THERMODYNAMICAL PROPERTIES OF BOSONS AND FERMIONS FOR LATTICE MOTIVATED DISPERSION RELATIONSHIPS

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ABSTRACT

THERMODYNAMICAL PROPERTIES OF BOSONS AND FERMIONS FOR LATTICE MOTIVATED DISPERSION RELATIONSHIPS

In this thesis, we have studied the coupled simple harmonic oscillator physics of one-dimensional strings, for acoustical phonons, and n-dimensional physics for the optical case (for arbitrary n).

For the acoustical modes, we have calculated only the Bosonic Simple Harmonic Oscillator (BSHO), for the optical mode, we have included both BSHO and Fermionic Simple Harmonic Oscillator (FSHO). For the optical modes, for both BSHO's and FSHO's, we have found that the problem is reduced to the physics of a single oscillator with a partial vibration frequency.

For the FSHO's in the optical cases, we have encountered the presence of negative temperatures for all n. In both cases, we have discovered the presence of correct asymptotical behavior as $T \to 0$ and $T \to \infty$. In the acoustical case, we have used Mellin Transform and a summation formula due to Euler to calculate the partition function and the thermodynamical properties thereof.

Again we have obtained the correct asymptotical behavior as $T \to 0$ and $T \to \infty$. We note that whenever possible, we have included more than one method of calculation and obtained similar results.

ÖZET

KAFES YAPILARINDAN HAREKETLE ELDE EDİLEN DAĞILIM İLİŞKİSİ İÇİN BOZONLAR VE FERMİYONLARIN TERMODİNAMİK ÖZELLİKLERİ

Bu tezde akustik ve optik fononlar için sicimlerin veya optik fononlar için n-boyutlu sistemlerin basit harmonic hareketlerini inceleyeceğiz. Akustik modlar için sadece bozonik basit harmonik hareketleri, optik modlar için ise hem bozonik hem fermiyonik basit harmonik hareketleri üzerinde durduk. Optik modlar için her iki durumda da problemin tek bir titreşime indirgendiğine şahit olduk.

Optik fermiyonik sistemler için, negatif sıcaklıklarla karşı karşıya kaldık. Her iki durumda da $T \to 0$ veya $T \to \infty$ için doğru sınır değerlerini elde ettik. Akustik modlar için Mellin transformları, Euler'e ait bir toplam formül ve iki diğer analitik metod kullanarak fonksitona ailt diğer termodinamik büyüklükleri hesapladık. Bu durumda da $T \to 0$ veya $T \to \infty$ için doğru sınır değerlerini elde ettik.

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LIST OF SYMBOLS

a, d	Lattice spacing
A	Helmholtz free energy
B_n	Bernoulli number
c	Speed of sound
c_v	Specific heat capacity at constant volume
c_p	Specific heat capacity at constant pressure
E	Energy
I_0	Modified Bessel function of the first kind and order zero
J_0	Bessel function of order zero
k_1, k_2	Spring constants
K_T	Compressiblity at constant temperature
L	Length
L_0	Modified Struve function
m	Spring contant
N	Number of particles
p	Pressure
Q	Partition function
S	Entropy
T	Temperature
z	Partition function
α	ω_0/kT
β	1/kT
$\varDelta$	Spring constant
$\varGamma$	Gamma function
κ	Boltzmann constant
λ	Wavelength
ρ	Density

ω_0	Modified frequency
ζ	Riemann-Zeta functin

LIST OF ACRONYMS/ABBREVIATIONS

1-d	One Dimensional
n-d	n Dimensional
BSHO	Bosonic Simple Harmonic OScillators
FSHO	Fermionic Simple Harmonic Oscillator
SHO	Simple Harmonic Oscillator

1. INTRODUCTION

In this thesis, we will study the physics of phonons as in condensed matter physics, in mainly one dimension (also in n-dimensions for optical phonons). These phonons are low lying independent excitations representing the behavior of crystals. The Hamiltonian of such a system consists of a sum of terms, each representing an independent harmonic oscillator, each term corresponding to a pattern vibration of the crystal (normal mode).

As a whole, each mode with a particular (possibly degenerate) frequency, such that all the oscillations behave independently of each other. When we go to higher orders in the interaction, we study the system as a system of phonons interacting with each other.

