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On Mossbauer dynamics in Nb_3Sn

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Abstract. We compare the anharmonic Lamb Mossbauer factor and the q-Lamb Mossbauer factor by studying the anharmonicity observed in the f-factor data of Nb_3Sn. We also show that this anharmonicity does not arise due to the presence of potential.

Keywords. Anharmonicity; lattice dynamics; Mossbauer spectroscopy; superconductor.

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1. Introduction

Before the advent of high temperature oxide superconductivity, several intermetallic compounds possessing A15 crystal structure [1] have been known to be good superconductors; namely V_3Si (T_c=17.1 K), V_3Ga (T_c=16.8 K), Nb_3Sn (T_c=18 K), Nb_3Al (T_c=18.5 K) and $Nb_3Al_{0.75}$ $Ge_{0.75}$ (T_c=20 K). A15 group of compounds are only intermetallic material known at present to possess transition temperature in excess of 18 K. In fact Nb_3Sn has been used in the development of superconducting magnets for fields in excess of 100 kOe, inspite of diffculties involved in fabricating long continuous leads of the brittle material [2].

In addition to high transition temperature these materials frequently display anomalies in their electronic and elastic properties. These anomalies manifest themselves as strong temperature dependence of properties like electronic specific heat, magnetic susceptibility, knight shift etc [1–3]. Although in the past decade interest have been mainly focussed on ceramic oxides there are many unresolved questions related to the above mentioned anomalies.

Mossbauer spectroscopy has also been employed to study Nb_3Sn, a A15 superconductor. The recoil free factor f and isomer shift of ^{119}Sn in Nb_3Sn have been measured by Shier and Taylor [4]. The f-factor of Nb_3Sn is rather small and its temperature dependence is not very strong, implying that mean square displacement (msd) of the Sn atom is fairly large and not very temperature dependent. Sheir and Taylor [4] argued that tin atom moves in a highly anharmonic potential well and Nb_3Sn is a case of low temperature anharmonicity. However, no evidence of unusual overall softness in the phonon spectrum has been observed in specific heat measurements [5,6], resistivity measurements [7] and x-ray Debye–Waller factor [8] measurements. In particular, the x-ray studies of Debye–Waller factor of Sn in Nb_3Sn by Vieland [8] yield values of msd of Sn atoms which are about half the values derived from Mossbauer experiments. The msd of the Sn atom evaluated from X-ray studies show a normal temperature dependence and can fit with Debye temperature θ_D= 262 K for Sn atom and θ_D= 318 K for Nb atoms [8]. The X-ray results are supported by calculations based on the elastic constant [9]. Earlier Hearne *et al* [10] made a precision recoil free measurement of Sn atom in Nb_3Sn and compared the Mossbauer data obtained by all experiments. Although these measured values of the data disagreed with each other yet all the measured values pointed towards the presence of pronounced anharmonicity in Nb_3Sn. The discrepancy, that of x-ray data pointing towards a harmonic solid whereas Mossbauer data pointing towards an anharmonic solid has been attributed to the sensitivity of the Mossbauer technique to anharmonic contributions due to higher order terms [10]. It has been argued that anharmonicity is an essential feature of both intermetallic [18,19,24] and metal oxide supercondutors [20–23].

In this paper our first aim is to show that anharmonicity experienced in Nb_3Sn Mossbauer data may not arise due to the presence of any potential. In order to do so we re-analyse the experimental f factor data of Nb_3Sn to look for presence of anharmonicity in the Mossbauer data at high temperatures also and study its temperature dependence. Our second aim is to study comparison between conventional anharmonic Lamb Mossbauer factor and q Lamb Mossbauer factor on the same experimental f factor data of Nb_3Sn. Earlier q Lamb Mossbauer factor has been used [16] to study anharmonicity in antimony and prussian blue analogues. Thus apart from studying anharmonicity in Nb_3Sn, our interest also lies in studying the physics behind the q structures and hence look for similarities (if any) between parameter q and anharmonic coefficient ϵ.

