14] from a slightly different angle. In his work, the quantum algebras appeared in the context of the solution of the Yang-Baxter Equation (YBE).

There is no universally accepted definition of a quantum group. There are several approaches [15-17]. As we have seen, in Drinfeld's approach, the quantum group is defined as a deformation of the Universal Enveloping Algebra (UEA) of a Lie algebra. This approach is similar to the study of Lie groups via their Lie

algebras. Jimbo also gave almost the same definition. The new algebraic structures are called Quantised Universal Enveloping Algebras (QUEA). In Manin's work [18], quantum groups are defined as symmetries of non-commutative or quantum spaces. We discuss this point in detail in Section 1.2. Woronowicz [19–21] gave an entirely different approach to quantum groups, based on non-commutative C^* algebras. This is analogous to the classical theory of topological groups. He called these groups, pseudo-groups. His approach is popular among mathematicians. The theory of Faddeev and the Leningrad school [22] introduces quantum groups in terms of R-matrices which are solutions of the Quantum Yang-Baxter Equation (QYBE). This approach is directly connected to integrable quantum field theories and has no classical analogue.

In all the four approaches, quantum groups have the structure of a Hopf algebra [15]. The word 'quantum' in quantum groups is different from the canonical quantisation. It comes from the Yang-Baxter Equation. Solutions of the classical YBE are closely related to the notion of classical groups while solutions of the QYBE are related to quantum groups. Thus the relation of quantum groups to ordinary Lie groups is analogous to that between quantum mechanics and classical mechanics. The structure of quantum group is much more complex than that of Lie group.

1.1 Quantum groups and non-commutative spaces

The quantum algebras have been linked to geometries that have non-commutative structures [23&24]. The concept of space-time continuum has been fundamental to all successful physical theories. However there are arguments that on a submicroscopic level, this concept has to be abandoned [25]. There is no experimental proof for the assumption that space-time is smooth down to arbitrarily small distances. Perhaps it may be because of this idealisation of space-time concept that one comes across tremendous problems in the unification of various interactions [26]. This motivates one to look for a new space-time concept. Quantum mechanical phase-space is only partially non-commuting, only co-ordinates and momenta non-commute, co-ordinates themselves are commuting. If at a sufficiently small length scale, co-ordinates become non-commuting operators, it will be impossible to measure the position of a particle exactly. In this way, one may hope to remove the ultra-violet divergences of conventional quantum field theory which are due to the possibility of measuring field oscillations at one point. Thus non-commutativity is introduced as a necessary condition in the generalised space-time concept. It has been argued that physics at the Planck scale may be understood only with the help of non-commutative geometry [26&27].

In a non-commutative space with real co-ordinates (x,y,z) , a unit of

length along the x-direction is defined as

$$\Delta x = (q - 1) x \quad (1.1)$$

or equivalently

$$\Delta x = (q - q^{-1}) x \quad (1.2)$$

where q is some parameter which is real. The width of the interval Δx is not a constant. In the limit $q \rightarrow 1$, the interval $\Delta x \rightarrow 0$ and we have space-time continuum.

Consider a system with two degrees of freedom. The quantum mechanical phase-space of the system is spanned by the co-ordinates x, y and conjugate momenta p_x and p_y . This phase-space is only partially non-commuting:

$$[x, p_x] = i\hbar = [y, p_y] \quad (1.3)$$

$$[x, y] = 0 = [p_x, p_y] \quad (1.4)$$

i.e, the x - y plane and p_x - p_y plane have continuum structure and only x - p_x and y - p_y planes may have discrete structure. In a non-commutative space, non-commutativity is prescribed for co-ordinates also:

$$x y = q y x \quad (1.5)$$

The q-commutator

$$[x, y]_q = x y - q y x = 0 \quad (1.6)$$

Eq.(1.5) should remain co-variant under a co-ordinate transformation $(x, y) \rightarrow (x', y')$. Let

$$T = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \quad (1.7)$$

be the matrix effecting the transformation. a, b, c and d are in general non-commuting elements. Then

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} ax + by \\ cx + dy \end{pmatrix}.$$

$$x' y' = q y' x'$$

implies

$$(ax + by)(cx + dy) = q(cx + dy)(ax + by) \quad (1.8)$$

If we assume that a, b, c, d commute with (x, y) , we can write

$$(x' \ y') = (x \ y) \begin{pmatrix} a & b \\ c & d \end{pmatrix} = (ax + cy \quad bx + dy)$$

Then invariance of (1.5) implies

$$(ax + cy)(bx + dy) = q(bx + dy)(ax + cy) \quad (1.9)$$

Relations (1.8) and (1.9) give a complete set of conditions to be obeyed by the non-commuting objects a, b, c, d to preserve the structure of the quantum plane:

$$ab = qba ;$$

$$cd = qdc ;$$

$$ac = qca ;$$

$$bd = qdb ;$$

$$bc = cb ;$$

$$ad - da = (q - q^{-1}) bc \tag{1.10}$$

These are commutation relations obeyed by a, b, c, d . T is called a quantum matrix.

It is shown that [28] the matrices T satisfy all the axioms of a non-commutative Hopf algebra and thus constitute a quantum group. It is denoted by $GL_q(2)$, the quantum linear general group in two dimensions. It is the group of linear transformations in two-dimensional non-commutative space that preserves the commutation relation (1.5). The additional relation

$$ad - qbc = 1 \tag{1.11}$$

yields the quantum unimodular group $SL_q(2)$. The object defined by

$$\det_q(T) = ad - qbc \tag{1.12}$$

is called the quantum determinant or q-determinant.

1.2 q-deformed numbers and q-differential calculus

The q-deformation of numbers was introduced by Heine [29] in 1878. The q-basic number $[n]_q$ is defined as

$$[n]_q = \frac{q^n - 1}{q - 1} \tag{1.13}$$

or alternatively,

$$[n]_q = \frac{q^n - q^{-n}}{q - q^{-1}} \quad (1.14)$$

$$\lim_{q \rightarrow 1} [n]_q = n, \text{ the ordinary number.} \quad (1.15)$$

The q-functions are also defined [30]. For example, the q-exponential function

$$e_q(x) = \sum_{n=0}^{\infty} \frac{x^n}{[n]_q!} \quad (1.16)$$

where

$$[n]_q! = [n]_q [n-1]_q \dots [2]_q [1]_q \quad (1.17)$$

It follows that

$$[1]_q = 1 ;$$

$$[0]_q = 0 ;$$

$$[0]_q! = 1 \quad (1.18)$$

The q-sine and q-cosine functions are defined as

$$\sin_q(x) = \sum_{r=0}^{\infty} \frac{x^{2r+1}}{[2r+1]_q!} = \frac{1}{2i} (e_q^{ix} - e_q^{-ix}) \quad (1.19)$$

$$\cos_q(x) = \sum_{r=0}^{\infty} \frac{x^{2r}}{[2r]_q!} = \frac{1}{2} (e_q^{ix} + e_q^{-ix}) \quad (1.20)$$

q-differential calculus is a generalisation of ordinary differential calculus. It was developed in the nineteenth century by Jackson [31&32].

Let $f(x)$ be a function of the real variable x . Its q-derivative is defined

as

$$\mathcal{D}_x f(x) = \frac{f(qx) - f(x)}{x(q-1)} \quad (1.21)$$

where q is in general some complex parameter. $\mathcal{D}_x f$ is a difference quotient $\frac{\Delta f}{\Delta x}$ where $\Delta f = f(qx) - f(x)$ and $\Delta x = x(q - 1)$ under the scaling $x \rightarrow qx$. q is called the base. An alternative definition of q -derivative is

$$\mathcal{D}_x f(x) = \frac{f(qx) - f(q^{-1}x)}{x(q - q^{-1})} \quad (1.22)$$

This defines a difference quotient $\frac{\Delta f}{\Delta x}$ under the scaling $q^{-1}x \rightarrow qx$ or $x \rightarrow q^2x$.

The q -derivative becomes the ordinary derivative as $q \rightarrow 1$.

$$\lim_{q \rightarrow 1} \mathcal{D}_x(f) = \frac{\partial f}{\partial x} = \partial_x f \quad (1.23)$$

Thus q -differentiation defines a finite differential calculus where the intervals Δx are finite. As $q \rightarrow 1$, $\Delta x \rightarrow 0$ and the variation of x is continuous. In this respect, q -differential calculus is convenient for the description of non-commutative space.

The q -derivative satisfies the following properties:

$$\mathcal{D}_x(x) = 1 \quad (1.24)$$

$$\mathcal{D}_x(x^n) = [n]_q x^{n-1} \quad (1.25)$$

$$\mathcal{D}_x(ax^n) = a [n]_q x^{n-1} \quad (1.26)$$

$$\mathcal{D}_x(af + bg) = a\mathcal{D}_x(f) + b\mathcal{D}_x(g) \quad (1.27)$$

$$\mathcal{D}_x(fg) = g(x)\mathcal{D}_x(f) + f(qx)\mathcal{D}_x(g) \quad (1.28)$$

$$\mathcal{D}_x x - q^{-1} x \mathcal{D}_x = q^{x\partial_x} \quad (1.29)$$

$$[x \partial_x, x] = x \quad (1.30)$$

$$[x \partial_x, \mathcal{D}_x] = -\mathcal{D}_x \quad (1.31)$$

Here a and b are constants and f and g are functions of x . In proving these properties, we assume definitions (1.13) and (1.21).

The q -analogue of integration in the case of finite limits a, b is also defined as

$$\int_a^b f(x) d(qx) = (1-q) \left\{ b \sum_{r=0}^{\infty} q^r \phi(q^r b) - a \sum_{r=0}^{\infty} q^r \phi(q^r a) \right\} \quad (1.32)$$

1.3 Simple examples of quantum groups and quantum algebras

Two well-known examples of quantum group are $SL_q(2)$ and $SU_q(2)$.

$SL_q(2)$:

This group has already been introduced in Section 1.1. It is the system of 2×2 matrices $T = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$ with non-commuting matrix elements, i.e, the algebra \mathcal{A}_q generated by the four elements a, b, c, d satisfy the relations (1.10):

$$ab = qba ; \quad bd = qdb$$

$$cd = qdc ; \quad ac = qca$$

$$bc = cb ; \quad ad - da = (q - q^{-1})bc$$

The matrix elements a, b, c, d cannot have a realisation in ordinary numbers.

However when $q \rightarrow 1$, these elements commute and the matrix T turns to an ordinary

matrix that belongs to the group $GL(2)$ or $SL(2)$ if $\det(T) = 1$. If T_1 and T_2 are two matrices with non-commuting matrix elements satisfying the above relations and if elements of T_1 commute with those of T_2 , then the elements of the product matrix T_1T_2 also satisfy the above relations. In this sense, the set of matrices T has one of the properties of the groups—the closure property. It is to be noted that T_1T_2 is not the usual matrix product but the coproduct:

$$T_1T_2 = \begin{pmatrix} a_1 & b_1 \\ c_1 & d_1 \end{pmatrix} \otimes \begin{pmatrix} a_2 & b_2 \\ c_2 & d_2 \end{pmatrix} = \begin{pmatrix} a_1 \otimes a_2 + b_1 \otimes c_2 & a_1 \otimes b_2 + b_1 \otimes d_2 \\ c_1 \otimes a_2 + d_1 \otimes c_2 & c_1 \otimes b_2 + d_1 \otimes d_2 \end{pmatrix}$$

However in order to form a group, for every matrix T , there should exist an inverse T^{-1} such that

$$TT^{-1} = T^{-1}T = I,$$

the unit matrix. The matrix T^{-1} obtained from T by the standard methods does not satisfy this property. However, for every matrix T satisfying relations (1.10), a corresponding matrix

$$S(T) = \begin{pmatrix} d & -q^{-1}b \\ -qc & a \end{pmatrix} \quad (1.33)$$

can be defined such that

$$S(T)T = TS(T) = I \det_q(T) \quad (1.34)$$

where $\det_q(T) = ad - qbc$. The quantum determinant $\det_q(T)$ commutes with all elements of the algebra \mathcal{A}_q . $S(T)$ can be considered as the analogue of the inverse matrix except for $\det_q(T)$ and is called *antipode*.

Thus the set of matrices T is not exactly a matrix group, but something like a group. Woronowicz labelled it as ‘compact matrix pseudo group’. However, in the limit $q \rightarrow 1$, it turns into the $SL(2)$ group. For $q \neq 1$, the set of matrices T can be considered a q -deformation of the group $GL(2)$ and is called the quantum group $GL_q(2)$. Physically it represents the set of all linear transformations in the $x - y$ quantum plane satisfying the relation $x y = q y x$. In particular, if $\det_q(T) = 1$, it forms the quantum group $SL_q(2)$.

$SU_q(2)$:

The other well-studied quantum group is $SU_q(2)$ which is the q -deformation of the classical group $SU(2)$, the group of angular momentum. The Lie algebra $su(2)$ consists of three elements L_+ , L_- and L_z which satisfy the commutation relations

$$[L_z, L_{\pm}] = \pm L_{\pm} \quad (1.35)$$

$$[L_+, L_-] = 2 L_z \quad (1.36)$$

with

$$L_+^\dagger = L_- \quad (1.37)$$

Kulish and Reshetikhin [7], while studying the solution of YBE, introduced the algebra of three elements J_+ , J_- and J_z :

$$[J_z, J_{\pm}] = \pm J_{\pm} ;$$

$$[J_+, J_-] = [2J_z]_q \quad (1.38)$$

In the limit $q \rightarrow 1$, this algebra goes into the $su(2)$ algebra. Thus it is called q -deformation of $su(2)$ algebra and is denoted by $su_q(2)$.

Both $su_q(2)$ and $sl_q(2)$ are quantum algebras with a single deformation parameter q . Going to higher dimensions with more than two non-commuting coordinates, one has to use more than one deformation parameter. Several authors have worked on two parameter deformations [33&34].

Chapter 2

q-DEFORMED HARMONIC OSCILLATOR

2.1 Introduction

The Simple Harmonic Oscillator (SHO) problem has an indispensable role in physics. It is customary to use the SHO to illustrate the basic concepts and new methods in classical as well as quantum physics. The wave mechanical theory of oscillators provides the basis for understanding the properties of a wide variety of systems which are analysable in terms of harmonic oscillators. It is useful not only in the study of vibrations of diatomic and polyatomic molecules, but also in the study of vibrations of other more complicated systems expressed in terms of their normal modes. Thus its applications are not limited to molecular spectroscopy, but extend to a variety of branches of modern physics such as solid state physics, nuclear structure, quantum field theory, quantum optics, quantum statistical mechanics and so forth.

Our study is essentially based on the q -deformed oscillator introduced by Biedenharn [2] and Macfarlane [3]. They have investigated the connection between q -oscillators and q -deformed algebras. Since then, there has been an increasing interest in the study of physical systems using the concept of q -oscillators. We start with a discussion of Heisenberg-Weyl algebra and its q -deformation.

2.2 Harmonic oscillator as a realisation of Heisenberg-Weyl algebra

For simplicity, we consider the one-dimensional harmonic oscillator. In classical mechanics, its Hamiltonian H is expressed in terms of the co-ordinate x and the conjugate momentum p as

$$H = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2 \quad (2.1)$$

where m is the mass and ω is the angular frequency of the oscillator. The transition to the quantum mechanical scenario is carried out by replacing x and p with their operator analogues:

$$\begin{aligned} x &\rightarrow \hat{x} \\ p &\rightarrow \hat{p} = -i\hbar \frac{\partial}{\partial x}. \end{aligned}$$

x and p satisfy the commutation relation

$$[x, p] = i\hbar \quad (2.2)$$

or in the case of a system with many degrees of freedom,

$$[\hat{Q}_\mu, \hat{P}_\nu] = i\hbar \delta_{\mu\nu} \hat{I} \quad (2.3)$$

where Q_μ and P_μ are co-ordinates and conjugate momenta and \hat{I} is the identity operator. The set of elements \hat{Q}_μ , \hat{P}_μ and $\hbar \hat{I}$ close an algebra known as the *Heisenberg algebra* \mathcal{H} [35].

The Hamiltonian can also be represented in terms of the abstract operators a and a^\dagger :

$$a = \sqrt{\frac{m\omega}{2\hbar}} \hat{x} + \frac{i}{\sqrt{2m\omega\hbar}} \hat{p} \quad (2.4)$$

$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \hat{x} - \frac{i}{\sqrt{2m\omega\hbar}} \hat{p} \quad (2.5)$$

Then

$$[a, a^\dagger] = 1 \quad (2.6)$$

The operator

$$N = a^\dagger a \quad (2.7)$$

also plays an important role. It is hermitian, i.e, $N = N^\dagger$. It satisfies the relations

$$[N, a^\dagger] = a^\dagger \quad (2.8)$$

$$[N, a] = -a \quad (2.9)$$

The four elements a , a^\dagger , N and I , satisfying the above commutation relations, constitute what is known as *Heisenberg-Weyl algebra*, denoted by \mathcal{H}_4 .

The quantum mechanics of the system is based on the Heisenberg-Weyl algebra.

In terms of the new operators,

$$\begin{aligned} H &= \hbar \omega \left(a^\dagger a + \frac{1}{2} \right) \\ &= \hbar \omega \left(N + \frac{1}{2} \right) \end{aligned} \quad (2.10)$$

Thus H commutes with N and hence H and N possess simultaneous eigen functions.

It is well-known that the spectrum of N consists of the set of non-negative integers

$$n = 0, 1, 2, \dots, \infty \quad (2.11)$$

The normalised eigenvector of N belonging to the eigenvalue n is denoted by the ket $|n\rangle$. i.e,

$$N |n\rangle = n |n\rangle \quad (2.12)$$

The set $\{|n\rangle\}$ of vectors for n varying from 0 to ∞ constitutes a complete orthonormal set and defines a representation called *occupation number representation*. The operators N and H are diagonal in this representation.

$$\langle m | N | n \rangle = n \delta_{mn} \quad (2.13)$$

The Hilbert space spanned by $\{|n\rangle\}$ is called *Fock space*. The state $|n\rangle$ is obtained by a^\dagger , acting n times on the state $|0\rangle$:

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}} |0\rangle \quad (2.14)$$

$$a^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle \quad (2.15)$$

$$a |n\rangle = \sqrt{n} |n-1\rangle \quad (2.16)$$

$$a |0\rangle = 0 \quad (2.17)$$

The matrices representing the operators a , a^\dagger , N and H are respectively

$$a = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \dots \\ 0 & 0 & \sqrt{2} & 0 & 0 & \dots \\ 0 & 0 & 0 & \sqrt{3} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$a^\dagger = \begin{pmatrix} 0 & 0 & 0 & 0 & \dots \\ \sqrt{1} & 0 & 0 & 0 & \dots \\ 0 & \sqrt{2} & 0 & 0 & \dots \\ 0 & 0 & \sqrt{3} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$N = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \dots \\ 0 & 1 & 0 & 0 & 0 & \dots \\ 0 & 0 & 2 & 0 & 0 & \dots \\ 0 & 0 & 0 & 3 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$H = \hbar\omega \begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & \dots \\ 0 & \frac{3}{2} & 0 & 0 & 0 & \dots \\ 0 & 0 & \frac{5}{2} & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

The energy values $\frac{1}{2}\hbar\omega, \frac{3}{2}\hbar\omega, \frac{5}{2}\hbar\omega\dots$ are equally spaced.