In our systems of harmonic oscillators, we have a particular relationship relating the frequency of vibration ω_k to a function of the wavevector (crystal momentum). There exists in the literature different relationships. The most famous of these are the Einstein model of the Debye model (both of these are quantum systems). In the Einstein model, we have a single of vibration. In the Debye model, we have a collection of acoustical phonons ($\omega = ck$ where c is the speed of sound and k is the wavevector) such that the total number of these modes equals to 3N where N is the number of particles in 3-dimensions.

As such there is an upper limit to the frequency of vibrations. The total partition function of such a system is the product of the partition functions for each oscillation.

There are two kinds of phonons which are optical and acoustical. For the acoustical phonons (branch), we have $\omega \simeq ck$, as in the case of sound. In acoustical modes, all atoms within a primitive call move in phase as a unit. In optical modes on the other hand, $\omega = m_o + ck^2$ and the ions in a primitive cell execute a molecular vibration out of phase each other.

In this thesis, we study the thermodynamic properties of systems of bosons, and fermions obeying dispersion relations such that

$$\omega^2 = m^2 + \Delta^2 \sin^2 (ka/2), \tag{1.1}$$

$$\omega = \Delta \sin (ka/2), \tag{1.2}$$

and

$$\omega^2 = m^2 + \sum_i {\Delta_i}^2 \sin^2 (k_1 \pi a/2). \tag{1.3}$$

Dispersion relationships similar to the above forms occur in condensed matter of physics. For instance, in the phenomena of plasma oscillations, we have

$${\omega_k}^2 = {\omega_p}^2 + c^2 k^2. \tag{1.4}$$

The similarity with our case is obvious for small k. On the other hand for a system of lattice vibrations [1] monatomic, we have

$$\omega = \Delta \sin ka/2. \tag{1.5}$$

Also for a system of oscillations of a diatomic basis, we have the dispersion relationship

$$\omega^2 = \frac{k_1 + k_2}{m}[1 \pm (1 - \frac{4k_1k_2}{(k_1 + k_2)^2} \sin^2 ka/2)^{1/2}], \tag{1.6}$$

where k_1 and k_2 are the spring constants. The $\pm$ sign corresponds to the optical (acoustical) mode and for $\frac{k_1k_2}{(k_1+k_2)^2} << 1$ or for $k_1 = k_2$ is similar to our dispersion relationship. For one dimension, we will take k to be a continuous variable and calculate the thermodynamical properties of our system using elementary statistical mechanics, and certain analytical methods.

These methods are the theory of Bose-Einstein and Fermi-Dirac functions [2], [3], [4] a summation formula due to Euler [5] and Mellin transform [6]. We first make a brief review of oscillatory systems in Section 2.

In Section 3, we calculate the partition function of Bosonic oscillators for the case of optical modes in one dimension. From there on we calculate the thermodynamical quantities such as the ground state energy, energy, specific heat at constant volume, entropy, and pressure. We obtain the correct asymptotical behavior as $T \to 0$ and $T \to \infty$. Proceeding forward, in section four, we focus on the properties of fermionic oscillators in one dimension.

Again we obtain expressions for the energy, entropy, and specific heat at constant volume. Since the energy of the system is bounded from above, we can have negative temperatures. We note that our results for the case of FSHO's show us that a different behavior is obtained. For fermions in contrast to BSHO's. In sections three and four, we see that the system behaves as N-independent oscillators with a particular frequency of vibration. This corresponds to the Einstein solid in one dimension i.e we have that a collection of optical harmonic oscillators behaves as an Einstein solid. We have not been able to obtain the same behavior for acoustical phonons.

In Section 5, we have calculated the partition function of Bosonic oscillators in an arbitrary number of dimensions, again for the optical modes. We also note that our system of FSHO's behaves precisely as the paramagnetic spin 1/2 1 system in a uniform magnetic field.

In Sections 5 and 6, we focus on the behavior of our systems of BSHO's and FSHO's in an arbitrary number of dimensions. Again, we obtain the correct asymptotic behavior as $T \to \infty$, and $T \to 0$. We also note that in n-dimensions as in the case of 1-dimension, the system behaves as independent oscillations with a particular frequency related to the parameters of our system. We also calculated the pressure and its variation with temperature and volume, and we obtained for our system the gruncisen parameter. We again discovered the presence of negative temperatures for the FSHO's.