2. Theory

q-Bosonic algebra has found wide range applications in nuclear physics, molecular physics, non-linear optics ([26], and refrences therein). Its application in condensed matter physics include derivation of q specific heat. It has been argued that parameter q in q-specific heat is a measure of degree of anharmonicity [25]. In recent studies [27] it has been shown that specific heat measurements in ^{4}He superfluid can be explained only if phonons follow q-deformation algebra. q-Harmonic oscillator Hamiltonian can be written as [14,15]

$$H = \frac{1}{2}\hbar\omega(a^+ a + a a^+), \tag{1}$$

where a^+ and a are q-creation and q-annihilation operators which satisfy the commutation relations

$$a a^+ - q a^+ a = 1. \tag{2}$$

q defines the quantum deformation of the Bose operators. We have used a square bracket as the q-number. For any number, say n, the q-number is defined by

$$[n] = \frac{(q^n - (1/q)^n)}{(q - (1/q))}. \tag{3}$$

Equation (3) holds for $q > 1$. q Lamb Mossbauer factor can be written as [16]

$$f = \exp\left\{ -\frac{E_\gamma^2}{3mc^2} \int_0^{\omega_{\max}} \left(\frac{1}{2} + n_q \right) 9 \left\{ \frac{\hbar}{k} \right\}^3 \frac{\omega_i^2}{\theta_{\rm D}^3} \frac{{\rm d}\omega_i}{\hbar\omega_i} \right\}, \tag{4}$$

where

$$n_q = \frac{\sum_{n=0}^{\infty} \frac{1}{2} \{[n+1]+[n]-1\} \exp\left\{ -\frac{1}{2} x \{[n+1]+[n]-1\} \right\}}{\sum_{n=0}^{\infty} \exp\left\{ -\frac{1}{2} x \{[n+1]+[n]-1\} \right\}}$$

and $x = \hbar\omega/kT$, $\hbar\omega_{\max} = k\theta_{\rm D}$. Earlier eq. (4) has been numerically solved for q being real and positive. It has been shown (figure 1 of ref. [16]) that parameter q decides the shape of the f-factor.

3. Conventional approach

Maradudin and Flinn have derived a relationship which describes the effect of anharmonicity on the recoil free factor f. This relationship is given as [12,13]

$$\ln f = -\frac{6RT}{\theta_{\rm D}^2} (1 + \epsilon T + \cdots). \tag{5}$$

In eq. (5) R is the recoil energy of the nucleus, ϵ is the anharmonic coefficient and $\theta_{\rm D}$ is the Debye temperature. For ^{57}Fe nucleus, $R = 22.6$ K. The anharmonic coefficient ϵ can be theoretically calculated by using Maradudin and Flinn theory. Experimentally ϵ can be measured from recoil free factor versus temperature curves. Steyart and Taylor [12] have compared theoretically calculated values and measured values of ϵ (by using eq. (5)) of ^{57}Fe nucleus in various host systems like Ir, Pt, Pd, Au, Ti, etc. Equation (5) holds for temperature $T \geq 50$ K for Debye temperature $\theta_{\rm D} = 300$ K.

In figure 1 we have plotted recoil free factor as obtained from eq. (4) for different values of q but for fixed value of Debye temperature $\theta_{\rm D}$ =300 K. It is evident from figure 1 that as the value of Debye temperature increases, recoil free fraction decreases. Again in figure 1 we have also plotted eq. (5) (anharmonic Lamb Mossbauer factor) for the same value of the Debye temperature ($\theta_{\rm D} = 300$ K) but for different values of anharmonic coefficient ϵ. It is clear from figure 1 that both q and ϵ affect f factor in similar manner i.e. larger the value of q or ϵ, larger is their effect on f factor and vice versa. Again it is important to note that value of ϵ needed to affect the change in f factor depends on the value of Debye temperature i.e. larger the value of Debye temperature, larger is the value of ϵ needed to affect the nature of f factor and vice versa. This is also true of q parameter [16]. Thus anharmonic coefficient shares a similar relationship with Debye temperature as parameter q does. This behaviour points towards a qualitative (if not quantitative) but important similarity in the nature of q and ϵ. Anharmonicity affects the recoil free factor f ($-\ln f$) by decreasing (increasing) it more rapidly than in the case of a normal Debye solid which is also evident from figure 1.