This abstract operator analysis permits the following interpretation:

The oscillator in the state $|n\rangle$ is an assembly of n non-interacting particles, each of energy $\hbar\omega$. The different states of the oscillator correspond to different numbers of the particles. The operator a^\dagger raises the particle number by 1 whereas the operator a lowers the particle number by 1. Hence a^\dagger and a are referred to as *creation operator* and *annihilation operator* respectively. N is interpreted as the *number operator* since its eigenvalue gives the number of particles in the given state. The state $|0\rangle$ corresponds to no particle and is called the *vacuum state*. $a|0\rangle = 0$ and $a^\dagger|0\rangle \sim |1\rangle$ are consistent with this interpretation since a particle cannot be destroyed when no particle is initially present, whereas a particle can be created even when no particle is initially present.

The operators a, a^\dagger and N are usually referred to as *boson operators* since there is no restriction to the number of particles occupying any state.

If one deforms the underlying algebra (2.6–2.9), the quantum mechanics based on the deformed algebra will have a different form.

2.3 q-deformed Heisenberg-Weyl algebra (q-oscillator algebra)

The algebra of the three elements N_q , a_q and a_q^\dagger is referred to as a q-deformed Heisenberg-Weyl algebra \mathcal{H}_{q} if they satisfy the commutation relations

$$\begin{aligned} [N_q, a_q^\dagger] &= a_q^\dagger ; \\ [N_q, a_q] &= -a_q ; \\ [a_q, a_q^\dagger]_q &= a_q a_q^\dagger - q a_q^\dagger a_q = q^{-N_q} \end{aligned} \quad (2.18)$$

This definition was given by Beidenharn [2]. The operators a_q^\dagger , a_q and N_q are referred to as q-boson creation operator, q-boson annihilation operator and q-boson number operator respectively. N_q is hermitian but

$$N_q \neq a_q^\dagger a_q \quad (2.19)$$

$[a_q, a_q^\dagger]_q$ is called the q-commutator. In general, for any two operators A and B ,

$$[A, B]_q = A B - q B A \quad (2.20)$$

where q is some parameter which may be real or complex. It satisfies the properties

$$[A, B]_q = -q [B, A]_{q^{-1}} \quad (2.21)$$

and

$$\lim_{q \rightarrow 1} [A, B]_q = [A, B] , \quad (2.22)$$

the usual commutator in quantum mechanics.

The q -commutators do not satisfy the Jacobi identity. Quesne [36] has shown that q -commutators satisfy some q -deformed Jacobi identity.

The algebra (2.18) is also referred to as q -oscillator algebra or q -boson algebra. In the limit $q \rightarrow 1$, it tends to the standard oscillator algebra or Heisenberg-Weyl algebra and the q -deformed quantum mechanics will tend to the standard quantum mechanics. This is a manifestation of the correspondence principle.

There exist other equivalent definitions of q -deformed Heisenberg-Weyl algebra in terms of other sets of operators [35] which differ from (2.18). In some cases, they have some advantages from a practical point of view.

The q -oscillator algebra is proved to be a quantum group. Its Hopf algebraic structure also has been set up [37].

2.4 q -oscillator description of $SU_q(2)$ and $SU_q(1, 1)$

The harmonic oscillator is a convenient tool to obtain representations of some Lie algebras. The concept of q -deformed harmonic oscillator was introduced by Biedenharn [2] and independently by Macfarlane [3] in 1989. Biedenharn had developed a new realisation of the quantum group $SU_q(2)$ using a q -analogue of the Jordan-Schwinger mapping. To achieve this, he postulated the q -oscillator algebra (2.18) which is a generalisation of the Heisenberg-Weyl algebra. To realise the Lie algebra of the generators of $SU_q(2)$, a pair of mutually commuting q -harmonic oscillator systems with operators a_{iq}^\dagger and a_{iq} with $i = 1, 2$ is considered. Then the

q-analogue of the Jordan-Schwinger map is defined:

$$\begin{aligned}
J_+ &= a_{1q}^\dagger a_{2q} \\
J_- &= a_{2q}^\dagger a_{1q} = J_+^\dagger \\
J_z &= \frac{1}{2}(N_{1q} - N_{2q})
\end{aligned} \tag{2.23}$$

These generators satisfy the $su_q(2)$ algebra (1.38):

$$\begin{aligned}
[J_z, J_\pm] &= \pm J_\pm; \\
[J_+, J_-] &= [2J_z]_q
\end{aligned}$$

The algebra generated by the three elements K_+ , K_- and K_0 such that

$$\begin{aligned}
[K_0, K_\pm] &= \pm K_\pm; \\
[K_+, K_-] &= -2K_0
\end{aligned} \tag{2.24}$$

is referred to as $su(1,1)$ algebra. In the quantum case, the generators of $su_q(1,1)$ satisfy the commutation relations [38&39]

$$\begin{aligned}
[K_0, K_\pm] &= \pm K_\pm; \\
[K_+, K_-] &= -[2K_0]_q
\end{aligned} \tag{2.25}$$

The generators K_+ , K_- and K_0 of $SU_q(1,1)$ accept the following q-boson representation:

$$\begin{aligned}
K_+ &= a_{1q}^\dagger a_{2q}^\dagger; \\
K_- &= a_{1q} a_{2q}; \\
K_0 &= \frac{1}{2}(N_{1q} + N_{2q} + 1)
\end{aligned} \tag{2.26}$$

2.5 Properties of q-boson operators

From the defining relations (2.18), the following properties of q-boson operators can be deduced.

(1)

$$a_q^\dagger f(N_q) = f(N_q - 1) a_q^\dagger \quad (2.27)$$

$$a_q f(N_q) = f(N_q + 1) a_q \quad (2.28)$$

$$[N_q, a_q^\dagger a_q] = [N_q, a_q a_q^\dagger] = 0 \quad (2.29)$$

or in general,

$$[a_q a_q^\dagger, f(N_q)] = [a_q^\dagger a_q, f(N_q)] = 0 \quad (2.30)$$

where $f(N_q)$ is an arbitrary function of N_q .

To prove relation (2.27), we consider the algebraic relation

$$[N_q, a_q^\dagger] = a_q^\dagger$$

i.e.,

$$\begin{aligned} N_q a_q^\dagger - a_q^\dagger N_q &= a_q^\dagger \\ a_q^\dagger N_q &= (N_q - 1) a_q^\dagger \\ a_q^\dagger N_q^2 &= (N_q - 1) a_q^\dagger N_q \\ &= (N_q - 1)^2 a_q^\dagger \end{aligned}$$

and by induction,

$$a_q^\dagger N_q^k = (N_q - 1)^k a_q^\dagger$$

Let

$$f(N_q) = \sum_s c_s N_q^s$$

Then

$$\begin{aligned} a_q^\dagger f(N_q) &= \sum_s c_s a_q^\dagger N_q^s \\ &= \sum_s c_s (N_q - 1)^s a_q^\dagger \\ &= f(N_q - 1) a_q^\dagger \end{aligned}$$

Relation (2.28) can be proved in a similar way by considering the defining relation

$$[N_q, a_q] = -a_q$$

Relation (2.29) immediately follows from relations (2.27) and (2.28).

(2) The parameter q is either real or is a pure phase.

To prove this, we take the defining relation

$$a_q a_q^\dagger - q a_q^\dagger a_q = q^{-N_q}$$

Taking the hermitian conjugate,

$$a_q a_q^\dagger - q^* a_q^\dagger a_q = (q^*)^{-N_q}$$

In order that these two equations coincide, either $q^* = q$ or $q^* = q^{-1}$. i.e., either q is real or q is a pure phase.

If q is real, it can be expressed as

$$q = e^\eta, \quad (2.31)$$

η being real. Then the q -number

$$\begin{aligned} [x]_q &= \frac{q^x - q^{-x}}{q - q^{-1}} \\ &= \frac{e^{\eta x} - e^{-\eta x}}{e^\eta - e^{-\eta}} \\ &= \frac{\sinh(\eta x)}{\sinh(\eta)} \end{aligned} \quad (2.32)$$

If q is a pure phase, of the form

$$q = e^{i\eta}, \quad (2.33)$$

$$\begin{aligned} [x]_q &= \frac{e^{i\eta x} - e^{-i\eta x}}{e^{i\eta} - e^{-i\eta}} \\ &= \frac{\sin(\eta x)}{\sin(\eta)} \end{aligned} \quad (2.34)$$

(3) The bilinear forms become

$$a_q^\dagger a_q = [N_q]_q \quad (2.35)$$

$$a_q a_q^\dagger = [N_q + 1]_q \quad (2.36)$$

(4) The above properties remain invariant w.r.t. the symmetry $q \rightarrow q^{-1}$.

(5) In the limit $q \rightarrow 1$, the q -numbers (or operators) tend to the ordinary numbers (or operators).

$$\lim_{q \rightarrow 1} [x]_q = \lim_{\eta \rightarrow 0} \frac{\sin(\eta x)}{\sin(\eta)} = x$$

$$\begin{aligned}\lim_{q \rightarrow 1} (a_q^\dagger a_q) &= \lim_{q \rightarrow 1} [N_q]_q = N_q \\ \lim_{q \rightarrow 1} (a_q a_q^\dagger) &= \lim_{q \rightarrow 1} [N_q + 1]_q = N_q + 1\end{aligned}$$

(6) In general, $N_q \neq a_q^\dagger a_q$. However, Polychronakos [40] have shown that there exists a classical realisation of the q-oscillator algebra in which $N_q = N = a^\dagger a$.

We call this as the *boson realisation* of q-oscillator algebra. In this,

$$a_q^\dagger = \sqrt{\frac{[N]_q}{N}} a^\dagger \quad (2.37)$$

$$a_q = \sqrt{\frac{[N+1]_q}{N+1}} a \quad (2.38)$$

$$a_q a_q^\dagger - q a_q^\dagger a_q = q^{-N} \quad (2.39)$$

and

$$N_q = N \quad (2.40)$$

Then

$$a_q^\dagger a_q = [N] \quad (2.41)$$

$$a_q a_q^\dagger = [N+1] \quad (2.42)$$

In this realisation, the eigenstates of N_q are the same as those of N .

It is worth noting that there is an isomorphism between the q-oscillator algebra and the q-differential operator algebra. The q-oscillator algebraic relations

$$\begin{aligned}[N_q, a_q] &= -a_q \\ [N_q, a_q^\dagger] &= a_q^\dagger \\ a_q a_q^\dagger - q a_q^\dagger a_q &= q^{-N_q}\end{aligned}$$

possess a one-to-one correspondence to the commutation relations in q-differential calculus:

$$\begin{aligned} [x\partial_x, \mathcal{D}_x] &= -\mathcal{D}_x \\ [x\partial_x, x] &= x \\ \mathcal{D}_x x - q^{-1} x \mathcal{D}_x &= q^{x\mathcal{D}_x} \end{aligned}$$

Here \mathcal{D}_x is the q-derivative w.r.t. x .

Thus

$$x \leftrightarrow a_q^\dagger, \quad \mathcal{D}_x \leftrightarrow a_q, \quad x\partial_x \leftrightarrow N_q \quad (2.43)$$

2.6 Eigenstates of N_q

In the classical realisation of the q-oscillator algebra introduced by Polychronakos [40], $N_q = N = a^\dagger a$ and the basis vectors $|n\rangle_q$ of N_q are chosen to be the same as those of the usual harmonic oscillator:

$$N_q |n\rangle_q = N |n\rangle_q = n |n\rangle_q \quad (2.44)$$

i.e, the eigenvalues of N_q are also the integers from 0 to ∞ , and hence N_q is interpreted as the number of q-deformed bosons. In order to obtain the representation of the q-deformed boson algebra bounded below, it is postulated that there exists a vector $|0\rangle_q$ with the properties

$$\begin{aligned} a_q |0\rangle_q &= a_q |0\rangle = 0; \\ N_q |0\rangle_q &= N |0\rangle_q = 0 \end{aligned} \quad (2.45)$$

$|0\rangle_q$ is referred to as the q-deformed vacuum state and is interpreted as a state without bosons. The interpretation of a_q^\dagger and a_q as raising and lowering operators or as creation and annihilation operators also holds.

The eigenstates $|n\rangle_q$ are orthonormal.

$$|n\rangle_q = \frac{(a_q^\dagger)^n}{\sqrt{[n]_q!}} |0\rangle_q \quad (2.46)$$

It can be easily seen that

$$a_q |n\rangle_q = \sqrt{[n]_q} |n-1\rangle_q \quad (2.47)$$

$$a_q^\dagger |n\rangle_q = \sqrt{[n+1]_q} |n+1\rangle_q \quad (2.48)$$

$${}_q\langle n+1 | a_q^\dagger | n \rangle_q = \sqrt{[n+1]_q} \quad (2.49)$$

$${}_q\langle n-1 | a_q | n \rangle_q = \sqrt{[n]_q} \quad (2.50)$$

In general, the operators a_q^\dagger and a_q can be represented as infinite dimensional matrices

$$a_q^\dagger = \begin{pmatrix} 0 & \sqrt{[1]_q} & 0 & 0 & 0 & \dots \\ 0 & 0 & \sqrt{[2]_q} & 0 & 0 & \dots \\ 0 & 0 & 0 & \sqrt{[3]_q} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$a_q = \begin{pmatrix} 0 & 0 & 0 & 0 & \dots \\ \sqrt{[1]_q} & 0 & 0 & 0 & \dots \\ 0 & \sqrt{[2]_q} & 0 & 0 & \dots \\ 0 & 0 & \sqrt{[3]_q} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

The Hilbert space spanned by $\{|n\rangle_q\}$ is positive definite only if $|q| \leq 1$. For larger values of $|q|$, states with negative squared norm arise and the probability interpretation of quantum mechanics is lost.

When one tries to apply the q -deformed algebras for the description of real physical systems, it is seen that good agreement with experimental data is obtained only if q is chosen as a pure phase, of the form $e^{i\eta}$ and η is chosen to be small.

2.7 Energy spectrum of q -deformed harmonic oscillator

The Hamiltonian of the q -deformed harmonic oscillator is

$$H_q = \frac{p_q^2}{2m} + \frac{1}{2} m \omega^2 x_q^2 \quad (2.51)$$

where the q -position x_q and the q -momentum p_q of the oscillator are related to the q -creation and q -annihilation operators a_q^\dagger and a_q as in eqs.(2.4) and (2.5).

$$x_q = \sqrt{\frac{\hbar}{2m\omega}} (a_q^\dagger + a_q) \quad (2.52)$$

$$p_q = \sqrt{\frac{\hbar m \omega}{2}} (a_q^\dagger - a_q) \quad (2.53)$$

where a_q and a_q^\dagger satisfy the q-oscillator algebra (2.18). In terms of a_q and a_q^\dagger , the Hamiltonian reads

$$\begin{aligned} H_q &= \frac{1}{2} \hbar\omega (a_q^\dagger a_q + a_q a_q^\dagger) \\ &= \frac{1}{2} \hbar\omega ([N]_q + [N+1]_q) \end{aligned} \quad (2.54)$$

Here we are using the boson realisation of the q-oscillator algebra in which $N_q = N$. The number and energy eigenstates of the q-oscillator are then the same as those of the usual harmonic oscillator and are q-independent. Only eigenvalues are q-dependent. The energy eigenvalues are given by the eigenvalue equation

$$\begin{aligned} H_q |n\rangle &= E_{qn} |n\rangle \\ \frac{1}{2} \hbar\omega ([N]_q + [N+1]_q) |n\rangle &= E_{qn} |n\rangle \end{aligned}$$

Thus

$$E_{qn} = \frac{1}{2} \hbar\omega ([n]_q + [n+1]_q) |n\rangle \quad (2.55)$$

i.e, the energy levels of the q-oscillator are not uniformly spaced for $q \neq 1$. The behaviour of the energy spectra is completely different in the cases $q = e^\eta$ and $q = e^{i\eta}$. When q is real ($q = e^\eta$), the separation between the levels increases with the value of n . i.e, the spectrum is *extended*. On the other hand, when q is a pure phase, the separation between the levels decreases with increasing n . i.e, the spectrum is *squeezed*. The spectrum in this case exhibits many characteristic features of the anharmonic oscillator. The energy levels of the anharmonic oscillator are not equidistant but their separation decreases when the value of the oscillator quantum

number v increases:

$$E_v = \hbar\omega \left(v + \frac{1}{2}\right) - \hbar\omega x_e \left(v + \frac{1}{2}\right)^2 + \hbar\omega y_e \left(v + \frac{1}{2}\right)^3 - \dots \quad (2.56)$$

where $\omega y_e \ll \omega x_e \ll \omega$ and v takes only a limited number of values ($v \leq v_{max}$) because of the finite depth of the potential well. The energy values of the q-deformed harmonic oscillator can be written as

$$\begin{aligned} E_{qv} &= \frac{1}{2} \hbar\omega \left([v]_q + [v+1]_q \right) \\ &= \begin{cases} \frac{1}{2} \hbar\omega \left(\frac{\sinh \eta(v+\frac{1}{2})}{\sinh(\frac{\eta}{2})} \right) & \text{if } q = e^\eta \\ \frac{1}{2} \hbar\omega \left(\frac{\sin \eta(v+\frac{1}{2})}{\sin(\frac{\eta}{2})} \right) & \text{if } q = e^{i\eta} \end{cases} \end{aligned} \quad (2.57)$$

The second expression on expanding, we get

$$E_{qv} = \frac{1}{2} \hbar\omega \frac{\eta}{\sin(\frac{\eta}{2})} \left[\left(v + \frac{1}{2}\right) - \frac{\eta^2}{6} \left(v + \frac{1}{2}\right)^3 + \dots \right] \quad (2.58)$$

Comparing this with the expression (2.56), we see that there is a great similarity between the spectrum of the q-deformed harmonic oscillator and that of the anharmonic oscillator describing the vibrational spectra of diatomic molecules. However, the coincidence is only a qualitative one. Expression (2.58) contains only the odd powers of $(v + \frac{1}{2})$ whereas expression (2.56) contains odd as well as even powers of $(v + \frac{1}{2})$.

$$\lim_{q \rightarrow 1} E_{qv} = \hbar\omega \left(v + \frac{1}{2}\right) \quad (2.59)$$

i.e, in the limit $q \rightarrow 1$, the energy spectrum of the q-deformed harmonic oscillator coincides with that of the standard harmonic oscillator.

Besides the energy spectrum, other properties of q-oscillators are also well studied. For example, coherent states and squeezed states of q-harmonic oscillators have been investigated by many authors [41--43].