In Section 7, we studied the statistical mechanics of the chain of atoms, interacting via a simple harmonic potential. We have calculated the partition function thereof in three different methods in the form of an infinite series of modified Struve functions of order zero, and modified Bessel functions of the first kind of zeroth order.

In one of these, we used a summation formula due to Euler [5], in the other two methods we used elementary analysis. Proceeding we used Mellin transforms to calculate the partition function, and thermodynamical quantities in the form of an infinite series, and to extract the asymptotic behavior out of these series. Again we have obtained the correct asymptotic behavior (with respect to temperature) out of these series, i.e.

$$c_v \propto T \quad \text{as} \quad T \to 0, \tag{1.7}$$

$$c_v \propto k \quad \text{as} \quad T \to \infty, \tag{1.8}$$

$S \to 0$ as $T \to 0$, and

$$S \to N(1 + \log(kT/\Delta)) \quad \text{as} \quad T \to \infty. \tag{1.9}$$

In Section 8.1, we obtained another method for calculating the partition function for 1-d acoustical phonons. Here we made the approximation $\zeta(2k) \sim 1$, which is an excellent one for $k > 3$. Elementary analytical methods lead us to a closed form for the partition function for $z = \Delta\beta/2\pi < 1$. We again obtained the correct behaviour a $z \to 0$ $(T \to \infty)$ i.e E $\propto$ NkT is represented as

$$S = Nk(1 + \log(2kT/\Delta)). \tag{1.10}$$

In Section 8.2, we have calculated the partition function for our system of BSHO's using still another method.

Here in addition to the approximation that $\zeta(2k) \sim 1$, we have also used an asymptotic formula for the Γ-functions in the infinite series. As a result, we obtained a Fermi-Dirac function of order 3/2 for the partition function in terms of $z = \Delta\beta/2\pi < 1$. Again we obtained the correct asymptotic behavior, and we emphasize that for those formulas to be valid z must be less than one. In Section 8.3, we compare the results of the Sections 8.1 and 8.2, and we see that the two expressions are similar to each other.

2. A BRIEF REVIEW OF OSCILLATORY SYSTEMS

In this thesis, for the most part, we are going to study the physics of one-dimensional strings of atoms connected by springs attached to each other such that the interatomic potential between the atoms is approximately a simple harmonic potential. In addition, we have considered the n-dimensional optical modes with the same potential.

We have as the relevant parameters a set of mass values $(m_1, m_2, ...)$ and a set of values for the spring constants $(k_1, k_2, ...)$. We are concerned with optical modes in 1-d in addition to the acoustical modes if there are more than one parameter for these sets. When there is only one parameter in 1-d, we are concerned with acoustical modes.

A similar way of expressing the same idea is that when there is a monatomic basis, we have an acoustical mode; on the other hand, when we have a polyatomic basis, we have an optical mode(s) in addition to the acoustical mode(s). We include only nearest-neighbor interactions and we study longitudinal and/or transverse oscillations.

We will first construct the Hamiltonian for this system. For the potential energy we have

$$V(q_1, ..., q_N) = V_0(q_1, ..., q_N) + \sum_i \frac{\partial V}{\partial q_{i0}} \eta_i + \frac{1}{2!} \sum_{i,j} \frac{\partial^2 V}{\partial q_{i0} \partial q_{j0}} \eta_i \eta_j \tag{2.1}$$

$$+ \frac{1}{3!} \sum_{i,j,k} \frac{\partial^3 V}{\partial q_{i0} \partial q_{j0} \partial q_{k0}} \eta_i \eta_j \eta_k + J(m^4), \tag{2.2}$$

where $q_i = q_{i0} + \eta_i$, and η_i being the displacement relative to the position of equilibrium q_{i0}. Thus we have expanded the potential energy around the position of equilibrium. Thus the second term vanishes. We ignore the third-order term (plus the remainder) for small displacements (small η_i). We also absorb the first term in the zero-point energy. Now, for the kinetic energy we read,

$$T = \frac{1}{2}\sum_{i,j} T_{ij} m_i m_j, \tag{2.3}$$

where $T_{ij} = T_{ji}$. Now, we write the potential energy as the sum over the interactions between the j'th and $(j+1)'$th particles, i.e.