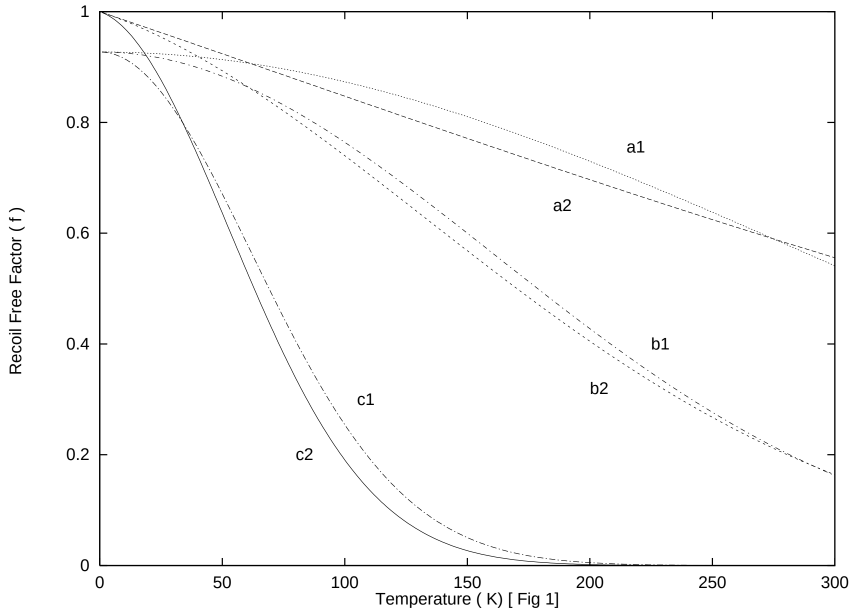

Figure 1. q Lamb–Mossbauer factor and anharmonic Lamb Mossbauer factor versus temperature for fixed value of Debye temperature $\theta_{\rm D} = 300$ K but for different values of q parameter: (a1) $q = 1.1$, (b1) $q = 3.0$, (c1) $q = 50.0$, and different values of anharmonic coefficient ϵ: (a2) $\epsilon = 0.001$, (b2) $\epsilon = 0.01$, (c2) $\epsilon = 0.1$.

4. Results

Absolute values of Sn recoil free factor in the A15 superconductor, Nb_3Sn, have been reported [11]. We are using this published data as experimental inputs in this paper. The experimental recoil free factor data shown in figure 1 of ref. [11] is normalized at 77 K. We have multiplied the data obtained from figure 1 of ref. [11] by 0.375 (which is recoil free factor at 77 K) to denormalize it to make it compatible with other measurements [10]. The results are shown in figure 2 in which we have plotted recoil free factor ($-\ln f$) versus temperature for fixed value of Debye temperature equal to 300 K [11] but for various values of q-parameter. This is the same value of Debye temperature which has been obtained from x-ray Debye–Waller factor measurements of Nb_3Sn. The hollow squares in figure 2 represent experimental data. It is clear from this figure that the temperature dependence of experimental values is very weak even at higher temperatures suggesting the apparent temperature dependence of Debye temperature. Fitting conventional Lamb Mossbauer factor is not possible because each experimental data value corresponds to recoil free factor curve for different values of Debye temperature. This apparent temperature dependence of Debye temperature reflects anharmonicity. It is evident from figure 2 that with the decrease in temperature, the value of q corresponding to different curves increases. Values of parameter q, corresponding to the curves of figure 2 which fit to the experimental data have been plotted against temperature in figure 3. Again figure 4 has been obtained