2.8 Statistical mechanics of q-harmonic oscillator

Neskovic and Urosevic [44] have studied the statistical mechanics of q-deformed harmonic oscillators. Using the boson realisation of q-oscillator algebra and taking q to be real, they have calculated the partition function Z and thermodynamic potentials such as Gibb's free energy F , entropy S and internal energy U for a Slightly Deformed Oscillator (SDO). Taking $q = e^\eta$ and for small values of η , they obtained the following results for Hamiltonian and the themodynamic functions:

$$H_{SDO} = H_0 + \frac{\eta^2}{3!} H_1 \quad (2.60)$$

where

$$H_1 = \frac{1}{2} \hbar \omega \left[N^3 + (N+1)^3 - (2N+1) \right] \quad (2.61)$$

and

$$Z_{SDO} = Z_0 \left\{ 1 + \beta \frac{\eta^2}{3!} E_1 \right\}; \quad (2.62)$$

$$F_{SDO} = F_0 - \frac{\eta^2}{3!} E_1; \quad (2.63)$$

$$U_{SDO} = U_0 - \frac{\eta^2}{3!} \left\{ E_1 - T \frac{\partial E_1}{\partial T} \right\}; \quad (2.64)$$

$$S_{SDO} = S_0 + \frac{\eta^2}{3!} \frac{\partial E_1}{\partial T} \quad (2.65)$$

where Z_0 , F_0 , U_0 and S_0 are the corresponding quantities for the usual harmonic oscillator and

$$E_1 = - \langle H_1 \rangle_0 \quad (2.66)$$

2.9 Description of some physical systems in terms of q-oscillator algebra

Numerous applications of quantised algebra to real physical systems have been worked out by various authors. Here we cite a few of them.

The $su_q(1, 1)$ quantum algebra has been used to describe the vibrational spectra of diatomic molecules [45]. It is seen that when q is chosen as a phase, the results show fair agreement with the experimental data in the case of vibrational spectra of diatomic molecules such as H_2 , for $\eta \simeq .06$. The second order Casimir operator of $su_q(1, 1)$ corresponds to a special form of the Dunham expansion containing all powers of $(v + \frac{1}{2})$ while in the classical case of $su(1, 1)$, only the first two non-vanishing powers of $(v + \frac{1}{2})$ are obtained.

A q-rotator model with $SU_q(2)$ quantum symmetry has been set up to describe the rotational spectra of diatomic molecules [46]. For deformation parameter $\eta \simeq .01$, the spectra of the q-rotator model coincide with the observed spectra to satisfactory accuracy. A complete quantum group theoretic treatment of vibrating and rotating diatomic molecules has also been given [47] by assuming the deformation parameter q of the q-oscillator algebra to depend on the rotational quantum number J .

The coincidence between the predictions of the model and conventional phenomenological formulae is remarkable. The dependence of q on J seems to characterise the interaction between vibration and rotation.

The $su_q(2)$ algebra has been used for the description of energy spectra of the deformed even-even nuclei [48], and it is shown that there is good agreement with experimental results when q is chosen as a phase ($q = e^{i\eta}$) with $\eta \simeq .04$

The many-body problem of q -oscillators has been investigated by several authors [49–51]. The spectra of the system are found to be rich, exhibiting interactions between the levels of the individual oscillators. The deformed algebra has also been employed to the many-body problem of composite particles [52]. The deformation parameter is interpreted as a measure of the effects of the statistics of the internal degrees of freedom of the composite particles.

The q -oscillator models in two and higher dimensions is applied to the spectra of triatomic molecules such as H_2O and superdeformed nuclei [53].

The $sc_q(4)$ algebra has been used for the description of a q -analogue of the hydrogen atom [54] and it is seen that the spectrum and degeneracy of the q -analogue of the hydrogen atom is different from that of the real systems.

The nature of an electromagnetic field of high intensity , modelled by q-oscillators has been discussed and it is shown that the non-linearity of such an electromagnetic field may produce in the electrostatic regime, a deviation from the Coulomb law and a form-factor of a charged particle [55].

Chapter 3

q-ANHARMONIC OSCILLATOR WITH QUARTIC INTERACTION

3.1 Introduction

The q-harmonic oscillator algebra discussed in detail in the second chapter, is a well studied topic. In real physical systems, one cannot dismiss the role of anharmonicity. For example, the assumption of molecular and crystalline vibrations to be of harmonic type is an idealisation and experimental observations indicate deviations from the predictions based on harmonic approximation. The discrepancy between theoretical predictions and experimental results, to a certain extent, can be removed by assuming that the vibrations are of anharmonic type. In this chapter, we present the study of q-deformations of an anharmonic oscillator with quartic interaction in first order perturbation theory. The energy spectrum and statistical mechanics of q-Anharmonic Oscillators (q-AO) are discussed.

3.2 Anharmonic oscillator and its energy spectrum

We consider the anharmonic oscillator described by the Hamiltonian

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 + \frac{\lambda}{4!} x^4 \quad (3.1)$$

where λ is positive and assumed to be very small.

In the Fock-space representation, H takes the form [56]

$$H = \hbar\omega(N + \frac{1}{2}) + \frac{\lambda}{4!} \left(\frac{\hbar}{2m\omega}\right)^2 (6N^2 + 6N + 3) \quad (3.2)$$

where N is the number operator having eigenvalues $0, 1, 2, \dots, \infty$. The second expression on the RHS of eq.(3.2) makes sense only for low-lying levels

3.3 Energy spectrum of q-AO

The Hamiltonian of the q-analogue of the anharmonic oscillator is taken to be

$$\bar{H} = \frac{\bar{p}^2}{2m} + \frac{1}{2} m\omega^2 \bar{x}^2 + \frac{\lambda}{4!} \bar{x}^4 \quad (3.3)$$

The q-position operator \bar{x} and the q-momentum operator \bar{p} of the q-AO are related to the q-boson operators a_q and a_q^\dagger in the same way as in the case of q-deformed harmonic oscillators (see eqs.(2.52) and (2.53)). We work in the boson realisation

in which $N_q = N = a^\dagger a$ and the eigenstates are those of the usual harmonic oscillator. Hereafter we drop the suffix q for q -deformed operators and q -numbers for convenience. Thus

$$\bar{x} = \sqrt{\frac{\hbar}{2m\omega}} (a + a^\dagger) \quad (3.4)$$

$$\bar{p} = i \sqrt{\frac{\hbar m\omega}{2}} (a - a^\dagger) \quad (3.5)$$

where

$$[N, a^\dagger] = a^\dagger ;$$

$$[N, a] = -a ;$$

$$a a^\dagger - q a^\dagger a = q^{-N} \quad (3.6)$$

In terms of these operators, the Hamiltonian takes the form

$$\bar{H} = \frac{1}{2} \hbar\omega (a^\dagger a + a a^\dagger) + \frac{\lambda}{4!} \left(\frac{\hbar}{2m\omega}\right)^2 (a + a^\dagger)^4 \quad (3.7)$$

What we are interested in, is the expectation values of \bar{H} in the eigenstates $|n\rangle$. The terms in \bar{H} containing different powers of a^\dagger and a have zero contribution to the expectation values:

$$\langle n | a | n \rangle = \sqrt{[n]} \langle n | n-1 \rangle = 0$$

$$\langle n | a^2 | n \rangle = \sqrt{[n][n-1]} \langle n | n-2 \rangle = 0$$

$$\langle n | a^\dagger a^2 | n \rangle = \sqrt{[n][n-1]} \langle n | n-1 \rangle = 0 \quad \text{and so on.}$$

Thus in expanding $(a + a^\dagger)^4$, we keep only those terms having same powers of a and a^\dagger . Using properties (2.27) and (2.28) of q -bosonic operators, we simplify these terms

as follows:

$$\begin{aligned}
a^2 a^{\dagger 2} &= [N+1] [N+2] \\
a^{\dagger 2} a^2 &= [N] [N-1] \\
a a^{\dagger} a a^{\dagger} &= [N+1] [N+1] \\
a a^{\dagger 2} a &= [N+1] [N] \\
a^{\dagger} a^2 a^{\dagger} &= [N] [N+1] \\
a^{\dagger} a a^{\dagger} a &= [N] [N]
\end{aligned}$$

Using these, eq.(3.7) becomes

$$\begin{aligned}
\bar{H} &= \frac{1}{2} \hbar\omega ([N+1] + [N]) \\
&+ \frac{\lambda}{4!} \left(\frac{\hbar}{2m\omega} \right)^2 \{ [N+1] [N+2] + [N+1] [N+1] \\
&+ 2[N+1] [N] + [N] [N] + [N] [N-1] \} \tag{3.8}
\end{aligned}$$

In the limit $q \rightarrow 1$, the q -number operators become ordinary operators and

$$\begin{aligned}
\bar{H} &\longrightarrow \frac{1}{2} \hbar\omega (2N+1) \\
&+ \frac{\lambda}{4!} \left(\frac{\hbar}{2m\omega} \right)^2 \{ (N+1)(N+2) + (N+1)^2 + 2(N+1)N + N^2 + N(N-1) \} \\
&= \left(N + \frac{1}{2} \right) \hbar\omega + \frac{\lambda}{4!} \left(\frac{\hbar}{2m\omega} \right)^2 (6N^2 + 6N + 3)
\end{aligned}$$

which is the same as (3.2), the Hamiltonian of the ordinary anharmonic oscillator.

To get an explicit expression for the Hamiltonian \bar{H} of the q -AO, we consider only slight deformations. Also q is chosen to be real:

$$q = e^\eta$$

or

$$\eta = \ln (q) \quad (3.9)$$

Then

$$[N] = \frac{\sinh (N\eta)}{\sinh (\eta)}$$

and

$$\begin{aligned} \bar{H} &= \frac{1}{2} \hbar \omega \left\{ \frac{\sinh (N\eta) + \sinh (N+1)\eta}{\sinh (\eta)} \right\} \\ &+ \frac{\lambda}{4!} \left(\frac{\hbar}{2m\omega} \right)^2 \frac{1}{\sinh^2(\eta)} \left\{ \sinh (N+2)\eta \sinh (N+1)\eta \right. \\ &+ \sinh^2(N+1)\eta + 2 \sinh (N+1)\eta \sinh (N\eta) \\ &+ \left. \sinh^2(N\eta) + \sinh (N\eta) \sinh (N-1)\eta \right\} \end{aligned} \quad (3.10)$$

For a Slightly Deformed Anharmonic Oscillator (SDAO), the deformation parameter q is very close to unity or η is very close to zero. Then the hyperbolic functions are expanded in Taylor series in powers of η and we retain only terms upto $O(\eta)^2$ in \bar{H} .

$$\sinh(x) = x + \frac{x^3}{3!} + \frac{x^5}{5!} + \frac{x^7}{7!} + \dots \quad (3.11)$$

$$\begin{aligned} &\frac{\sinh (N\eta) + \sinh (N+1)\eta}{\sinh (\eta)} \\ &= \frac{(N\eta) + \frac{(N\eta)^3}{3!} + \dots + (N+1)\eta + \frac{(N+1)^3\eta^3}{3!} + \dots}{\left(\eta + \frac{\eta^3}{3!} + \dots\right)} \\ &\approx \frac{\eta \left\{ (2N+1) + \frac{\eta^2}{3!} (N^3 + (N+1)^3) \right\}}{\eta \left(1 + \frac{\eta^2}{3!}\right)} \\ &\approx \left\{ (2N+1) + \frac{\eta^2}{3!} (N^3 + (N+1)^3) \right\} \left(1 - \frac{\eta^2}{3!}\right) \\ &\approx (2N+1) + \frac{\eta^2}{3!} (N^3 + (N+1)^3 - (2N+1)) \end{aligned} \quad (3.12)$$

$$\begin{aligned}
& \frac{\sinh(N+2)\eta \sinh(N+1)\eta}{\sinh^2\eta} \\
&= \frac{\left\{ (N+2)\eta + \frac{(N+2)^3\eta^3}{3!} + \dots \right\} \left\{ (N+1)\eta + \frac{(N+1)^3\eta^3}{3!} + \dots \right\}}{\left(\eta + \frac{\eta^3}{3!}\right)^2} \\
&\approx \frac{\eta \left\{ (N+2) + \frac{\eta^2}{3!} (N+2)^3 \right\} \eta \left\{ (N+1) + \frac{\eta^2}{3!} (N+1)^3 \right\}}{\eta^2 \left(1 + \frac{\eta^2}{3!}\right)^2} \\
&\approx (N+2)(N+1) + \frac{\eta^2}{3!} \left\{ (N+2)^3(N+1) \right. \\
&\quad \left. + (N+1)^3(N+2) - 2(N+2)(N+1) \right\} \tag{3.13}
\end{aligned}$$

Similarly

$$\left(\frac{\sinh(N+1)\eta}{\sinh\eta} \right)^2 \approx (N+1)^2 + \frac{\eta^2}{3!} \left\{ 2(N+1)^4 - 2(N+1)^2 \right\} \tag{3.14}$$

$$\begin{aligned}
\frac{\sinh(N+1)\eta \sinh(N)\eta}{\sinh^2\eta} &\approx N(N+1) + \frac{\eta^2}{3!} \left\{ N^3(N+1) \right. \\
&\quad \left. + (N+1)^3N - 2N(N+1) \right\} \tag{3.15}
\end{aligned}$$

$$\left(\frac{\sinh(N)\eta}{\sinh\eta} \right)^2 \approx N^2 + \frac{\eta^2}{3!} \left\{ 2N^4 - 2N^2 \right\} \tag{3.16}$$

$$\begin{aligned}
\frac{\sinh(N)\eta \sinh(N-1)\eta}{\sinh^2\eta} &\approx N(N-1) + \frac{\eta^2}{3!} \left\{ N^3(N-1) \right. \\
&\quad \left. + (N-1)^3N - 2N(N-1) \right\} \tag{3.17}
\end{aligned}$$

Substituting eqs. (3.12)-(3.17) in eq.(3.10), the Hamiltonian of the SDAO is obtained as

$$\begin{aligned}
\bar{H}_{SDAO} &= \frac{1}{2} \hbar\omega (2N+1) + \frac{\eta^2}{3!} \frac{1}{2} \hbar\omega \left((N+1)^3 + N^3 - (2N+1) \right) \\
&+ \frac{\lambda}{4!} \left(\frac{\hbar}{2m\omega} \right)^2 (6N^2 + 6N + 3) \\
&+ \frac{\eta^2}{3!} \frac{\lambda}{4!} \left(\frac{\hbar}{2m\omega} \right)^2 (12N^4 + 24N^3 + 36N^2 + 24N + 6) \tag{3.18}
\end{aligned}$$

As $q \rightarrow 1$ or $\eta \rightarrow 0$, this expression tends to (3.2), the Hamiltonian of the usual boson anharmonic oscillator. The quartic anharmonic correction (to first order in λ) to the energy levels of the boson realisation of the q-oscillator follow at once by calculating $\langle n | \bar{H}_{SDAO} | n \rangle$ where $|n\rangle$'s are the unperturbed eigenstates.

3.4 Statistical Mechanics of q-AO

The quantity which is of prime interest in the study of thermodynamics of systems is the partition function

$$Z = \text{Tr}(e^{-\beta H}) \quad (3.19)$$

where $\beta = \frac{1}{k_B T}$, k_B being the Boltzmann's constant, T, the absolute temperature of the system and H, the Hamiltonian of the system. In the case of an assembly of SDAOs, H is given by eq.(3.18). For convenience, we write it in the form

$$\bar{H}_{SDAO} = H_0 + \frac{\eta^2}{3!} H_1 + H' + \frac{\eta^2}{3!} H'' \quad (3.20)$$

where

$$H_0 = \frac{1}{2} \hbar \omega (2N + 1) \quad (3.21)$$

$$H_1 = \frac{1}{2} \hbar \omega \left((N + 1)^3 + N^3 - (2N + 1) \right) \quad (3.22)$$

$$H' = \frac{\lambda}{4!} \left(\frac{\hbar}{2m\omega} \right)^2 (6N^2 + 6N + 3) \quad (3.23)$$

$$H'' = \frac{\lambda}{4!} \left(\frac{\hbar}{2m\omega} \right)^2 (12N^4 + 24N^3 + 36N^2 + 24N + 6) \quad (3.24)$$

H_0 is the Hamiltonian of the unperturbed harmonic oscillator. η and λ are assumed to be very small. Hence the last term in \bar{H}_{SDAO} which contains both η^2 and λ is very very small and is neglected. We consider the boson realisation in which the $|n\rangle$ are the eigenstates of H_0 . The partition function for the SDAO is then given by

$$\begin{aligned}
Z_{SDAO} &= \text{Tr.} \exp(-\beta \bar{H}_{SDAO}) \\
&\approx \sum_n \langle n | \exp(-\beta (H_0 + \frac{\eta^2}{3!} H_1 + H')) | n \rangle \\
&= \sum_n \langle n | \exp(-\beta H_0) \exp(-\beta (\frac{\eta^2}{3!} H_1 + H')) | n \rangle \\
&= \sum_n \langle n | \exp(-\beta H_0) \left\{ 1 - \beta (\frac{\eta^2}{3!} H_1 + H') \right\} | n \rangle \\
&= \sum_n \langle n | \exp(-\beta H_0) | n \rangle - \beta \sum_n \langle n | \frac{\eta^2}{3!} H_1 + H' | n \rangle \\
&= Z_0 \left\{ 1 - \beta (\frac{\eta^2}{3!} \langle H_1 \rangle + \langle H' \rangle) \right\} \tag{3.25}
\end{aligned}$$

where

$$Z_0 = \sum_n \langle n | \exp(-\beta H_0) | n \rangle \tag{3.26}$$

is the partition function of the ordinary harmonic oscillator and $\langle H_1 \rangle$ and $\langle H' \rangle$ are the thermal averages of H_1 and H' respectively:

$$\langle H_1 \rangle = \frac{\sum_{n=0}^{\infty} \langle n | H_1 \exp(-\beta H_0) | n \rangle}{\sum_{n=0}^{\infty} \langle n | \exp(-\beta H_0) | n \rangle} \tag{3.27}$$

$$\begin{aligned}
&= \frac{\sum_{n=0}^{\infty} \langle n | \frac{1}{2} \hbar \omega \left\{ (N+1)^3 + N^3 - (2N+1) \right\} \exp(-\beta(N + \frac{1}{2})\hbar\omega) | n \rangle}{\sum_{n=0}^{\infty} \langle n | \exp(-\beta(N + \frac{1}{2})\hbar\omega) | n \rangle} \\
&= \frac{1}{2} \hbar \omega \frac{\sum_{n=0}^{\infty} \left[(n+1)^3 + n^3 - (2n+1) \right] \exp(-(n + \frac{1}{2})x)}{\sum_{n=0}^{\infty} \exp(-(n + \frac{1}{2})x)} \tag{3.28}
\end{aligned}$$

where we have put

$$\beta \hbar \omega = x \quad (3.29)$$

Now

$$\begin{aligned} \sum_{n=0}^{\infty} (n+1)^3 \exp\left(-\left(n+\frac{1}{2}\right)x\right) &= \exp\left(\frac{x}{2}\right) \sum_{n=0}^{\infty} (n+1)^3 e^{-(n+1)x} \\ &= \exp\left(\frac{x}{2}\right) \sum_{n=0}^{\infty} n^3 e^{-nx} \end{aligned}$$

$$\begin{aligned} \langle H_1 \rangle &= \frac{1}{2} \hbar \omega \left\{ e^{x/2} \sum_{n=0}^{\infty} n^3 e^{-nx} + e^{-x/2} \sum_{n=0}^{\infty} n^3 e^{-nx} \right. \\ &\quad \left. - 2e^{-x/2} \sum_{n=0}^{\infty} n e^{-nx} - e^{-x/2} \sum_{n=0}^{\infty} e^{-nx} \right\} / e^{-x/2} \sum_{n=0}^{\infty} e^{-nx} \\ &= \frac{1}{2} \hbar \omega \left\{ \sum_{n=0}^{\infty} n^3 e^{-nx} (e^x + 1) \right. \\ &\quad \left. - 2 \sum_{n=0}^{\infty} n e^{-nx} - \sum_{n=0}^{\infty} e^{-nx} \right\} / \sum_{n=0}^{\infty} e^{-nx} \quad (3.30) \end{aligned}$$