$$V_{j,j+1} = \frac{1}{2}{\omega_0}^2 (q_{j+1} - q_j)^2. \tag{2.4}$$

We note here that the physics of the system should be independent of the boundary conditions imposed on the system for very large N. We employ periodic boundary conditions. Our case of strings is analogous to a pearl necklace in one dimension. In two dimensions, we have a torus. In three or more dimensions no similar picture exists. From the Lagrangian, which can be constructed by way of the Hamiltonian of the system, for the equations of motion we have (for acoustical phonons)

$$\omega^2 q_j = v^2 (q_{j+1} - 2q_j + q_{j-1}). \tag{2.5}$$

Clearly, we have a linear difference equation with constant coefficients, in direct analogy to a linear differential equation with again constant coefficients. Thus we make the conjecture

$$q_j = a_j e^{-i\omega t} = A e^{i(j\beta - \omega t)}, \tag{2.6}$$

j is the position of the j'th particle. We thus obtain the equation

$$\omega = \mathit{\Delta} \sin(\beta/2). \tag{2.7}$$

Employing the periodic boundary conditions such that α is an integer, we get

$$\omega = \mathit{\Delta} \sin(\frac{\pi\alpha}{N}) \qquad 0 \le \alpha \le N-1. \tag{2.8}$$

Thus, we have a set of frequencies for each α, for the normal modes of our system, and a particular pattern of vibrations for each mode. Thus we say that we have diagonalized our system of equations. Now, we can write the Lagrangian as follows

$$L = \frac{1}{2}\sum_{\alpha=1}^{N} \dot{Q}^*_\alpha \dot{Q}_\alpha - \omega^2_\alpha Q^*_\alpha Q_\alpha, \tag{2.9}$$

where $Q^*_\alpha = Q_{-\alpha}$ and

$$Q_k = \frac{1}{\sqrt{N}}\sum_{j=1}^{N} a_j e^{ikx_j}, \tag{2.10}$$

being the transformed (normal) coordinates. Thus we have a set of N one-dimensional decoupled normal modes.

We have a total of N modes, equal to the number of oscillators. For some modes we can have such that some frequencies are zero, these modes correspond to the uniform translational or rotational displacements of the system as a whole. For optical phonons, a similar result is obtained, the main difference being that the zero wavenumber eigenfrequency is nonzero.

Up to now, we have focused on the physics of a discrete chain of atoms. Now we can go on to the continuum case. We have such that each atom oscillates with a phase difference relative to the adjacent atoms as such. We associate a wavelength to describe the motion of our chain, as follows from the relation for a_{j0}. The wave number corresponding to this is equal to

$$k = \frac{2\pi}{\lambda} = \frac{2\pi\alpha}{Nd} \qquad 0 \leq \alpha \leq N-1, \tag{2.11}$$

where the range of α is given above. Then we have as the variables of the behavior of our system

$$q_j = \frac{1}{\sqrt{N}} \sum_{k=1}^{N} Q_k e^{-ikx_j} \rightarrow \text{originial coordinates}, \tag{2.12}$$

$$Q_k = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} q_j e^{ikx_j} \rightarrow \text{transformed coordinates}, \tag{2.13}$$

$$a_{jk} = \frac{1}{\sqrt{N}} e^{ikx_j} \rightarrow \text{passage from original to transformed coordinates}, \tag{2.14}$$

$$\omega_k = \mathit{\Delta} \sin(\frac{kd}{2}). \tag{2.15}$$

We now assume that $kd << 1$ where $\omega \sim kc$. We have the expressions giving the physical properties of our system

$$\sum_{j=1}^{N} (\quad) = \frac{N}{L} \int_0^L dx(\quad) \rightarrow \text{summation over the coordinates}, \tag{2.16}$$

$$\sum_{k=1}^{N} (\quad) = \frac{L}{2\pi} \int_0^{2\pi/d} dk(\quad) \rightarrow \text{summation over the wave numbers}. \tag{2.17}$$