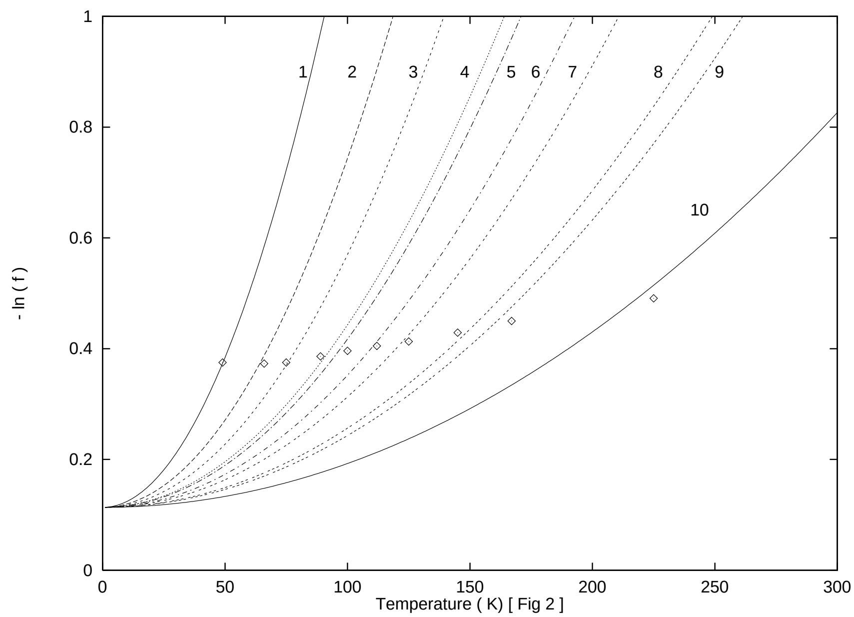

Figure 2. The temperature dependence of qf-factor (-ln f)for Debye temperature $\theta_{\rm D} = 200$ K for various values of q : (1) $q = 23.0$ (2) $q = 9.0$, (3) $q = 6.5$, (4) $q = 4.75$, (5) $q = 3.74$, (6) $q = 3.20$, (7) $q = 2.7$, (8) $q = 2.0$ (9) $q = 1.65$, (10) $q = 1.30$.

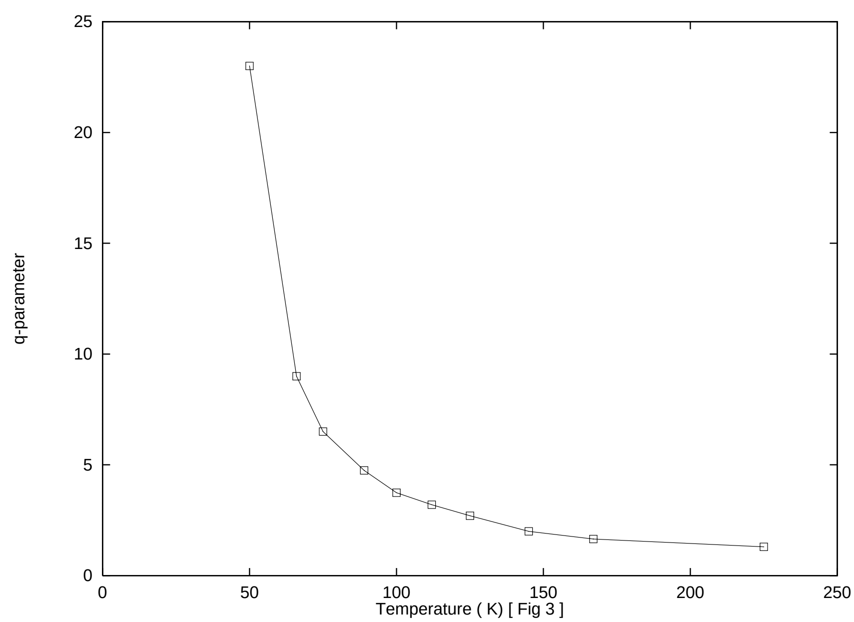

Figure 3. This figure depicts values of parameter q (of various curves of figure 2, which fit to the experimental data) against temperature.