Using the results

$$\sum_{n=0}^{\infty} n^3 e^{-nx} = \frac{e^{3x} + 4e^{2x} + e^x}{(e^x - 1)^4} \quad (3.31)$$

$$\sum_{n=0}^{\infty} n e^{-nx} = \frac{e^{-x}}{(1 - e^{-x})^2} \quad (3.32)$$

and

$$\sum_{n=0}^{\infty} e^{-nx} = \frac{1}{1 - e^{-x}}, \quad (3.33)$$

eq.(3.30) gets simplified as

$$\langle H_1 \rangle = -\frac{1}{2} \hbar \omega - \frac{\hbar \omega}{(e^{\beta \hbar \omega} - 1)} + \hbar \omega \sinh(\beta \hbar \omega) g(\beta \hbar \omega) \quad (3.34)$$

where

$$g(\beta\hbar\omega) = \frac{e^{3\beta\hbar\omega} + 4e^{2\beta\hbar\omega} + e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega} - 1)^4}. \quad (3.35)$$

$$\begin{aligned} \langle H' \rangle &= \frac{\sum_{n=0}^{\infty} \langle n | H' \exp(-\beta H_0) | n \rangle}{\sum_{n=0}^{\infty} \langle n | \exp(-\beta H_0) | n \rangle} \quad (3.36) \\ &= \frac{\sum_{n=0}^{\infty} \langle n | \frac{\lambda}{4!} \left(\frac{\hbar}{2m\omega}\right)^2 (6N^2 + 6N + 3) \exp(-\beta(N + \frac{1}{2})\hbar\omega) | n \rangle}{\sum_{n=0}^{\infty} \langle n | \exp(-\beta(N + \frac{1}{2})\hbar\omega) | n \rangle} \\ &= \frac{\lambda}{4!} \left(\frac{\hbar}{2m\omega}\right)^2 \frac{\sum_{n=0}^{\infty} (6n^2 + 6n + 3) e^{-x(n+\frac{1}{2})}}{\sum_{n=0}^{\infty} e^{-x(n+\frac{1}{2})}} \\ &= \frac{\lambda\hbar^2}{32m^2\omega^2} \coth^2\left(\frac{\beta\hbar\omega}{2}\right) \quad (3.37) \end{aligned}$$

where we have used eqs.(3.32),(3.33) and also the result

$$\sum_{n=0}^{\infty} n^2 e^{-nx} = \frac{1 + e^{-x}}{(1 - e^{-x})^3} \quad (3.38)$$

Thus we find the partition function of the SDAO as

$$\begin{aligned} Z_{SDAO} &= Z_0 \left[1 + \beta \frac{\eta^2}{3!} \left\{ \frac{1}{2} \hbar\omega + \frac{\hbar\omega}{\exp(\beta\hbar\omega) - 1} \right. \right. \\ &\quad \left. \left. - \hbar\omega \sinh(\beta\hbar\omega) g(\beta\hbar\omega) \right\} - \frac{\beta\lambda\hbar^2}{32m^2\omega^2} \coth^2\left(\frac{\beta\hbar\omega}{2}\right) \right] \quad (3.39) \end{aligned}$$

In the limit $q \rightarrow 1$, this expression reduces to that of the usual anharmonic oscillator [56].

A knowledge of the partition function enables us to evaluate other thermodynamical quantities such as free energy F , internal energy U and entropy S which are defined by [57]

$$F = -k_B T \ln(Z) \quad (3.40)$$

$$U = k_B T^2 \frac{\partial}{\partial T} \ln(Z) = \frac{S}{\beta} + F \quad (3.41)$$

$$S = \beta^2 \frac{\partial F}{\partial \beta} \quad (3.42)$$

The partition function given by eq.(3.39) can be written as

$$Z_{SDAO} = Z_0 \left(1 + \beta \frac{\eta^2}{3!} U_1 + \frac{\lambda}{4!} \beta U_2 \right) \quad (3.43)$$

where

$$U_1 = \frac{1}{2} \hbar \omega + \frac{\hbar \omega}{\exp(\beta \hbar \omega) - 1} - \hbar \omega \sinh(\beta \hbar \omega) g(\beta \hbar \omega) \quad (3.44)$$

i.e.,

$$U_1 = U_0 - \hbar \omega \sinh(\beta \hbar \omega) g(\beta \hbar \omega) \quad (3.45)$$

with

$$U_0 = \frac{1}{2} \hbar \omega + \frac{\hbar \omega}{\exp(\beta \hbar \omega) - 1} \quad (3.46)$$

and

$$U_2 = -\frac{3\hbar^2}{4m^2\omega^2} \coth^2\left(\frac{\beta \hbar \omega}{2}\right) \quad (3.47)$$

The free energy F of the SDAO is then given by

$$\begin{aligned} F_{SDAO} &= -k_B T \ln(Z_{SDAO}) \\ &= -k_B T \ln Z_0 \left(1 + \beta \frac{\eta^2}{3!} U_1 + \beta \frac{\lambda}{4!} U_2 \right) \\ &= -k_B T \left(\ln Z_0 + \beta \frac{\eta^2}{3!} U_1 + \beta \frac{\lambda}{4!} U_2 \right) \end{aligned} \quad (3.48)$$

where we have used the result

$$\ln(1+x) \approx x \quad \text{when } x \ll 1 \quad (3.49)$$

Thus

$$F_{SDAO} = F_0 - \frac{\eta^2}{3!} U_1 - \frac{\lambda}{4!} U_2 \quad (3.50)$$

where

$$F_0 = -k_B T \ln(Z_0) \quad (3.51)$$

is the free energy of the usual harmonic oscillator.

The entropy S of the SDAO is

$$\begin{aligned} S_{SDAO} &= \beta^2 \frac{\partial}{\partial \beta} F_{SDAO} \\ &= \beta^2 \frac{\partial F_0}{\partial \beta} - \beta^2 \frac{\eta^2}{3!} \frac{\partial U_1}{\partial \beta} - \beta^2 \frac{\lambda}{4!} \frac{\partial U_2}{\partial \beta} \\ &= S_0 - \beta^2 \frac{\eta^2}{3!} \frac{\partial U_1}{\partial \beta} - \beta^2 \frac{\lambda}{4!} \frac{\partial U_2}{\partial \beta} \end{aligned} \quad (3.52)$$

Here

$$S_0 = \beta^2 \frac{\partial F_0}{\partial \beta} \quad (3.53)$$

is the entropy of the ordinary harmonic oscillator and

$$\frac{\partial U_1}{\partial \beta} = \frac{3(\hbar\omega)^2}{(exp\beta\hbar\omega - 1)^5} \left\{ e^{4\beta\hbar\omega} + 3e^{3\beta\hbar\omega} - 3e^{2\beta\hbar\omega} - e^{\beta\hbar\omega} \right\} \quad (3.54)$$

and

$$\frac{\partial U_2}{\partial \beta} = \frac{3\hbar^3}{4m^2\omega} \coth\left(\frac{\beta\hbar\omega}{2}\right) \operatorname{cosech}^2\left(\frac{\beta\hbar\omega}{2}\right) \quad (3.55)$$

The internal energy U of the SDAO is given by

$$\begin{aligned} U_{SDAO} &= \frac{S_{SDAO}}{\beta} + F_{SDAO} \\ &= \frac{S_0}{\beta} - \beta \frac{\eta^2}{3!} \frac{\partial U_1}{\partial \beta} - \beta \frac{\lambda}{4!} \frac{\partial U_2}{\partial \beta} \end{aligned}$$

$$\begin{aligned}
& + F_0 - \frac{\eta^2}{3!} U_1 - \frac{\lambda}{4!} U_2 \\
& = U_0 - \frac{\eta^2}{3!} \left(U_1 + \beta \frac{\partial U_1}{\partial \beta} \right) - \frac{\lambda}{4!} \left(U_2 + \beta \frac{\partial U_2}{\partial \beta} \right) \quad (3.56)
\end{aligned}$$

Here

$$U_0 = \frac{S_0}{\beta} + F_0 \quad (3.57)$$

is the internal energy of the usual harmonic oscillator.

Thus we find that the expressions of thermodynamic quantities of the q -deformed anharmonic oscillator consist of q -dependent correction terms and in the limit $q \rightarrow 1$, the results coincide with the classical results.

3.5 Conclusion

The effect of anharmonicity is well studied in classical and quantum physics. The study of q -AO and its thermodynamics carried out here is expected to be of relevance to investigations of anharmonic effects in molecular and condensed matter systems.

Chapter 4

LATTICE HEAT CAPACITY OF CRYSTALS—A q -OSCILLATOR DEBYE MODEL

4.1 Introduction

In this chapter, we present a model for lattice heat capacity of solids based on q -oscillator algebra. 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 harmonic oscillator. The lattice heat capacity is evaluated in the high and low temperature limits. A comparison of the theoretical results with experimental data is also presented.

The two basic experimental facts about the heat capacity of solids which any theory must explain are:

- (i) At room temperature, the heat capacity of most solids is close to $3k_B$ per atom so that for molecules consisting of n atoms, the molar heat capacity is close to

$3nR$ where R is the universal gas constant. Accurate measurements indicate temperature dependence of heat capacity in this region.

- (ii) At low temperatures, the heat capacities decrease and vanish at $T = 0$. The decrease goes as T^3 .

The Debye model for lattice heat capacity of solids has been remarkably successful in describing the experimental observations at low temperatures in many pure crystalline solids. In the low temperature regime, the Debye's theory predicts $C_v \propto T^3$ in agreement with experimental results. In the high temperature region ($T \gg \Theta_D$), the Debye model leads to the Dulong-Petit law: $C_v = 3R/\text{g.atom}$, a constant for all monoatomic crystals and is independent of temperature. This is not in exact agreement with experimental observations which show an increase of heat capacity with temperature.

Debye's theory involves three basic assumptions [58]: (i) isotropy of the solid (ii) nondispersion of sound waves in the medium and (iii) degeneracy of different branches of allowed modes. Above all, it is based on the harmonic approximation. Real crystals do exhibit anharmonic effects such as thermal expansion; the adiabatic and isothermal elastic constants are in general different and dependent on temperature and pressure. The influence of the anharmonicity on the various quantities for specific cases has been dealt with in a number of papers [59–62].

The concept of q-deformed harmonic oscillators has been discussed in

the second chapter. It is found that the energy levels of the q-oscillator are not equally spaced, but the energy spectrum is ‘squeezed’ when q is chosen as a pure phase. The q-oscillator model has been found to be suitable in accounting for the measurements on the infra-red spectrum of a number of molecules [45]. Thus there is already some appreciation of the fact that q-deformation can take care of anharmonicity effects to some extent. Motivated by this, we try to explain the temperature dependence of lattice heat capacity in the temperature region $T \gg \Theta_D$ by suggesting a q-oscillator Debye model.

Before presenting the q-oscillator Debye model, we recall the harmonic oscillator Debye model [63].

4.2 Heat capacity of a Harmonic crystal-Debye model

The solid is assumed to be a crystal lattice of atoms whose oscillations generate elastic waves. There are as many normal modes as the number of degrees of freedom. These normal modes behave as independent harmonic oscillators. The propagation of elastic waves in crystalline solids retaining their atomic structure is a difficult problem. However, for the propagation of sound waves which are elastic waves of low frequency, the wavelength λ is very large compared with the interatomic spacing a of the crystal ($\lambda \gg a$) and one can ignore the discrete atomic structure of the solid and describe it as a homogeneous elastic medium. Thus it is assumed that

only waves of low frequencies lying within a certain range $0 < \omega < \omega_D$ can propagate through the crystal. The cut-off frequency ω_D is called the Debye frequency. For simplicity, it is assumed that the medium is isotropic so that the velocity of propagation of elastic waves is independent of direction. To find the normal modes for low frequencies, we then need only find the different modes of standing waves possible in the medium. For each wave vector \vec{k} , there are two independent transverse directions of polarisation and one longitudinal polarisation. It is also assumed that for sufficiently low frequency, the velocity v of sound waves does not depend on frequency, i.e., there is no dispersion of sound waves in the crystal. Then the number of modes of each polarisation type with frequency between (ω) and $(\omega + d\omega)$ is given by

$$D(\omega) d\omega = \frac{V \omega^2}{2\pi^2 v^3} d\omega \quad (4.1)$$

where V is the volume of the crystal. It is further assumed that the phonon velocity is the same for the three directions of polarisation.

The total number (N_0) of atoms in the specimen is then related to the cut-off frequency ω_D through

$$\int_0^{\omega_D} D(\omega) d\omega = 3N_0 \quad (4.2)$$

i.e.,

$$\int_0^{\omega_D} \frac{V \omega^2}{2\pi^2 v^3} d\omega = 3N_0.$$

This gives

$$\omega_D = \left(\frac{6\pi^2 v^3 N_0}{V} \right)^{\frac{1}{3}} \quad (4.3)$$

Here it is assumed that the number of modes is so large that summations can be replaced by integrations.

The partition function of a harmonic oscillator with angular frequency ω_i at temperature T is given by [57]

$$\begin{aligned} z_i &= \sum_{n=0}^{\infty} \langle n | \exp(-\beta(N + \frac{1}{2})\hbar\omega) | n \rangle \\ &= \frac{\exp(-\frac{1}{2}\beta\hbar\omega_i)}{1 - \exp(-\beta\hbar\omega_i)} \end{aligned} \quad (4.4)$$

The contribution to the internal energy of the crystal from the i^{th} oscillator is

$$\begin{aligned} U_i &= k_B T^2 \frac{\partial}{\partial T} (\ln z_i) \\ &= \frac{1}{2} \hbar\omega_i + \frac{\hbar\omega_i}{\exp(\beta\hbar\omega_i) - 1} \end{aligned} \quad (4.5)$$

The total internal energy of the crystal is

$$\begin{aligned} U = \sum_i U_i &= \sum_i \left(\frac{1}{2} \hbar\omega_i + \frac{\hbar\omega_i}{\exp(\beta\hbar\omega_i) - 1} \right) \\ &= \sum_i \frac{1}{2} \hbar\omega_i + 3 \int_0^{\omega_D} \frac{\hbar\omega}{\exp(\beta\hbar\omega) - 1} D(\omega) d\omega \end{aligned}$$

The summation in the second sum has been replaced by integration. The factor 3 takes care of the three independent directions of polarisation. Substituting for $D(\omega)$ from (4.1), we get

$$U = U_0 + \frac{3\hbar V}{2\pi^2 v^3} \int_0^{\omega_D} \frac{\omega^3}{\exp(\beta\hbar\omega) - 1} d\omega \quad (4.6)$$

The zero point energy U_0 , being a constant, can be ignored in heat capacity calculations.

Putting

$$\begin{aligned}x &= \frac{\hbar\omega}{k_B T} = \frac{\Theta}{T}, \\x_D &= \frac{\hbar\omega_D}{k_B T} = \frac{\Theta_D}{T}, \\d\omega &= \frac{k_B T}{\hbar} dx,\end{aligned}\tag{4.7}$$

$$U = 9N_0 k_B T \left(\frac{T}{\Theta_D}\right)^3 \int_0^{x_D} \frac{x^3 dx}{e^x - 1}\tag{4.8}$$

Θ_D is called the *Debye temperature* of the solid.

The lattice heat capacity at constant volume (C_v) is defined by the relation

$$C_v = \frac{\partial U}{\partial T}\tag{4.9}$$

Now we discuss the results in the high and low temperature limits.

(i) The high temperature limit defined by $T \gg \Theta_D$ or $x_D \ll 1$:

In this case, we may expand the exponential function in the integrand of eq.(4.8)

and retain only the first order terms. This gives

$$C_v = 3 N_0 k_B\tag{4.10}$$

Thus lattice heat capacity becomes a constant = $3R/g.\text{atom}$ at high temperatures for monoatomic solids. However, measurements indicate a temperature dependence of C_v in this region.

(ii) The low temperature limit defined by $T \ll \Theta_D$ or $x_D \gg 1$:

In this limit, we may replace the upper limit of integration in eq.(4.8) to infinity.

One obtains

$$C_v = \frac{12 \pi^4}{5} N_0 k_B \left(\frac{T}{\Theta_D} \right)^3 \quad (4.11)$$

This is the Debye T^3 law and it works well for most solids at low temperatures.

The discrepancy in the high temperature limit is usually explained on the basis of anharmonic terms in the potential energy function. We explain it by treating the modes as q-oscillator modes.