We also have

$$q_{j+1}(t) - q_j(t) \simeq d(\frac{\partial u}{\partial x}), \tag{2.18}$$

where d is the lattice spacing, and $u(x,t)$ is the continuum coordinate. Now the expression for the Lagrangian in terms of the continuous variables $u(x,t)$ can be written as

$$L = \frac{1}{2}\rho \int_0^L dx(\frac{\partial u}{\partial t})^2 - \frac{\rho c^2}{2}\int_0^L dx(\frac{\partial u}{\partial \gamma})^2, \tag{2.19}$$

where $c = \Delta d$, $\rho = m/d$ which is the mass density. For the Fourier transform of $u(k,t)$, we obtain

$$u(k,t) = \int_0^L dx u(x,t)e^{ikx}. \tag{2.20}$$

In terms of these variables we have

$$L = \frac{1}{2}\rho \int \frac{dk}{2\pi}(\frac{\partial u(k,t)}{\partial t})^2 - \frac{\rho c^2}{2}\int \frac{dk}{2\pi}k^2 u(k,t). \tag{2.21}$$

Now for the relevant equation of motion, we obtain

$$\rho(\frac{\partial^2 u}{\partial t^2}) = \rho c^2(\frac{\partial^2 u}{\partial x^2}), \tag{2.22}$$

where we repeat that we have taken $\omega = ck$.

Up to now, we have determined the eigenfrequencies of the motion, which are the same for classical and quantum mechanical cases. Now we go on to the quantum mechanics of a line of atoms. For the Feynman propagator in Quantum Mechanics, we have

$$K = \int .. \int \mathcal{D}(q_1(t))...\mathcal{D}(q_N(t))exp\frac{i}{2\hbar}[\int dt(\sum_{i=1}^{N} \dot{q_i}^2 - \sum_{j,k} v_{j,k}\int dt q_j(t)q_k(t))]. \tag{2.23}$$

In terms of the normal coordinates

$$K = \int .. \int \mathcal{D}(Q_1(t))...\mathcal{D}(Q_N(t))exp\frac{i}{2\hbar}\sum_{\alpha=1}^{N}\int dt(\dot{Q}^2 - \omega_\alpha Q_\alpha^2), \tag{2.24}$$

and

$$K = \Pi_{\alpha=1}^{N}(exp\frac{i}{2t}\int dt(\dot{Q}^2 - \omega_\alpha Q_\alpha^2))\mathcal{D}(Q_\alpha(t)). \tag{2.25}$$

So the total path integral for the Kernel can be separated into a product of independent kernels. The same result follows for the wavefunctions. It follows that the sum of the individual energies gives the total energy.

Now we pass on imaginary time (Temperature) formulation. We have for the relevant case partition function with normal frequency ω_k, in terms of temperature. For Bosons

$$Q_k = -N \log 2 \sinh(\omega/2\pi), \tag{2.26}$$

and for Fermions

$$Q_k = N \log 2 \cosh(\omega/2kT). \tag{2.27}$$

For the ground state energy of the discrete system, we have

$$E_{ground} = \sum_k \frac{\omega_k}{2}. \tag{2.28}$$

Using the approximation of continuity setting $\omega \sim ck$,

$$E_{ground} = \int_0^{k_{max}} \frac{kc}{2} dk. \tag{2.29}$$

We have set $\omega = kc$. To avoid infinities, we have inserted a cutoff wave number. We can make a better approximation by denoting the energy as

$$E_{ground} = \sum_{k=-k_{max}}^{+k_{max}} \frac{\Delta}{2} \sin(kd/2). \tag{2.30}$$

For very large N, we have

$$E_{ground} = cL\frac{1}{\pi d^2}, \tag{2.31}$$

given a particular speed of sound and a length (volume), the ground state energies diverge as d goes to zero. In such case, we prefer to ignore it, for d nonzero on the other hand, we have

$$E_{ground} = \frac{\Delta}{\pi} N, \tag{2.32}$$

(i.e. independent of d).