by using anharmonic Lamb Mossbauer factor for Debye temperature $\theta_D = 300$ K but for different values of anharmonic coefficient ϵ. The hollow squares represent experimental data. The values of ϵ, corresponding to the curves of figure 4 which fit to the experimental data have been plotted against temperature in figure 5. It is clear from figures 3 and 5 that anharmonicity is present even at high temperature and becomes maximum at low temperature because all the experimental data fits for $\epsilon \neq 0$ (or $q \neq 1$). The case $\epsilon = 0$ (or $q = 1$) corresponds to a harmonic solid. Thus in this study we have shown that anharmonicity in Nb_3Sn is temperature dependent on nature and increases gradually with the decrease of temperature.

5. Discussion

Earlier it had been argued that unusual behaviour of Mossbauer data of Nb_3Sn is a case of low temperature anharmonicity due to the presence of an anharmonic potential. But no model of potential has been actually fitted to the experimental data, however some suggestions on the nature of potential have been made [11]. Again, there has been no discussion as to why low temperature anharmonicity (if due to potential) should be unique only to Nb_3Sn? In this paper we have shown that it is not possible to fit conventional anharmonic Lamb Mossbauer factor to the experimental f factor data (of Nb_3Sn) for a single value of anharmonic coefficient ϵ. The anharmonic coefficient ϵ can be theoretically

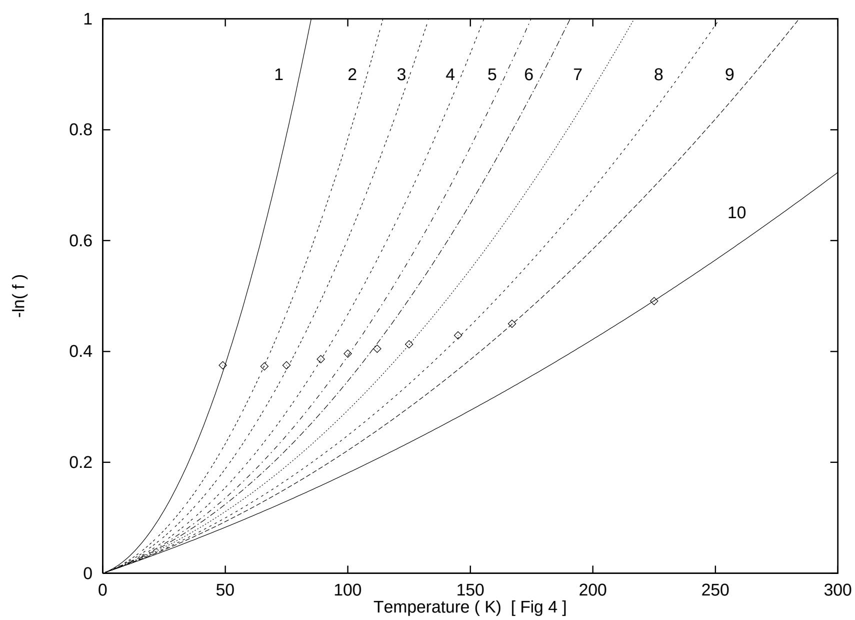

Figure 4. This figure depicts recoil free factor (-ln f) for fixed value of Debye temperature $\theta_D = 300$ K but for various values of anharmonic coefficients ϵ: (1) $\epsilon = 0.08$, (2) $\epsilon = 0.042$, (3)$\epsilon = 0.03$, (4) $\epsilon = 0.021$, (5) $\epsilon = 0.016$, (6) $\epsilon = 0.013$, (7) $\epsilon = 0.0095$, (8) $\epsilon = 0.0065$, (9) $\epsilon = 0.0047$ (10) $\epsilon = 0.002$.