4.3 Heat capacity of a slightly q-deformed harmonic crystal (q-oscillator Debye model)

The properties of q-deformed harmonic oscillators have been discussed at length in chapter 2. The eigenstates and eigenvalues of its Hamiltonian H_q are in general q-dependent. However, in the boson realisation, the eigenstates of H_q are q-independent and are the usual harmonic oscillator eigenstates. The q-oscillator Hamiltonian reads (See eq.2.54)

$$H_q = \frac{1}{2} \hbar \omega \left([N+1] + [N] \right)$$

where N is the number operator satisfying the commutation relations (2.18). Treating q as a pure phase, i.e, writing

$$q = e^{i\eta}, \quad \eta \in \mathcal{R}, \quad (4.12)$$

$$[N+1] = \frac{\sin(N+1)\eta}{\sin \eta}, \quad [N] = \frac{\sin N\eta}{\sin \eta}$$

and

$$\begin{aligned} H_\epsilon &= \frac{1}{2} \hbar\omega \left[\frac{\sin(N+1)\eta}{\sin \eta} + \frac{\sin N\eta}{\sin \eta} \right] \\ &= \frac{1}{2} \hbar\omega \left[\frac{(N+1)\eta - \frac{\eta^3}{3!}(N+1)^3 + \dots + N\eta - \frac{\eta^3}{3!}N^3 + \dots}{\eta - \frac{\eta^3}{3!} + \dots} \right] \end{aligned}$$

We treat the phonon modes as slightly deformed q-oscillators (SDO). i.e, η is taken to be very small, close to zero. Then we may retain only terms upto $O(\eta^2)$. Doing this, the Hamiltonian of the slightly deformed oscillator is obtained as

$$\begin{aligned} H_{SDO} &= \frac{1}{2} \hbar\omega (2N+1) - \frac{\eta^2}{3!} \frac{1}{2} \hbar\omega \{ (N+1)^3 + N^3 - (2N+1) \} \\ &= H_0 - \frac{\eta^2}{3!} H_1 \end{aligned} \quad (4.13)$$

where

$$H_0 = \frac{1}{2} \hbar\omega (2N+1) \quad (4.14)$$

is the Hamiltonian of the usual harmonic oscillator and

$$H_1 = \frac{1}{2} \hbar\omega \{ (N+1)^3 + N^3 - (2N+1) \} \quad (4.15)$$

The partition function for the SDO is then given by

$$\begin{aligned} (z)_{SDO} &= \text{Tr.} \exp(-\beta H_{SDO}) \\ &= \sum_{n=0}^{\infty} \langle n | \exp(-\beta (H_0 - \frac{\eta^2}{3!} H_1)) | n \rangle \\ &= \sum_{n=0}^{\infty} \langle n | \exp(-\beta H_0) \exp(\beta \frac{\eta^2}{3!} H_1) | n \rangle \end{aligned}$$

$$\begin{aligned}
&= \sum_{n=0}^{\infty} \langle n | \exp(-\beta H_0) \left\{ 1 + \beta \frac{\eta^2}{3!} H_1 \right\} | n \rangle \\
&= \sum_{n=0}^{\infty} \langle n | \exp(-\beta H_0) | n \rangle + \beta \frac{\eta^2}{3!} \sum_{n=0}^{\infty} \langle n | H_1 \exp(-\beta H_0) | n \rangle \\
&= z_0 \left\{ 1 + \beta \frac{\eta^2}{3!} \langle H_1 \rangle \right\} \tag{4.16}
\end{aligned}$$

where z_0 is the partition function of the usual harmonic oscillator, of the form (4.4)

and

$$\langle H_1 \rangle = \frac{\sum_{n=0}^{\infty} \langle n | H_1 \exp(-\beta H_0) | n \rangle}{\sum_{n=0}^{\infty} \langle n | \exp(-\beta H_0) | n \rangle}$$

which is the same as eq.(3.27) and has been evaluated as

$$\langle H_1 \rangle = -\frac{1}{2} \hbar \omega - \frac{\hbar \omega}{(e^{\beta \hbar \omega} - 1)} + \hbar \omega \sinh(\beta \hbar \omega) g(\beta \hbar \omega)$$

(See eq.3.34). Thus

$$(z)_{SDO} = z_0 \left(1 - \beta \frac{\eta^2}{3!} U_1 \right) \tag{4.17}$$

where

$$U_1 = \frac{1}{2} \hbar \omega + \frac{\hbar \omega}{(e^{\beta \hbar \omega} - 1)} - \hbar \omega \sinh(\beta \hbar \omega) g(\beta \hbar \omega) \tag{4.18}$$

Here

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

See eq.(3.35). Thus for the i^{th} SDO,

$$\begin{aligned}
(U_1)_i &= \frac{1}{2} \hbar \omega_i + \frac{\hbar \omega_i}{(e^{x_i} - 1)} - \hbar \omega_i \left(\frac{e^{x_i} - e^{-x_i}}{2} \right) \left\{ \frac{e^{3x_i} + 4e^{2x_i} + e^{x_i}}{(e^{x_i} - 1)^4} \right\} \\
&= -3! \frac{1}{2} \hbar \omega_i \frac{e^{x_i}(e^{x_i} + 1)}{(e^{x_i} - 1)^3} \tag{4.19}
\end{aligned}$$

Here

$$x_i = \beta \hbar \omega_i = \frac{\hbar \omega_i}{k_B T} \tag{4.20}$$

The partition function for a slightly deformed harmonic crystal is

$$\begin{aligned}\bar{Z} &= \prod_i (z_{SDO})_i \\ &= \prod_i z_0 \left(1 - \beta \frac{\eta^2}{3!} (U_1)_i\right)\end{aligned}\quad (4.21)$$

The internal energy of the crystal is

$$\begin{aligned}\bar{U} &= k_B T^2 \frac{\partial}{\partial T} (\ln \bar{Z}) \\ &= k_B T^2 \frac{\partial}{\partial T} \ln \left\{ \prod_i z_0 \left[1 - \beta \frac{\eta^2}{3!} (U_1)_i\right] \right\} \\ &= k_B T^2 \frac{\partial}{\partial T} \left\{ \sum_i \left[\ln(z_0) + \ln \left(1 - \beta \frac{\eta^2}{3!} (U_1)_i\right) \right] \right\} \\ &= k_B T^2 \frac{\partial}{\partial T} (\ln Z) - k_B T^2 \sum_i \frac{\partial}{\partial T} \left\{ \beta \frac{\eta^2}{3!} (U_1)_i \right\}\end{aligned}\quad (4.22)$$

where we have used the result (3.49). $Z = \prod_i (z_0)$ is the partition function of the usual harmonic crystal. Simplifying,

$$\bar{U} = U + \frac{\eta^2}{3!} \left(U_1 - T \frac{\partial U_1}{\partial T} \right) \quad (4.23)$$

where U is the internal energy of the usual harmonic crystal and

$$U_1 = \sum_i (U_1)_i \quad (4.24)$$

Substituting for $(U_1)_i$ from (4.19) and simplifying, eq.(4.23) becomes

$$\bar{U} = U + \eta^2 3 \int_0^{\omega_D} \frac{1}{2} \hbar \omega \frac{e^x}{(e^x - 1)^4} \left\{ 1 + x + 4xe^x + e^{2x}(x - 1) \right\} D(\omega) d\omega \quad (4.25)$$

We have replaced the summation over ω_i by integration over ω . The factor 3 in the numerator arises because of the three polarisation types. Thus we have retained all

the fundamental premises of the Debye model except for the q -deformation. Incorporating (4.1) in (4.25),

$$\bar{U} = U + \frac{3}{4} \eta^2 \frac{\hbar V}{\pi^2 v^3} \int_0^{\omega_D} \frac{\omega^3 e^x}{(e^x - 1)^4} \{1 + x + 4xe^x + e^{2x}(x - 1)\} d\omega \quad (4.26)$$

Using (4.7),

$$\bar{U} = U + \frac{3}{4} \eta^2 \frac{V}{\hbar^3 \pi^2 v^3} (k_B T)^4 \int_0^{x_D} \frac{x^3 e^x}{(e^x - 1)^4} \{1 + x + 4xe^x + e^{2x}(x - 1)\} dx$$

and substituting for v from (4.3),

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

Using (4.8),

$$\begin{aligned} \bar{U} = 9N_0 k_B T \left(\frac{T}{\Theta}\right)^3 & \left\{ \int_0^{x_D} \frac{x^3 dx}{e^x - 1} \right. \\ & \left. + \frac{\eta^2}{2} \int_0^{x_D} (x^3 e^x + x^4 e^x + 4x^4 e^{2x} + x^4 e^{3x} - x^3 e^{3x}) \frac{dx}{(e^x - 1)^4} \right\} \end{aligned} \quad (4.27)$$

Here we have dropped the zero point energy term. The lattice heat capacity of the q -deformed crystal can now be evaluated as $\left(\frac{\partial \bar{U}}{\partial T}\right)$. We compute this quantity in the two limiting cases:

(a) $T \ll \Theta_D$: In this case, $x_D \gg 1$ and the upper limit of integration in (4.27) can be extended to infinity without introducing any appreciable error because the integrands decay very rapidly for higher values of x . The integrals are then reduced in terms of Riemann zeta function ζ . We use the results [64]

$$\int_0^{\infty} \frac{x^{\nu-1} dx}{e^{\mu x} - 1} = \frac{1}{\mu^{\nu}} \Gamma(\nu) \zeta(\nu) \quad \text{for } Re \mu > 0, Re \nu > 1 \quad (4.28.1)$$

$$\int_0^{\infty} \frac{x^{\nu-1} e^{-\mu x}}{(e^x - 1)^2} dx = \Gamma(\nu) [\zeta(\nu - 1, \mu + 1) - (\mu + 1) \zeta(\nu, \mu + 1)] \quad (4.28.2)$$

for $Re.\nu > 2, Re.\mu > -2$

where the Riemann zeta function

$$\zeta(\nu) = \zeta(\nu, 1) = \sum_{n=1}^{\infty} \frac{1}{n^{\nu}} \quad \text{for } Re.\nu > 1 \quad (4.28.3)$$

and the generalised zeta function

$$\zeta(\nu, \mu) = \sum_{n=0}^{\infty} \frac{1}{(\mu + n)^{\nu}} \quad \text{for } Re.\nu > 1 \quad Re.\mu > 0 \quad (4.28.4)$$

$$\zeta(2m) = \frac{2^{2m-1} \pi^{2m}}{(2m)!} |B_{2m}| \quad (4.28.5)$$

B_{2m} are the Bernoulli numbers:

$$B_0 = 1$$

$$B_2 = -\frac{1}{6}$$

$$B_4 = -\frac{1}{30} \quad (4.28.6)$$

Thus

$$\zeta(2) = \frac{2^{2-1} \pi^2}{2!} |B_2| = \frac{\pi^2}{6}$$

$$\zeta(4) = \frac{2^{4-1} \pi^4}{4!} |B_4| = \frac{\pi^4}{90} \quad (4.28.7)$$

The integrals in (4.27) are obtained as

$$\int_0^{x_D} \frac{x^3 dx}{e^x - 1} \longrightarrow \int_0^\infty \frac{x^3 dx}{e^x - 1} = \frac{1}{1^4} \Gamma(4) \zeta(4) = \frac{\pi^4}{15} \quad (4.28)$$

$$\int_0^{x_D} \frac{x^3 e^x dx}{(e^x - 1)^4} \longrightarrow \zeta(1) - 3 \zeta(2) + 2 \zeta(3) \quad (4.29)$$

$$\int_0^{x_D} \frac{x^4 e^x dx}{(e^x - 1)^4} \longrightarrow 4 \zeta(2) - 12 \zeta(3) + 8 \zeta(4) \quad (4.30)$$

$$\int_0^{x_D} \frac{4x^4 e^{2x} dx}{(e^x - 1)^4} \longrightarrow 16 \zeta(2) - 16 \zeta(4) \quad (4.31)$$

$$\int_0^{x_D} \frac{x^4 e^{3x} dx}{(e^x - 1)^4} \longrightarrow 8 \zeta(4) + 12 \zeta(3) + 4 \zeta(2) \quad (4.32)$$

$$\int_0^{x_D} \frac{x^3 e^{3x} dx}{(e^x - 1)^4} \longrightarrow 2 \zeta(3) + 3 \zeta(2) + \zeta(1) \quad (4.33)$$

Substituting (4.28)-(4.33) in eq.(4.27),

$$\bar{U} = 9 N_0 k_B T \left(\frac{T}{\Theta} \right)^3 \left[\frac{\pi^4}{15} + \frac{\eta^2}{2} 18 \zeta(2) \right] \quad (4.34)$$

and

$$\begin{aligned} C_v &= \left(\frac{\partial \bar{U}}{\partial T} \right)_V \\ &= \frac{12 \pi^4}{5} N_0 k_B \left(\frac{T}{\Theta_D} \right)^3 \left(1 + \frac{45}{2} \frac{\eta^2}{\pi^2} \right) \end{aligned} \quad (4.35)$$

where we have used (4.28.7). Comparing this expression with (4.11), we note that q-deformation brings in a q-dependent correction which is negligible. Thus this model coincides with the Debye model in the low temperature limit.

(b) $T \gg \Theta_D$: In this case, $x_D \ll 1$ so that we may expand the exponential functions in (4.27) and retain only the first order terms. Then

$$\int_0^{x_D} \frac{x^3 dx}{e^x - 1} \longrightarrow \frac{x_D^3}{3} \quad (4.36)$$

$$\int_0^{x_D} (x^3 e^x + x^4 e^x + 4 x^4 e^{2x} + x^4 e^{3x} - x^3 e^{3x}) \frac{dx}{(e^x - 1)^4} \longrightarrow 4 x_D + 6 x_D^2 \quad (4.37)$$

In the high temperature limit, eq.(4.27) becomes

$$\bar{U} = 9 N_0 k_B T \left(\frac{T}{\Theta}\right)^3 \left[\frac{x_D^3}{3} + \frac{\eta^2}{2}(4 x_D + 6 x_D^2)\right]$$

However, since $\eta \ll 1$ and $x_D \ll 1$, we neglect the terms containing $\eta^2 x_D^2$. Hence

$$\bar{U} = 9 N_0 k_B T \left(\frac{T}{\Theta}\right)^3 \left[\left(\frac{\Theta_D}{T}\right)^3 \frac{1}{3} + \frac{\eta^2}{2} 4 \frac{\Theta_D}{T}\right] \quad (4.38)$$

and

$$C_v = \left(\frac{\partial \bar{U}}{\partial T}\right)_v = 3 N_0 k_B \left(1 + \eta^2 \frac{18 T^2}{\Theta_D^2}\right) \quad (4.39)$$

This expression exhibits a T^2 dependence in contrast to eq.(4.10). Though η^2 is small, the correction term becomes significant for $T \gg \Theta_D$. The lattice heat capacity per g-atom for a monoatomic solid is

$$C_v = 3 R \left(1 + \eta^2 \frac{18 T^2}{\Theta_D^2}\right) \quad (4.40)$$

4.4 Comparison with experimental data

The lattice heat capacity per g-atom is calculated according to eq.(4.40) for three alkali elements namely Potassium, Rubidium and Caesium for which the Debye temperatures (Θ_D) are relatively low. The deformation parameter η is assigned

T(K)	Caesium $\theta_D = 38.4 \text{ K}$ $\eta = 8.5 \times 10^{-5}$		Rubidium $\theta_D = 55.6 \text{ K}$ $\eta = 9.0 \times 10^{-5}$		Potassium $\theta_D = 90.6 \text{ K}$ $\eta = 10^{-4}$	
	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	6.00				
110	6.049	6.01				
120	6.067	6.04				
130	6.085	6.08				
140	6.106	6.13	6.057	6.02		
150	6.127	6.16	6.072	6.04		
160	6.151	6.17	6.087	6.07		
170	6.176	6.18	6.104	6.09		
180	6.202	6.20	6.121	6.11	6.050	5.983
190	6.230	6.22	6.140	6.13	6.062	6.005
200	6.259	6.26	6.159	6.14	6.073	6.030
210	6.290	6.30	6.180	6.17	6.085	6.057
220	6.322	6.33	6.201	6.19	6.098	6.085
230	6.356	6.35	6.224	6.22	6.110	6.117
240	6.391	6.38	6.248	6.26	6.124	6.150
250	6.428	6.46	6.272	6.30	6.140	6.183
260	6.466	6.55	6.298	6.35	6.150	6.219
270	6.506	6.61	6.325	6.40	6.170	6.263
273.15	6.519	6.64	6.333	6.42	6.173	6.278
280	6.547	6.71	6.352	6.47	6.180	6.317
290	6.590	6.84	6.381	6.56	6.200	6.379
298.15	6.626	6.97	6.405	6.67	6.214	6.439
300	6.635	7.00	6.411	6.69	6.217	6.454

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

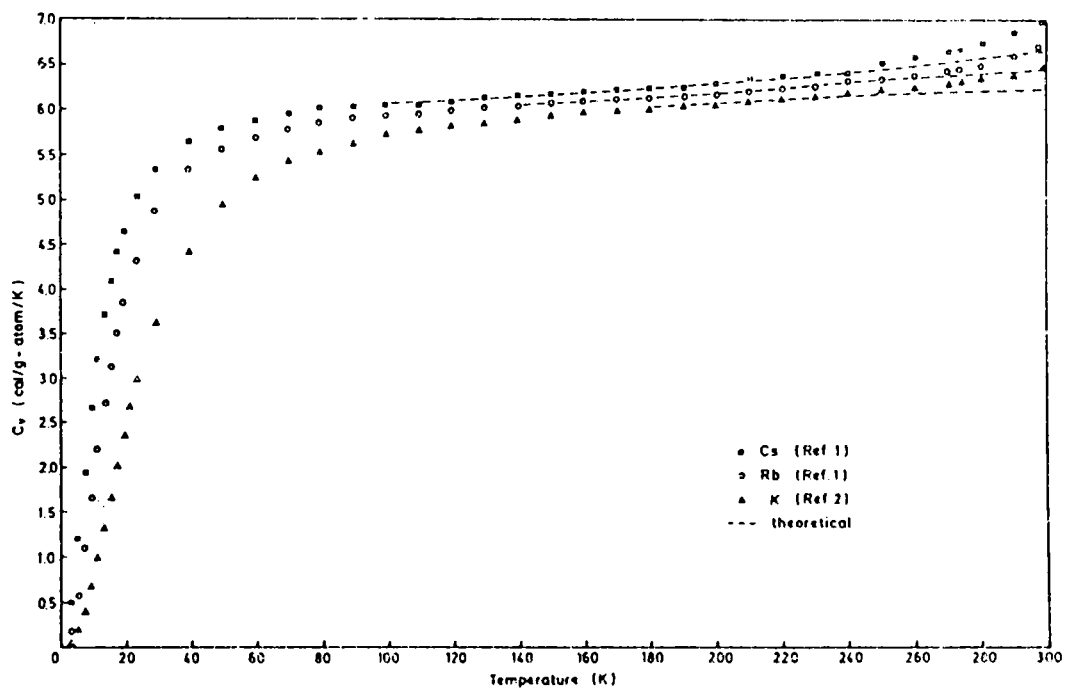


Fig. 1. Values of lattice heat capacity calculated in the q-harmonic approximation plotted as a function of temperature for alkali metals Cs, Rb and K. Experimental values are also shown.

values $\sim 10^{-5}$. The results are shown in Table 1. Experimental values [65,66] are also given. The results are plotted for the range 100-300K along with the experimental curves (Fig.1). It is observed that there is very good agreement for not too high values of T. As the temperature becomes higher, discrepancies arise , the heat capacity increases much more rapidly than predicted by the theory.

4.5 Conclusion

Thus the q-oscillator Debye model proposed here rectifies the weakness of the original model in the high temperature regime. The deformation, though marginal ($\eta \sim 10^{-5}$), produces excellent agreement in the three cases studied over a wide range of temperature. The investigations lend support to the view that phonons in crystals may be q-quantised excitations. Such phonons may be termed q-phonons. The deviations observed at higher temperatures may be explained taking into account quartic and higher order interactions possibly within the framework of a q-anharmonic oscillator model.

Chapter 5

THERMODYNAMIC PROPERTIES OF A q-DEFORMED HEISENBERG FERROMAGNET

5.1 Introduction

In this chapter, we present the study of the Heisenberg model of ferromagnetism using q -deformed oscillator algebra. The spinwave theory has been remarkably successful in predicting the low temperature properties of ferromagnets [67–70]. The theory is built upon the ideal model consisting of a lattice of identical spins with cubic symmetry and with isotropic exchange coupling between nearest neighbours. The notion of spin waves was introduced by Bloch [71&72]. He showed that low-lying excitations of a spin system with the above mentioned properties are wave-like in character. The energy of a spin wave is quantised and the quanta are known as magnons. Holstein and Primakoff [73] suggested the methods of field theory to spin

waves and this gave rise to the linear spin wave theory where the magnon interactions are neglected and the Hamiltonian is expressed as a sum of energies of uncoupled oscillators. The theory yields a $T^{\frac{3}{2}}$ dependence both for magnon heat capacity and spontaneous magnetisation of a ferromagnet.

The effect of spin-wave interaction on the energy levels of the crystal will be negligible only if the total number of spin-waves is small. Many authors [74-76] have tried to incorporate magnon interactions into the spin-wave theory. The most important among them is the work due to Dyson [75&76]. He perfected the spin-wave theory by introducing magnon interactions and showed that at low temperatures, the effect of spin-wave interaction is slight. The lowest order correction to the spontaneous magnetisation is proportional to T^4 , which for low temperatures is very small compared with the leading Bloch $T^{\frac{3}{2}}$ term. Thus the spin-wave theory remains as a genuine method for investigating the low temperature properties of materials with ordered elementary magnetic moments.