Now, we are going to discuss the case of an interacting system of quantum SHO's in one dimension in the context of the so-called Debye model. In this model, we have the dispersion relation

$$\omega = ck \qquad k \leq k_0, \tag{2.33}$$

$$\omega = 0 \qquad k > k_0, \tag{2.34}$$

where k_d is the wave number of the Debye model. Also, we have for the Debye frequency

$\omega_0 = ck_0$ where c is the speed of sound. Since the total number of modes equals to the number of particles which is given by the following expression

$$N = \frac{L}{2\pi c}\omega_0. \tag{2.35}$$

For the partition function in the discrete case, we have

$$-\log Q = \sum_k \log\left(1 - e^{-\beta\omega_k}\right). \tag{2.36}$$

In the continuum limit, we have (after integration by parts)

$$-\log Q = N\log(1 - e^{-\omega_0}) - N\frac{kT}{\omega_0}\int_0^{\omega_0/kT} dt \frac{t}{e^t - 1}. \tag{2.37}$$

With the relation $E = -\partial \log Q/\partial\beta$, we have for the energy

$$E = N\frac{(kT)^2}{\omega_0}\int_0^{\omega_0/kT} dt \frac{t}{e^t - 1}. \tag{2.38}$$

The specific heat at constant volume is given by

$$c_v = \frac{2E}{T} - Nk\frac{\omega_0/kT}{e^{\omega_0/kT} - 1}. \tag{2.39}$$

Both of these expressions are positive definite. Finally, for the entropy ($S = \frac{-\partial A}{\partial T}$) or $S = \frac{E}{T} - \frac{A}{T}$, we have

$$S = \frac{2E}{T} - Nk\log(1 - e^{-\beta\omega_0}). \tag{2.40}$$

Entropy is also positive definite for this model.

Now, consider the asymptotical behavior of these quantities. First consider $T \to 0$. We have

$$E = N\frac{(kT)^2}{\omega_0}\int_0^{\infty} dt \frac{t}{e^t - 1} = N\frac{\pi^2}{6}\frac{(kT)^2}{\omega_0}, \tag{2.41}$$

and

$$c_v = \frac{\pi^2}{3}Nk\left(\frac{kT}{\omega_0}\right) \to \text{correct behavior as T} \to 0. \tag{2.42}$$

On the other hand, for the entropy, we have

$$S = N\frac{\pi^2}{3}\frac{kT}{\omega_0}k + Nke^{-\beta\omega_0}, \tag{2.43}$$

which goes to zero as $T \to 0$. Reproducing the expressions above, we get

$$-\log Q = N\log(1 - e^{-\beta\omega_0}) - N\frac{kT}{\omega_0}\sum_n \frac{1}{n^2}\int_0^{n\omega_0/kT} te^{-t}detd\mu, \tag{2.44}$$

$$= N\frac{kT}{\omega_0}(g_2(e^{-\omega_0/kT}) - g(2)). \tag{2.45}$$

Now, we have from [7], [2],

$$g_m(e^-\alpha) = \frac{(-1)^{m-1}}{(m-1)!}(\sum_{k=1}^{m-1}\frac{1}{k} - \log\alpha)\alpha^{n-1} + \sum_{k=1}^{\infty}\frac{(-1)^k}{k!}\alpha^k\zeta(m-k). \tag{2.46}$$

For m=2,

$$g_2(e^{-\omega_0/kT}) = -(1-\log(\omega_0/kT))\frac{\omega_0}{kT} + \zeta(2) + \zeta(0)\frac{\alpha^2}{2} + \sum_{j=\beta}\frac{(-1)^j}{j!}\zeta(2-j)\alpha^j. \tag{2.47}$$

As a result,

$$\begin{aligned} -\log Q &= N[-(1-\log(\omega_0/kT)) + \zeta(0)\frac{\alpha}{2}], \\ &= N\log\omega_0/kT - \frac{1}{4}\frac{\omega_0}{kT}N - N. \end{aligned} \tag{2.48}$$

Thus, for the energy we have

$$E = NkT - \frac{1}{4}N\omega_0. \tag{2.49}$$

Adding to this the ground state energy $\frac{1}{4}N\omega_0$, we have,

$$E = NkT. \tag{2.50}$$

Now, we consider the remainder term R,

$$R = \sum_{j=3}^{\infty}\frac{(-1)^j}{j!}\zeta(2-j)\frac{\alpha^j}{\alpha} \quad (\alpha = \omega_0/kT), \tag{2.51}$$

only $2-j = 1-2k$ terms such that survives. Thus $j = 2k+1$, and

$$R = \sum_{k=1}^{\infty}(-1)\frac{1}{(2k+1)!}\zeta(1-2k)\alpha^{2k}. \tag{2.52}$$