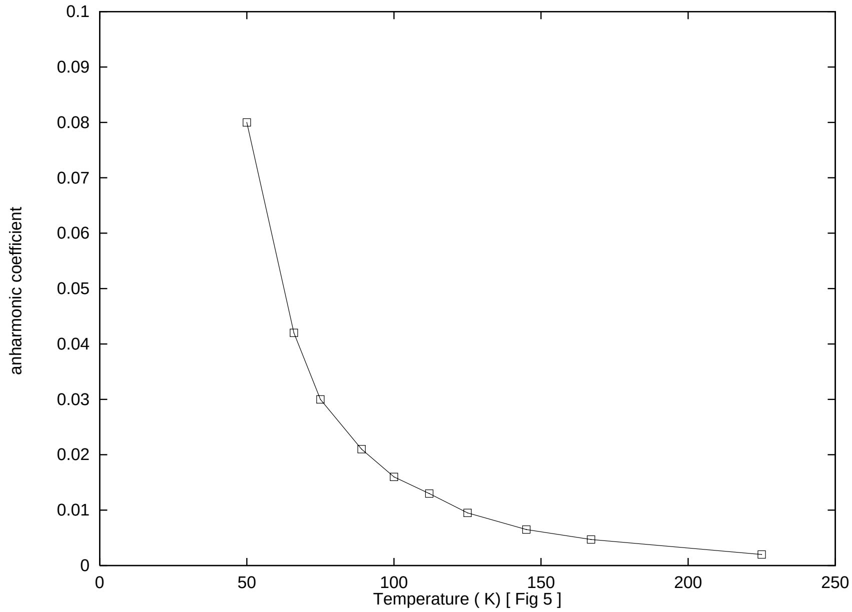

Figure 5. This figure depicts values of parameter ϵ (of various curves of figure 4, which fit to the experimental data) against temperature.

calculated by using Maradudin and Flinn theory for a given potential $\phi(r)$. So, for any typical value of ϵ, there is a corresponding potential $\phi(r)$. This apparent temperature dependence of anharmonic coefficient ϵ should mean that Mossbauer atoms experiences different potentials at different temperatures. But it is difficult to assume that nature of potential $\phi(r)$ will change with temperature. Hence it may not be possible to consider potential as a reason for anharmonicity observed in Nb_3Sn.

The origin of anharmonicity and other anomalies in the Nb_3Sn have been discussed in a recent paper [17] and have been attributed to the presence of sublattice relaxation. It has been argued that at high temperatures thermal motions wash away the structure of A15 superconductor and as the temperature is lowered sublattice relaxation sets in. This sublattice relaxation arises due to the internal strain and increases gradually as the temperature is decreased. The strongest instability has been observed in Nb_3Sn system among all A15 superconductors. Sublattice relaxation sets in at temperature $T \gg 0$ and gradually increases as the temperature is lowered, becoming maximum at 0 K.

In the present studies we have shown that f factor data of Nb_3Sn can not be explained on the basis of potential. Again we have shown that anharmonicity is maximum at lower temperatures and gradually decreases as the temperature increases i.e. anharmonicity in Nb_3Sn is temperature dependent. Our results compliment the above mentioned studies.

6. Conclusions

Anharmonicity is either a high temperature or a low temperature phenomena. But in the case of Nb_3Sn anharmonicity is present both at low and high temperatures. High temperature anharmonicity in Lamb Mossbauer factor occurs when small to moderate deviations take place in the parabolic nature of interatomic potential. In contrast to this low temperature anharmonicity results arises due to the presence of a non-parabolic potential. However, it has been proved that in the case of A15 superconductors in general and Nb_3Sn in particular, anharmonicity arises due to the sublattice relaxation [17].

In this paper, we have shown that Nb_3Sn is a case of temperature dependent anharmonicity which may not arise due to presence of any potential. We have also proved that Mossbauer experimental data can be explained for the same value of Debye temperature θ_{D} as obtained from x-ray Debye–Waller factor measurements. So there is no discrepancy between Debye temperature values of x-ray Debye–Waller factor data and Mossbauer data.

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