However, the agreement between the spin-wave theory based on Heisenberg exchange model of ferromagnetism and experimental observations is not perfectly satisfactory. Many attempts have been made to improve the model [77-80]. The work presented here is also one such attempt. Recently, Bonechi *et al.*[81] have investigated the one dimensional Heisenberg ferromagnet by means of quantum Galieli group and found that in this approach, some of the results provided by the Bethe-ansatz method emerge naturally. It is already appreciated that q-deformation

can characterise interaction between various degrees of freedom. For example, Zhe Chang and Hong Yan [46], in their description of rotation-vibration spectra of diatomic molecules using q -oscillator algebra, have shown that q -deformation characterises the rotation-vibration interaction. Motivated by this fact and by the fact that q -deformation brings in non-linear effects, we study the Heisenberg model of ferromagnetism using q -deformed oscillator algebras. In the linear spin-wave theory of ferromagnets [82], the Heisenberg Hamiltonian is diagonalised by transforming the spin operators into boson operators using the Holstein-Primakoff transformation [73]. We develop a q -deformed version of the spin-wave theory using the q -deformed Holstein-Primakoff transformation [83] for the spin variables, treating the magnons as q -bosons. The exchange Hamiltonian in the nearest neighbour approximation, is obtained for small values of the deformation parameter η . The thermodynamic quantities in the low temperature region are also evaluated. It is found that the spontaneous magnetisation and magnetic contribution to specific heat capacity have q -dependent $T^{\frac{1}{2}}$ terms in addition to the well-known Bloch $T^{\frac{3}{2}}$ term. In the limit $q \rightarrow 1$, our results coincide with the classical results. We have also made a comparative study of the theoretical results with experimental data in the case of the well-known Heisenberg ferromagnets EuO and EuS.

Before discussing the q -deformed model, we briefly recall the basic concepts in linear spin-wave theory.

5.2 Ferromagnetic magnons-basic concepts

We consider the simple case of a finite cubic crystal with periodic boundary conditions and with N atoms, each atom having z nearest neighbours. To each atom j is attached a spin vector \vec{s}_j of magnitude s . Then the Hamiltonian of the crystal with isotropic nearest neighbour exchange interaction can be written as

$$\mathcal{H} = -J \sum_{j=1}^N \sum_{\delta=1}^z \vec{s}_j \cdot \vec{s}_{j+\delta} - g \mu_B H \sum_j s_{jz} \quad (5.1)$$

The vectors $\vec{\delta}$ connect atom j with its δ^{th} nearest neighbour on the bravais lattice. J is the exchange integral between the j^{th} atom and its δ^{th} nearest neighbour and for ferromagnets, J is positive. μ_B is the Bohr magneton, g is the spectroscopic splitting factor. The first term in \mathcal{H} is the Heisenberg exchange energy expressed in terms of the atomic spin operators. The second term is the Zeeman contribution which gives the interaction energy of each atomic magnet with the external magnetic field H whose direction is taken as the positive z-direction. When the system is in the ground state, the magnetic moments are lined up along the positive z-axis. The dipole-dipole interaction and the interaction of higher order magnetic poles are neglected here.

The Hamiltonian (5.1) involves the three components of each spin vector \vec{s}_j :

$$\mathcal{H} = -J \sum_{j,\delta} \left\{ s_{jx} s_{(j+\delta)x} + s_{jy} s_{(j+\delta)y} + s_{jz} s_{(j+\delta)z} \right\} - g \mu_B H \sum_j s_{jz} \quad (5.2)$$

The components s_{jx} , s_{jy} , and s_{jz} are not independent, but are connected by the identity

$$\vec{s}_j \cdot \vec{s}_j = s(s+1) \quad (5.3)$$

The total spin

$$s^2 = \sum_j s_j^2$$

and the total z-component

$$S_z = \sum_{j=1}^N s_{jz}$$

are constants of motion of the spin. In the ground state $|0\rangle$ of the system,

$$\begin{aligned} s_z |0\rangle &= \sum_{j=1}^N s_{jz} |0\rangle \\ &= N S |0\rangle \end{aligned} \quad (5.4)$$

It is more convenient to work with the two operators s_j^+ and s_j^- which are independent and defined as

$$s_j^\pm = s_{jx} \pm i s_{jy} \quad (5.5)$$

Then the spin operators satisfy the $su(2)$ algebra:

$$\begin{aligned} [s_{jz}, s_{j'}^\pm] &= \pm \delta_{jj'} s_{j'}^\pm ; \\ [s_j^+, s_{j'}^-] &= 2 \delta_{jj'} s_{jz} \end{aligned} \quad (5.6)$$

Substituting (5.5) in (5.2),

$$\begin{aligned} \mathcal{H} = & - \frac{J}{2} \sum_{j=1}^N \sum_{\delta=1}^z [s_j^+ s_{j+\delta}^- + s_j^- s_{j+\delta}^+ + 2 s_{jz} s_{(j+\delta)z}] \\ & - g \mu_B H \sum_j s_{jz} \end{aligned} \quad (5.7)$$

The spin operators s_j^+ and s_j^- are now transformed to the boson creation and annihilation operators a_j^\dagger and a_j using the Holstein-Primakoff transformation [73]:

$$s_j^+ = \sqrt{2s(1 - \frac{a_j^\dagger a_j}{2s})} a_j; \quad (5.8)$$

$$s_j^- = a_j^\dagger \sqrt{2s(1 - \frac{a_j^\dagger a_j}{2s})} \quad (5.9)$$

where

$$[a_j, a_{j'}^\dagger] = \delta_{jj'} \quad (5.10)$$

Then

$$s_{jz} = s - a_j^\dagger a_j = s - n_j \quad (5.11)$$

The above transformation preserves the $su(2)$ algebra. In this representation, $n_j = (s - s_{jz})$ measures the deviation of the j^{th} spin from its maximum value s and hence is interpreted as the spin deviation operator.

Usually one describes the oscillatory system in terms of the normal modes. For this, one uses the Fourier expansion of the magnon operators a_j and a_j^\dagger :

$$\begin{aligned} a_j &= \frac{1}{\sqrt{N}} \sum_k \exp(-i\vec{k} \cdot \vec{x}_j) b_k; \\ a_j^\dagger &= \frac{1}{\sqrt{N}} \sum_k \exp(i\vec{k} \cdot \vec{x}_j) b_k^\dagger \end{aligned} \quad (5.12)$$

Here x_j is the position vector of the j^{th} atom. The operator b_k^\dagger creates a magnon of wave vector \vec{k} and the operator b_k destroys a magnon of wave vector \vec{k} . The discrete

values of \vec{k} summed over are those obtained from periodic boundary conditions. The operators b_k and b_k^\dagger satisfy the boson commutation relations:

$$\begin{aligned} [b_k, b_{k'}^\dagger] &= \delta_{kk'}; \\ [b_k^\dagger, b_{k'}^\dagger] &= [b_k, b_{k'}] = 0 \end{aligned} \quad (5.13)$$

Using the above transformations, the Hamiltonian can in principle be expressed in terms of the b_k 's and b_k^\dagger 's. In the linear spin wave theory, the following approximations are invoked[73]:

- (i). Only low-lying states of the system are considered so that one can neglect the magnon-magnon interactions and also one can assume the 'quasi-saturation approximation' - i.e, the fractional decrease in spontaneous magnetisation $M(T)$ from the maximum possible value $M(0)$ is small. i.e,

$$\frac{\langle n_j \rangle_{av}}{2s} \ll 1$$

or

$$\sqrt{1 - \frac{a_j^\dagger a_j}{2s}} = \sqrt{1 - \frac{n_j}{2s}} \approx 1 \quad (5.14)$$

This is valid at temperatures sufficiently below the Curie temperature.

- (ii). Terms proportional to $n_j n_{j'}$ are neglected. Assuming that there is no correlation in the location of the different spin deviations, the expectation value of these terms will be negligible in comparison with the expectation value of $2sn_j$.

(iii). Terms proportional to $\sqrt{2s}a_j^\dagger a_j a_j^\dagger$ are neglected. These are terms which cause the system to undergo transitions between states of different total spin. Unlike terms of the type $\sqrt{2s} a_j^\dagger a_j^\dagger$ which also cause such transitions, they are different from zero only for transitions taking place near atoms on which spin deviations are already present. The ratio of the number of transitions arising from the two types of terms is thus $\sim \frac{\langle n_j \rangle_{av}}{\sqrt{2s}} \ll 1$.

With the above assumptions, the Hamiltonian takes the form [81]

$$\begin{aligned} \mathcal{H} &= -J N z s^2 - g \mu_B H N s \\ &+ \sum_k [2 J s z (1 - \gamma_k) + g \mu_B H] b_k^\dagger b_k \end{aligned} \quad (5.15)$$

$$= \mathcal{H}_{00} + \mathcal{H}_0 \quad (5.16)$$

where

$$\mathcal{H}_{00} = -J N z s^2 - g \mu_B H N s \quad (5.17)$$

represents the minimum value of the Hamiltonian representing the completely ordered ground state $|0\rangle$ of the system and

$$\mathcal{H}_0 = \sum_k [2 J s z (1 - \gamma_k) + g \mu_B H] b_k^\dagger b_k \quad (5.18)$$

Here,

$$\gamma_k = \frac{1}{z} \sum_{\delta=1}^z \exp(i\vec{k} \cdot \vec{\delta}) \quad (5.19)$$

For crystals having a centre of symmetry, $\gamma_k = \gamma_{-k}$. Also $\sum_k \gamma_k = 0$. \mathcal{H}_0 is of the

form

$$\mathcal{H}_0 = \sum_k n_k \omega_k \quad (5.20)$$

where

$$\omega_k = 2 J s z (1 - \gamma_k) + g \mu_B H \quad (5.21)$$

For $|\vec{k} \cdot \vec{\delta}| \ll 1$ and for cubic lattices of lattice constant a ,

$$z(1 - \gamma_k) \approx \frac{1}{2} \sum_{\delta} (\vec{k} \cdot \vec{\delta})^2 = (ka)^2 \quad (5.22)$$

In this case,

$$\omega_k = D k^2 + g \mu_B H \quad (5.23)$$

where

$$D = 2 J s a^2 \quad (5.24)$$

Thus in the linear spin wave theory described here, the Hamiltonian takes the form

$$\mathcal{H} = \mathcal{H}_{00} + \sum_k n_k \omega_k \quad (5.25)$$

This leads to the following results for the magnon heat capacity per unit volume C_m and spontaneous magnetisation $M(T)$:

$$C_m = \frac{15}{4} k_B \left(\frac{k_B T}{4 \pi D} \right)^{\frac{3}{2}} \zeta\left(\frac{5}{2}\right) \quad (5.26)$$

$$M(T) = g \mu_B N s - \frac{g \mu_B}{4 \pi^2} \left(\frac{k_B T}{D} \right)^{\frac{3}{2}} \Gamma\left(\frac{3}{2}\right) \zeta\left(\frac{3}{2}\right) \quad (5.27)$$

The thermal decrease in spontaneous magnetisation is given by

$$\begin{aligned}
\Delta M &= M(0) - M(T) \\
&= \frac{g \mu_B}{4 \pi^2} \left(\frac{k_B T}{D} \right)^{\frac{3}{2}} \Gamma\left(\frac{3}{2}\right) \zeta\left(\frac{3}{2}\right)
\end{aligned} \tag{5.28}$$

This is the well-known Bloch $T^{\frac{3}{2}}$ law. Thus according to the simple linear spin wave theory based on Heisenberg's exchange model, both $\frac{C_m}{T^{\frac{3}{2}}}$ versus T plot and $\frac{\Delta M}{M(0)T^{\frac{3}{2}}}$ versus T plot are straight lines parallel to the temperature axis. However, if one retains all the terms in the expansion of $(1 - \gamma_k)$, one obtains $T^{\frac{5}{2}}, T^{\frac{7}{2}} \dots$ terms along with the leading $T^{\frac{3}{2}}$ term.

5.3 q-deformed Heisenberg ferromagnet

As in the case of q-oscillator Debye model, here also we retain all the basic assumptions in the linear spin wave theory except that the magnons here are treated as q-magnons. Thus the Hamiltonian (5.1) in the context of a q-deformed Heisenberg ferromagnet when expressed in terms of the spin raising and lowering operators takes the form

$$\begin{aligned}
\tilde{\mathcal{H}} &= - \frac{J}{2} \sum_{j,\delta} \left[\tilde{s}_j^+ \tilde{s}_{j+\delta}^- + \tilde{s}_j^- \tilde{s}_{j+\delta}^+ + 2 \tilde{s}_{jz} \tilde{s}_{(j+\delta)z} \right] \\
&\quad - g \mu_B H \sum_j \tilde{s}_{jz}
\end{aligned} \tag{5.29}$$

The operators $\tilde{s}_j^+, \tilde{s}_j^-$ and \tilde{s}_{jz} satisfy the $su_q(2)$ algebra:

$$\begin{aligned}
[\tilde{s}_{jz}, \tilde{s}_j^\pm] &= \pm \tilde{s}_j^\pm; \\
[\tilde{s}_j^+, \tilde{s}_j^-] &= 2 [\tilde{s}_{jz}]
\end{aligned} \tag{5.30}$$

Now we express the Hamiltonian in terms of the q-boson operators \tilde{a}_j and \tilde{a}_j^\dagger using the q-deformed Holstein-Primakoff transformation introduced by Kundu and Mallick [83]:

$$\begin{aligned}\tilde{s}_j^+ &= \sqrt{[2s - n_j]} \tilde{a}_j; \\ \tilde{s}_j^- &= \tilde{a}_j^\dagger \sqrt{[2s - n_j]};\end{aligned}\tag{5.31}$$

$$\tilde{s}_{jz} = s - n_j\tag{5.32}$$

\tilde{a}_j and \tilde{a}_j^\dagger satisfy the q-oscillator algebra:

$$\begin{aligned}[n_j, \tilde{a}_j^\dagger] &= \tilde{a}_j^\dagger, \\ [n_j, \tilde{a}_j] &= -\tilde{a}_j, \\ \tilde{a}_j \tilde{a}_j^\dagger - q \tilde{a}_j^\dagger \tilde{a}_j &= q^{-n_j}\end{aligned}\tag{5.33}$$

The above transformation preserves the $su_q(2)$ algebra (5.30). We choose q as a pure phase. i.e, we write

$$q = \exp(i\eta), \quad \eta \in \mathcal{R}\tag{5.34}$$

Then

$$\sqrt{[2s - n_j]} = \left\{ \frac{\sin \eta(2s - n_j)}{\sin \eta} \right\}^{\frac{1}{2}}$$

We consider only slight deformations (q very close to 1). Expanding the sine functions in Taylor series and keeping only terms upto $O(\eta^2)$,

$$\sqrt{[2s - n_j]} = \sqrt{2s} \left(1 - \frac{n_j}{4s}\right) \left\{ 1 + \frac{\eta^2}{2.3!} (1 - 4s^2 + 4sn_j) \right\}$$

Then eqs.(5.31) become

$$\begin{aligned}\tilde{s}_j^+ &\approx \sqrt{2s} \left\{ 1 + \frac{\eta^2}{2.3!} (1 - 4s^2) \right\} \tilde{a}_j ; \\ \tilde{s}_j^- &\approx \tilde{a}_j^\dagger \sqrt{2s} \left\{ 1 + \frac{\eta^2}{2.3!} (1 - 4s^2) \right\}\end{aligned}\quad (5.35)$$

i.e,

$$\begin{aligned}\tilde{s}_j^+ &\approx X \tilde{a}_j ; \\ \tilde{s}_j^- &\approx \tilde{a}_j^\dagger X\end{aligned}\quad (5.36)$$

where

$$X = \sqrt{2s} \left\{ 1 + \frac{\eta^2}{2.3!} (1 - 4s^2) \right\}\quad (5.37)$$

Here we have retained all the three assumptions so that terms in higher orders of boson operators are neglected. Now we use the Fourier expansion for the q-boson operators \tilde{a}_j , and \tilde{a}_j^\dagger :

$$\begin{aligned}\tilde{a}_j &= \frac{1}{\sqrt{N}} \sum_k \exp(-i\vec{k}\cdot\vec{x}_j) \tilde{b}_k ; \\ \tilde{a}_j^\dagger &= \frac{1}{\sqrt{N}} \sum_k \exp(i\vec{k}\cdot\vec{x}_j) \tilde{b}_k^\dagger\end{aligned}\quad (5.38)$$

The quantised spin wave excitations in this case are called q-magnons. The operators \tilde{b}_k and \tilde{b}_k^\dagger satisfy the q-boson commutation relations

$$\begin{aligned}[n_k, \tilde{b}_k] &= -\tilde{b}_k ; \\ [n_k, \tilde{b}_k^\dagger] &= \tilde{b}_k^\dagger ; \\ \tilde{b}_k^\dagger \tilde{b}_k &= [n_k] ;\end{aligned}$$

$$\begin{aligned}
\tilde{b}_k \tilde{b}_k^\dagger &= [n_k + 1] \\
\tilde{b}_k \tilde{b}_k^\dagger - q \tilde{b}_k^\dagger \tilde{b}_k &= q^{-n_k}
\end{aligned} \tag{5.39}$$

Also $n_k = b_k^\dagger b_k$. Using eqs.(5.36)–(5.39),

$$\begin{aligned}
\tilde{s}_j^+ \tilde{s}_{j+\delta}^+ &= X \frac{1}{\sqrt{N}} \sum_k \exp(-i\vec{k} \cdot \vec{x}_j) \tilde{b}_k X \frac{1}{\sqrt{N}} \sum_{k'} \exp(i\vec{k}' \cdot (\vec{x}_j + \vec{\delta})) \tilde{b}_{k'}^\dagger \\
&= \frac{X^2}{N} \sum_k \exp(i\vec{k} \cdot \vec{\delta}) \tilde{b}_k \tilde{b}_k^\dagger \\
&= \frac{X^2}{N} \sum_k \exp(i\vec{k} \cdot \vec{\delta}) [n_k + 1] \\
\tilde{s}_j^- \tilde{s}_{j+\delta}^+ &= \frac{X^2}{N} \sum_k \exp(-i\vec{k} \cdot \vec{\delta}) \tilde{b}_k^\dagger \tilde{b}_k \\
&= \frac{X^2}{N} \sum_k \exp(-i\vec{k} \cdot \vec{\delta}) [n_k] \\
\tilde{s}_{jz} \tilde{s}_{(j+\delta)z} &= (s - n_j)(s - n_{j+\delta}) \\
&\approx s^2 - s(n_j + n_{j+\delta}) \\
&= s^2 - s(a_j^\dagger a_j + a_{j+\delta}^\dagger a_{j+\delta}) \\
&= s^2 - \frac{s}{N} \sum_k 2b_k^\dagger b_k \\
&= s^2 - \frac{s}{N} \sum_k 2n_k \\
s_{jz} &= s - n_j \\
&= s - \frac{1}{N} \sum_k n_k
\end{aligned}$$

Here we have worked in the boson realisation of the q-oscillator algebra and used eq.(5.12). Substituting the above equations in (5.29),

$$\begin{aligned}\tilde{\mathcal{H}} = & -\frac{J}{2} \sum_{j,\delta} \left\{ \frac{X^2}{N} \sum_k \exp(i\vec{k}\cdot\vec{\delta}) [n_k + 1] + \frac{X^2}{N} \sum_k \exp(-i\vec{k}\cdot\vec{\delta}) [n_k] \right. \\ & \left. + 2 \left(s^2 - \frac{s}{N} \sum_k 2n_k \right) \right\} - g \mu_B H \sum_j \left(s - \frac{1}{N} \sum_k n_k \right)\end{aligned}$$

Using eq.(5.19),

$$\begin{aligned}\tilde{\mathcal{H}} = & -\frac{J}{2} \sum_{j,k} \left\{ \frac{X^2}{N} z \gamma_k [n_k + 1] + \frac{X^2}{N} z \gamma_{-k} [n_k] \right\} \\ & - J \sum_{j,\delta} \left(s^2 - \frac{s}{N} \sum_k 2n_k \right) - g \mu_B H N s + g \mu_B H \sum_k n_k \\ = & J N z s^2 - g \mu_B H N s + \sum_k n_k (2 J s z + g \mu_B H) \\ & - \frac{J}{2} X^2 z \sum_k \gamma_k \{ [n_k + 1] + [n_k] \}\end{aligned}\tag{5.40}$$

i.e,

$$\tilde{\mathcal{H}} = \mathcal{H}_{00} + \mathcal{H}_0' \tag{5.41}$$

where \mathcal{H}_{00} is the same as that given by eq.(5.17) and

$$\begin{aligned}\mathcal{H}_0' = & (2 J s z + g \mu_B H) \sum_k n_k \\ & - J s z \left\{ 1 + \frac{\eta^2}{3!} (1 - 4s^2) \right\} \sum_k \gamma_k \{ [n_k + 1] + [n_k] \}\end{aligned}\tag{5.42}$$

In the slightly deformed case ($\eta \rightarrow 0$), we may express $[n_k + 1]$ and $[n_k]$ in terms of sine functions and retain only terms upto $O(\eta^2)$. We get

$$[n_k + 1] + [n_k] = (2 n_k + 1) - \frac{\eta^2}{3!} (2 n_k^3 + 3 n_k^2 + n_k)$$

Using this in eq.(5.42),

$$\begin{aligned}
\mathcal{H}_0' &= (2 J s z + g \mu_B H) \sum_k n_k \\
&- J s z \left\{ 1 + \frac{\eta^2}{3!} (1 - 4s^2) \right\} \sum_k \gamma_k \left\{ (2 n_k + 1) - \frac{\eta^2}{3!} (2 n_k^3 + 3 n_k^2 + n_k) \right\} \\
&= \sum_k n_k \left\{ 2 J s z (1 - \gamma_k) + g \mu_B H \right\} + \frac{\eta^2}{3!} \sum_k \left\{ n_k J s z \gamma_k (8 s^2 - 1) \right. \\
&+ \left. 2 n_k^3 J s z \gamma_k + 3 n_k^2 J s z \gamma_k \right\} \\
&= \sum_k n_k \omega_k + \frac{\eta^2}{3!} \sum_k \left\{ n_k \omega_k' (8 s^2 - 1) + 2 n_k^3 \omega_k' \right. \\
&+ \left. 3 n_k^2 \omega_k' \right\} \tag{5.43}
\end{aligned}$$

where

$$\omega_k' = J s z \gamma_k \tag{5.44}$$

For cubic lattices of lattice constant a ,

$$\omega_k' = J s (z - k^2 a^2) = J s z - \frac{1}{2} D k^2 \tag{5.45}$$

Here D is given by eq.(5.24) and ω_k is given by eq.(5.23). Thus

$$\begin{aligned}
\tilde{\mathcal{H}} &= \mathcal{H}_{00} + \sum_k n_k \omega_k \\
&+ \frac{\eta^2}{3!} \sum_k \omega_k' \left\{ n_k (8s^2 - 1) + 3 n_k^2 + 2 n_k^3 \right\} \tag{5.46}
\end{aligned}$$

In the limit $q \rightarrow 1$, $\tilde{\mathcal{H}} \rightarrow \mathcal{H}$, the Hamiltonian of the usual Heisenberg ferromagnet as given in eq.(5.25).

5.4 Thermodynamics of q-deformed Heisenberg ferromagnet

The partition function \tilde{Z} of the q-deformed Heisenberg ferromagnet is given by

$$\begin{aligned}\tilde{Z} &= \text{Tr. } \exp(-\beta\tilde{\mathcal{H}}) \\ &= \sum_{n_k=0}^{\infty} \exp\left[-\beta\left\{E_{00} + \sum_k n_k \omega_k\right.\right. \\ &\quad \left.\left.+ \frac{\eta^2}{3!} \sum_k \omega_k' \left\{n_k(8s^2 - 1) + 3 n_k^2 + 2 n_k^3\right\}\right]\right]\end{aligned}$$

For small values of η , this reduces to

$$\begin{aligned}\tilde{Z} &= \exp(-\beta E_{00}) \prod_k \sum_{n_k} \exp(-\beta n_k \omega_k) \left\{1 - \right. \\ &\quad \left. \beta \frac{\eta^2}{3!} \omega_k' (n_k(8s^2 - 1) + 3 n_k^2 + 2 n_k^3)\right\}\end{aligned}\quad (5.47)$$

Writing

$$\beta \omega_k = x_k \quad (5.48)$$

and using the results

$$\begin{aligned}\sum_{n=0}^{\infty} e^{-nx} &= \frac{1}{1 - e^{-x}}; \\ \sum_{n=0}^{\infty} n e^{-nx} &= \frac{e^{-x}}{(1 - e^{-x})^2}; \\ \sum_{n=0}^{\infty} n^2 e^{-nx} &= \frac{1 + e^{-x}}{(1 - e^{-x})^3}; \\ \sum_{n=0}^{\infty} n^3 e^{-nx} &= \frac{e^{3x} + 4e^{2x} + e^x}{(e^x - 1)^4},\end{aligned}\quad (5.49)$$

eq.(5.47) becomes

$$\begin{aligned}
\tilde{Z} &= \exp(-\beta E_{00}) \prod_k \left\{ \frac{1}{1 - e^{-x_k}} - \beta \frac{\eta^2}{3!} \omega_k' \left[(8s^2 - 1) \frac{e^{-x_k}}{(1 - e^{-x_k})^2} \right. \right. \\
&\quad \left. \left. + \frac{3(1 + e^{-x_k})}{(1 - e^{-x_k})^3} + \frac{2(e^{3x_k} + 4e^{2x_k} + e^{x_k})}{(e^{x_k} - 1)^4} \right] \right\} \\
&= \exp(-\beta E_{00}) \prod_k Z_{0k} \left\{ 1 - \beta \frac{\eta^2}{3!} Z_{0k}^3 \omega_k' \left[3 + e^{-x_k}(1 + 8s^2) \right. \right. \\
&\quad \left. \left. + (7 - 16s^2)e^{-2x_k} + (1 + 8s^2)e^{-3x_k} \right] \right\} \quad (5.50)
\end{aligned}$$

where

$$Z_{0k} = \frac{1}{1 - \exp(-x_k)} \quad (5.51)$$

The free energy \tilde{F} of the system is

$$\begin{aligned}
\tilde{F} &= -k_B T \ln(\tilde{Z}) \\
&= E_{00} - k_B T \sum_k \left\{ \ln(Z_{0k}) + \ln \left[1 - \beta \frac{\eta^2}{3!} Z_{0k}^3 \omega_k'(\dots) \right] \right\} \\
&= E_{00} - k_B T \sum_k \ln(Z_{0k}) + \frac{\eta^2}{3!} \sum_k Z_{0k}^3 \omega_k'(\dots) \quad (5.52)
\end{aligned}$$

where we have used the result

$$\ln(1 - x) \approx -x \quad \text{when } x \ll 1.$$

To evaluate the sums in eq.(5.52), we put

$$\beta \omega_k = \beta (Dk^2 + g\mu_B H) = mk^2 + y \quad (5.53)$$

Then

$$m = \beta D = \frac{D}{k_B T} \quad (5.54)$$

$$y = \beta g\mu_B H \quad (5.55)$$

and the η^2 dependent terms in eq.(5.52) are

$$\begin{aligned}\sum_k 3 Z_{0k}^3 \omega_k' &= \sum_k \frac{3 \omega_k'}{(1 - e^{-x_k})^3} \\ &= \sum_k \frac{3 (Js z - \frac{1}{2} D k^2)}{\{1 - e^{-(mk^2+y)}\}^3}\end{aligned}$$

Replacing the summation over k by integration

$$\sum_k (\dots) = \frac{V}{(2\pi)^3} 4\pi \int_0^\infty (\dots) k^2 dk, \quad (5.56)$$

the above sum is

$$\begin{aligned}\sum_k 3 Z_{0k}^3 \omega_k' &= 3 \frac{V}{(2\pi)^3} 4\pi \left\{ Js z \int \frac{k^2 dk}{(1 - e^{-(mk^2+y)})^3} \right. \\ &\quad \left. - \frac{1}{2} D \int \frac{k^4 dk}{(1 - e^{-(mk^2+y)})^3} \right\} \quad (5.57)\end{aligned}$$

Similarly

$$\begin{aligned}\sum_k Z_{0k}^3 \omega_k' e^{-x_k} (1 + 8s^2) &= \frac{V}{(2\pi)^3} 4\pi (1 + 8s^2) \left\{ Js z \right. \\ &\quad \left. \int \frac{e^{-(mk^2+y)} k^2 dk}{(1 - e^{-(mk^2+y)})^3} - \frac{1}{2} D \int \frac{k^4 e^{-(mk^2+y)} dk}{(1 - e^{-(mk^2+y)})^3} \right\} \quad (5.58)\end{aligned}$$

$$\begin{aligned}\sum_k Z_{0k}^3 \omega_k' (7 - 16s^2) e^{-2x_k} &= \frac{V}{(2\pi)^3} 4\pi (7 - 16s^2) \left\{ Js z \right. \\ &\quad \left. \int \frac{e^{-2(mk^2+y)} k^2 dk}{(1 - e^{-(mk^2+y)})^3} - \frac{1}{2} D \int \frac{k^4 e^{-2(mk^2+y)} dk}{(1 - e^{-(mk^2+y)})^3} \right\} \quad (5.59)\end{aligned}$$

$$\begin{aligned}\sum_k Z_{0k}^3 \omega_k' (1 + 8s^2) e^{-3x_k} &= \frac{V}{(2\pi)^3} 4\pi (1 + 8s^2) \left\{ Js z \right. \\ &\quad \left. \int \frac{e^{-3(mk^2+y)} k^2 dk}{(1 - e^{-(mk^2+y)})^3} - \frac{1}{2} D \int \frac{k^4 e^{-3(mk^2+y)} dk}{(1 - e^{-(mk^2+y)})^3} \right\} \quad (5.60)\end{aligned}$$

Also

$$\begin{aligned}
\sum_k \ln(Z_{0k}) &= \sum_k \ln\left(\frac{1}{1 - e^{-x_k}}\right) \\
&= - \sum_k \ln(1 - e^{-x_k}) \\
&= \sum_k \sum_{n=1}^{\infty} \frac{e^{-nx_k}}{n} \\
&= \frac{V}{(2\pi)^3} 4\pi \sum_{n=0}^{\infty} \frac{1}{n} \int e^{-nx_k} k^2 dk \\
&= \frac{V}{(2\pi)^3} 4\pi \sum_{n=0}^{\infty} \frac{1}{n} \int_0^{\infty} e^{-n(mk^2+y)} k^2 dk \\
&= \frac{V}{(2\pi)^3} 4\pi \sum_{n=0}^{\infty} \frac{e^{-ny}}{n} \int_0^{\infty} e^{-nmk^2} k^2 dk \\
&= \frac{V}{(2\pi)^3} 4\pi \sum_{n=0}^{\infty} \frac{e^{-ny}}{n} \frac{1!!}{2(2nm)} \sqrt{\frac{\pi}{nm}} \\
&= \frac{V}{(2\pi)^3} 4\pi \frac{\sqrt{\pi}}{4} \left(\frac{k_B T}{D}\right)^{\frac{3}{2}} \sum_{n=1}^{\infty} \frac{e^{-ny}}{n^{\frac{5}{2}}} \tag{5.61}
\end{aligned}$$

where we have used the results

$$- \ln(1 - x) = \sum_{n=1}^{\infty} \frac{x^n}{n} \tag{5.62}$$

and

$$\int_0^{\infty} x^{2n} e^{-px^2} dx = \frac{(2n - 1)!!}{2(2p)^n} \sqrt{\frac{\pi}{p}} \tag{5.63}$$

Now we evaluate the integrals in eqs.(5.57)–(5.60) in the region of low temperatures:

$$e^{-(nk^2+y)} = e^{-\beta\omega_k} = e^{-\omega_k/k_B T} \rightarrow e^{-\infty} \rightarrow 0 \text{ as } T \rightarrow 0$$

The denominators in the integrands, i.e,

$$(1 - e^{-(nk^2+y)})^3 \rightarrow 1 \text{ as } T \rightarrow 0$$

Then the integrals

$$\begin{aligned}
I_1 &= \int k^2 dk \longrightarrow \infty ; \\
I_2 &= \int k^4 dk \longrightarrow \infty ; \\
I_3 &= \int e^{-(mk^2+y)} k^2 dk \longrightarrow \frac{\sqrt{\pi}}{4} e^{-y} \frac{1}{m^{\frac{3}{2}}} ; \\
I_4 &= \int e^{-(mk^2+y)} k^4 dk \longrightarrow \frac{3\sqrt{\pi}}{8} e^{-y} \frac{1}{m^{\frac{5}{2}}} ; \\
I_5 &= \int e^{-2(mk^2+y)} k^2 dk \longrightarrow \frac{\sqrt{\pi}}{8\sqrt{2}} e^{-2y} \frac{1}{m^{\frac{3}{2}}} ; \\
I_6 &= \int e^{-2(mk^2+y)} k^4 dk \longrightarrow \frac{3\sqrt{\pi}}{32\sqrt{2}} e^{-2y} \frac{1}{m^{\frac{5}{2}}} ; \\
I_7 &= \int e^{-3(mk^2+y)} k^2 dk \longrightarrow \frac{\sqrt{\pi}}{12\sqrt{3}} e^{-3y} \frac{1}{m^{\frac{3}{2}}} ; \\
I_8 &= \int e^{-3(mk^2+y)} k^4 dk \longrightarrow \frac{\sqrt{\pi}}{24\sqrt{3}} e^{-3y} \frac{1}{m^{\frac{5}{2}}} \tag{5.64}
\end{aligned}$$

Substituting eqs.(5.64) and (5.61) in eq.(5.52), we get the free energy of the system as

$$\begin{aligned}
\bar{F} &= E_{00} - \frac{V}{(2\pi)^3} 4\pi \frac{\sqrt{\pi}}{4} (k_B T) \left(\frac{k_B T}{D}\right)^{\frac{3}{2}} \sum_{n=1}^{\infty} \frac{\exp(-nuH/T)}{n^{\frac{5}{2}}} \\
&+ \frac{\eta^2}{3!} \frac{V}{(2\pi)^3} 4\pi \left\{ Jsz(1+8s^2)(I_3+I_7) \right. \\
&- \left. \frac{1}{2} D(1+8s^2)(I_4+I_8) + (7-16s^2) Jsz I_5 - (7-16s^2) \frac{D}{2} I_6 \right\} \tag{5.65}
\end{aligned}$$

where

$$u = \frac{g\mu_B}{k_B} \tag{5.66}$$

so that

$$y = \frac{g\mu_B H}{k_B T} = \frac{uH}{T} \tag{5.67}$$

The quantity which is of great interest is the spontaneous magnetisation defined by

$$M(T) = -\left(\frac{\partial \tilde{F}}{\partial H}\right)_{H=0, V=1} \quad (5.68)$$

Substituting eq.(5.65) in eq.(5.68) and using eqs.(5.64) and (5.67) and simplifying, we get

$$\begin{aligned} \tilde{M}(T) &= g\mu_B Ns - \frac{g\mu_B}{4\pi^2} \Gamma\left(\frac{3}{2}\right) \left\{ \left(\frac{k_B T}{D}\right)^{\frac{3}{2}} \zeta\left(\frac{3}{2}\right) \right. \\ &\quad \left. - \frac{\eta^2}{3!} \left(\frac{k_B T}{D}\right)^{\frac{3}{2}} \left[\frac{1}{k_B T} J_{sz} (6.527 + 1.305s^2) - (2.750 + 2.913s^2) \right] \right\} \end{aligned} \quad (5.69)$$

The thermal decrease in spontaneous magnetisation is given by

$$\begin{aligned} \Delta \tilde{M} &= \tilde{M}(0) - \tilde{M}(T) \\ &= \frac{g\mu_B}{4\pi^2} \Gamma\left(\frac{3}{2}\right) \left\{ \left(\frac{k_B T}{D}\right)^{\frac{3}{2}} \zeta\left(\frac{3}{2}\right) \right. \\ &\quad \left. - \frac{\eta^2}{3!} \left(\frac{k_B T}{D}\right)^{\frac{3}{2}} \left[\frac{1}{k_B T} J_{sz} (6.527 + 1.305s^2) - (2.750 + 2.913s^2) \right] \right\} \end{aligned} \quad (5.70)$$

As $q \rightarrow 1$,

$$\Delta \tilde{M} \rightarrow \Delta M = \frac{g\mu_B}{4\pi^2} \Gamma\left(\frac{3}{2}\right) \left(\frac{k_B T}{D}\right)^{\frac{3}{2}} \zeta\left(\frac{3}{2}\right)$$

which is the result given by the original model (See eq.5.28).

The internal energy U per unit volume of a system is defined by eq.(3.41). Thus for the q -deformed Heisenberg ferromagnet, it is given by

$$\tilde{U} = k_B T^2 \frac{\partial}{\partial T} (\ln \tilde{Z})$$

We evaluate it at $H = 0$ and obtain

$$\tilde{U} = E_{00} + \frac{3}{2} \frac{(k_B T)^{\frac{5}{2}}}{(4\pi D)^{\frac{3}{2}}} \zeta\left(\frac{5}{2}\right)$$

$$\begin{aligned}
& - \frac{\eta^2}{3!} \left(\frac{1}{4\pi}\right)^{\frac{3}{2}} \left(\frac{k_B T}{D}\right)^{\frac{3}{2}} \left\{ J_{sz} (1 + 8s^2) \left(\frac{1}{2} + \frac{1}{6\sqrt{3}}\right) \right. \\
& - \frac{1}{2} (1 + 8s^2) (k_B T) \left(\frac{9}{4} + \frac{1}{4\sqrt{3}}\right) + (7 - 16s^2) J_{sz} \frac{1}{4\sqrt{2}} \\
& \left. - \frac{1}{2} (7 - 16s^2) (k_B T) \left(\frac{9}{16\sqrt{2}}\right) \right\} \tag{5.71}
\end{aligned}$$

The magnon heat capacity per unit volume of the q-deformed Heisenberg ferromagnet is therefore

$$\begin{aligned}
\tilde{C}_m &= \left(\frac{d\tilde{U}}{dT}\right) \\
&= \frac{15}{4} k_B \left(\frac{k_B T}{4\pi D}\right)^{\frac{3}{2}} \zeta\left(\frac{5}{2}\right) \\
&- \frac{\eta^2}{3!} \left(\frac{k_B}{4\pi D}\right)^{\frac{3}{2}} \left\{ T^{\frac{1}{2}} J_{sz} (2.750 + 2.913s^2) \right. \\
&+ \left. k_B T^{\frac{3}{2}} (0.487 - 15.988s^2) \right\} \tag{5.72}
\end{aligned}$$

In the limit $q \rightarrow 1$, this expression coincides with eq.(5.26), the result in the original model.

Thus the present calculations bring in q-dependent corrections to the temperature dependence of spontaneous magnetisation and magnon heat capacity.

5.5 Comparison with experimental data

The simplest Heisenberg ferromagnets known are EuO and EuS. Both have fcc lattice structure and the magnetism is due to the well localised 4f electrons having $s = \frac{7}{2}$. The data required for the calculation of magnon heat capacity and spontaneous magnetisation [84] is furnished in Table 2. The Riemann zeta functions

$\zeta(\frac{3}{2}) = 2.612$; $\zeta(\frac{5}{2}) = 1.341$. With these data, we have calculated the magnetic contribution to the molar heat capacity \tilde{C}_m and the thermal decrease in spontaneous magnetisation for EuO and EuS for temperatures much below their Curie temperature T_c .

	s	z	g	T_c (K)	J (k_B)	a (Å)	molecular weight	density ($\times 10^3 \text{kg/m}^3$)
<i>EuO</i>	$7\frac{1}{2}$	12	2	69.15	0.606	5.14	167.96	8.216
<i>EuS</i>	$7\frac{1}{2}$	12	2	16.57	0.236	5.95	184.02	5.7

Table 2. Properties of EuO and EuS [84].

We obtain

for EuO,

$$\frac{\tilde{C}_m}{R T^{\frac{3}{2}}} = 10^{-3} \left\{ 3.24 + \eta^2 \left(20.94 - \frac{104.79}{T} \right) \right\} \quad (5.73)$$

$$\frac{\Delta \tilde{M}}{\tilde{M}(0) T^{\frac{3}{2}}} = 10^{-4} \left\{ 4.79 + \eta^2 \left(11.75 - \frac{171}{T} \right) \right\} \quad (5.74)$$

and for EuS,

$$\frac{\tilde{C}_m}{R T^{\frac{3}{2}}} = 10^{-3} \left\{ 13.52 + \eta^2 \left(87.55 - \frac{170.67}{T} \right) \right\} \quad (5.75)$$

$$\frac{\Delta \tilde{M}}{\tilde{M}(0) T^{\frac{3}{2}}} = 10^{-3} \left\{ 1.972 + \eta^2 \left(4.836 - \frac{28.08}{T} \right) \right\} \quad (5.76)$$

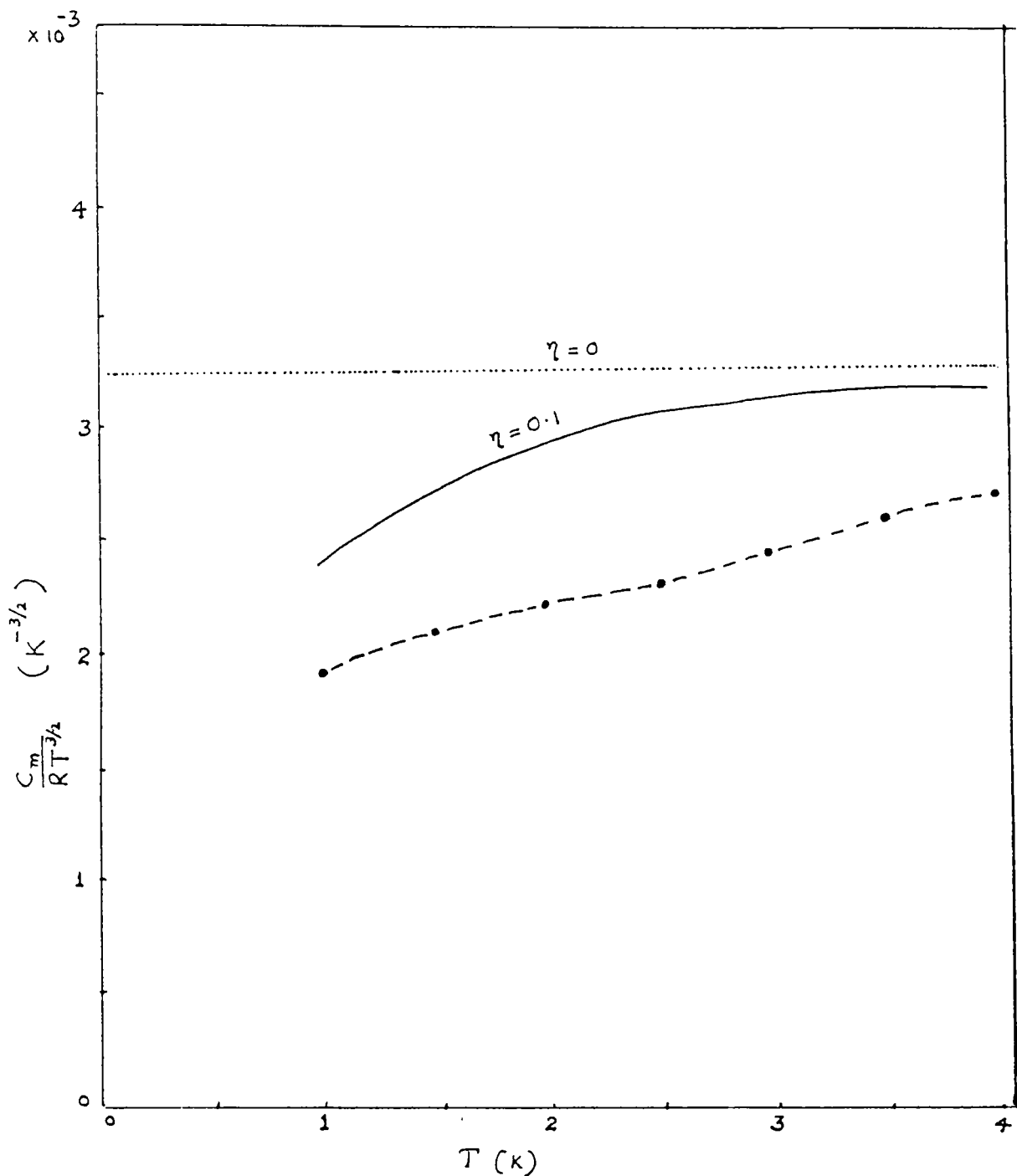


Fig. 2. Magnetic molar heat capacity divided by $T^{3/2}$ vs T in EuO. The solid curve represents theoretical results for $\eta = 0.1$. The dashed curve is the best fit to experimental data [85].

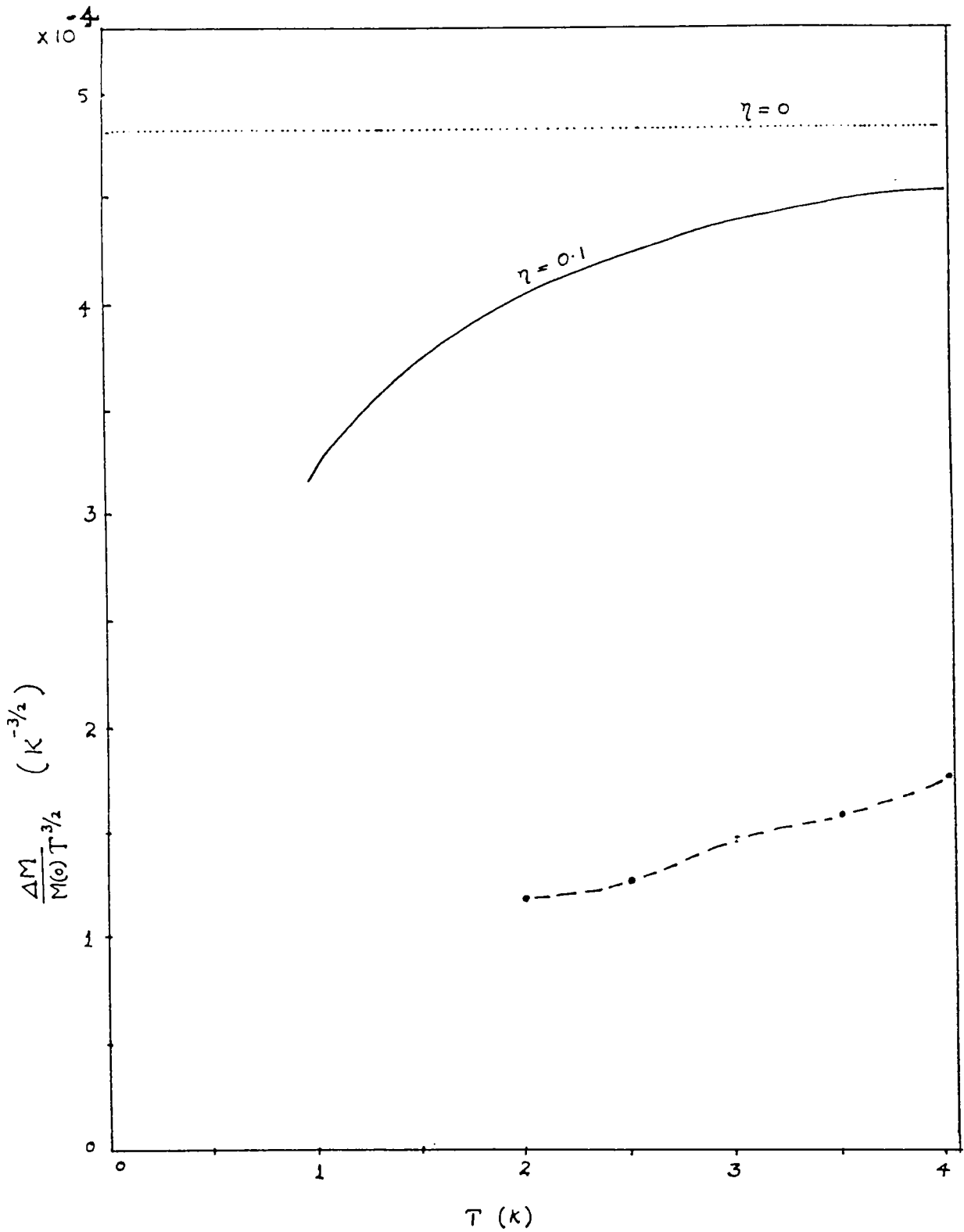


Fig. 3. Reduced magnetisation divided by $T^{3/2}$ vs T in EuO. The solid curve represents theoretical results for $\eta = 0.1$. The dashed curve is the best fit to experimental data [85].

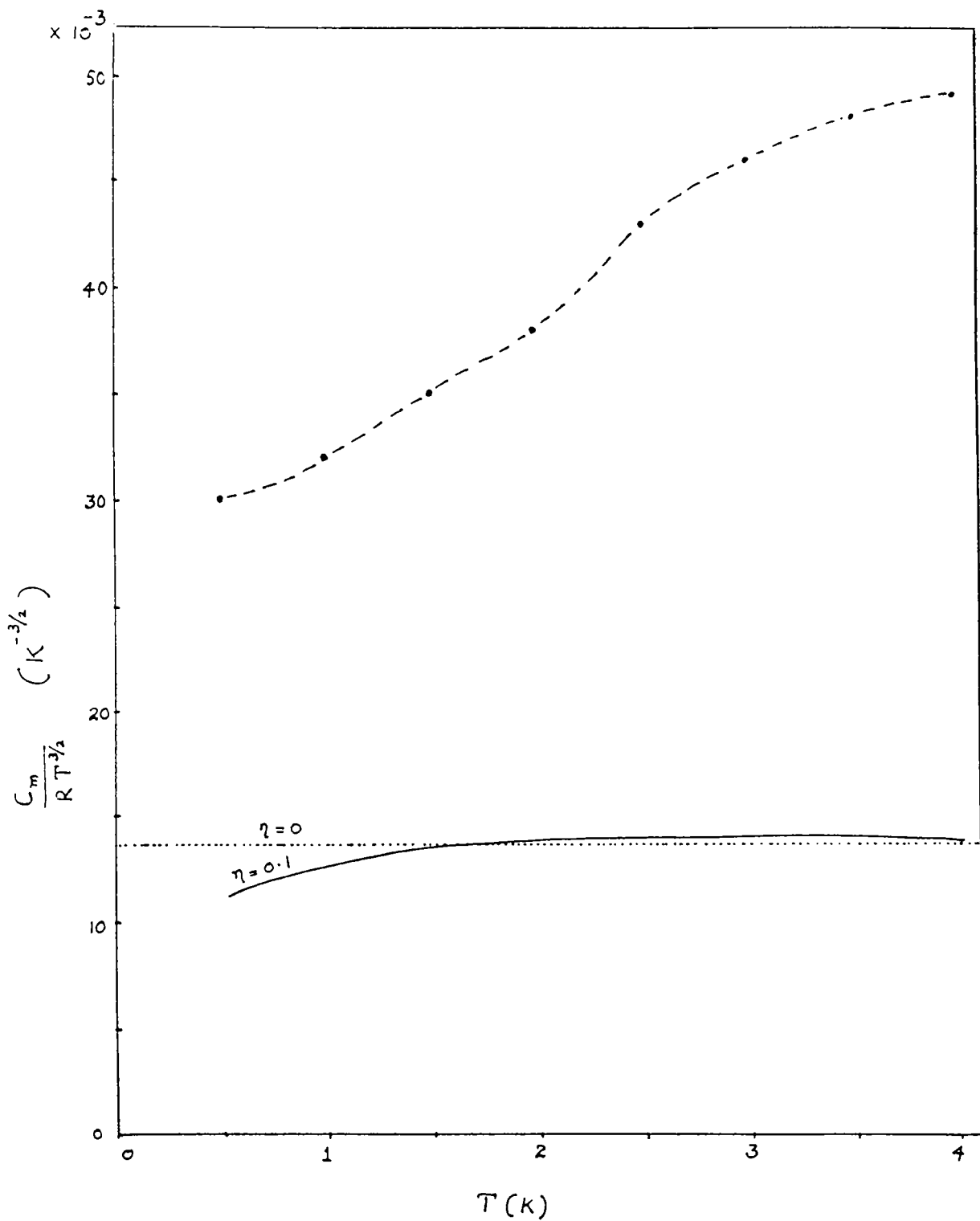


Fig. 4. Magnetic molar heat capacity divided by $T^{3/2}$ vs T in EuS. The solid curve represents theoretical results for $\eta = 0.1$. The dashed curve is the best fit to experimental data [85].

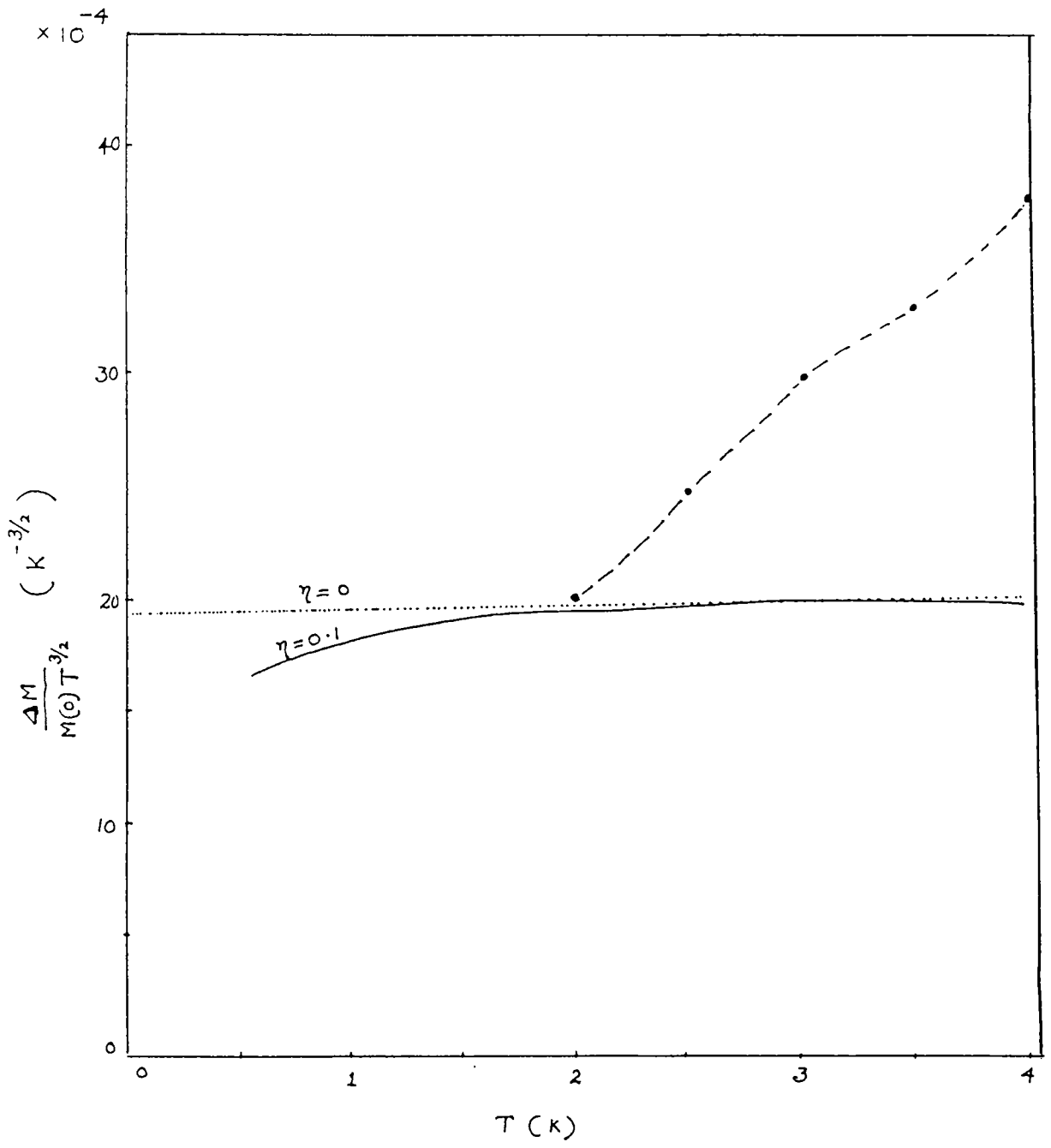


Fig. 5. Reduced magnetisation divided by $T^{3/2}$ vs T in EuS. The solid curve represents theoretical results for $\eta = 0.1$. The dashed curve is the best fit to experimental data [85].

The results for $\eta = 0.1$ are plotted graphically in Figs.(2-5). The results of linear spin wave theory ($\eta = 0$) are also shown. In the case of EuO, there is qualitative agreement between the present theoretical values and experimental values [85] whereas in the case of EuS, the agreement is poor.

5.6 Conclusion

The results of linear spin wave theory based on Heisenberg exchange model of ferromagnetism are not in perfect agreement with experimental observations. The present work is an attempt to improve the model using the concept of q-oscillators. We developed the model in the nearest neighbour approximation. The resulting Hamiltonian contains anharmonic contributions in addition to the uncoupled classical contribution. The additional terms may be interpreted as arising from q- magnon interactions. Only small deformations of the standard spin wave model are considered in the present work. The graphs indicate that the present model is an improvement over the linear spin wave theory and the general nature of temperature dependence of magnon heat capacity and spontaneous magnetisation is predicted by the model. Better results may be obtained if next nearest neighbour exchange interaction and dipole-dipole interaction are also taken into account.

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