From Riemann's identity, we obtain

$$R = -\sum_{k=1}^{\infty}\frac{2}{(2\pi)^{2k}}\frac{\zeta(2k)\Gamma(2k)}{(2k+1)^k}(-1)^k\alpha^{2k}, \tag{2.53}$$

$$= 2N\sum_{k=1}^{\infty}(\frac{\alpha}{2\pi})^{2k}(\frac{1}{2k+1} - \frac{1}{2k})(-1)^k\zeta(2k). \tag{2.54}$$

Again, set $\zeta(2k) \simeq 1$. We now have, (after setting $\frac{\alpha}{2\pi}$ =z) and taking the integral we have

$$R_n = [(\frac{1}{z}\tan^{-1}(z) - 1) + \frac{1}{2}\log(1+z^2)]2N, \tag{2.55}$$

for $0 < z < 1$. The remainder terms are negligible for $z < 1$ (the case we study here). Thus, asymptotically, we have as $T \to 0$, $c_v = Nk$ (E = NkT). Now, we are going to get motivated by our choice of a dispersion relation. We specialize in the case of a string of oscillators with a diatomic basis. In solid-state physics, we have the dispersion relation

$$\omega^2 = \frac{k_1 + k_2}{m}[1 \pm (1 - \frac{4k_1k_2}{(k_1+k_2)^2}\sin^2(\frac{ka}{2}))^{(1/2)}], \tag{2.56}$$

where k_1, k_2 are the spring constants for our system, and m gives the mass of a single mode. For $\frac{k_1k_2}{(k_1+k_2)^2} << 1$ and for the optical modes

$$\omega^2 = \frac{2(k_1+k_2)}{m}(1 - \frac{k_1k_2}{(k_1+k_2)^2}\sin^2(ka/2)). \tag{2.57}$$

For the acoustical mode

$$\omega^2 = \frac{2k_1k_2}{m(k_1+k_2)}\sin^2 ka/2. \tag{2.58}$$

We also have for $k_1 = k_2 = k_0$,

$$\omega^2 = \frac{4k_0}{m}\sin^2 ka/2, \tag{2.59}$$

or

$$\omega^2 = \frac{4k}{n}\cos^2 ka/2. \tag{2.60}$$

A similar result follows from the considerations of acoustical phonons in 1-d. Led by these considerations, we choose the dispersion relationships of our system.

$$\omega^2 = m^2 + \Delta^2 \sin^2 ka/2 \qquad \text{1-d optical case,} \tag{2.61}$$

$$\omega^2 = m^2 + \sum_i \Delta_i^2 \sin^2 k_i a/2 \qquad \text{n-d optical case,} \tag{2.62}$$

$$\omega = \Delta \sin(ka/2) \qquad \text{1-d acoustical mode.} \tag{2.63}$$

3. CALCULATION OF THE PARTITION FUNCTION OF BOSONIC OSCILLATORS IN ONE DIMENSION

3.1. Preliminaries

First we make the passage from the discrete case to the continuous case and determine exactly what we are going to calculate. From the above equations again since

$$\omega_k^2 = m^2 + \mathit{\Delta}^2 \sin(2)(\frac{\pi k a}{L}) \qquad 0 \leq k \leq \frac{L}{a}, \tag{3.1}$$

and

$$\log(Z) = \sum_k \log(Z_k) = -\sum_k \log(2\sinh(\frac{\beta\omega_k}{2})), \tag{3.2}$$

by enumeration of momentum states

$$\mathit{\Delta} k = \frac{L}{\pi a}\frac{\omega \mathit{\Delta}\omega}{\sqrt{(\omega^2 - m^2)(\mathit{\Delta}^2 + m^2 - \omega^2)}}, \tag{3.3}$$

we have

$$\log(Z) = \frac{-L}{\pi a}\int_m^{\sqrt{m^2+\mathit{\Delta}^2}} \frac{\omega d\omega}{\sqrt{(\omega^2 - m^2)(\mathit{\Delta}^2 + m^2 - \omega^2)}} \log(2\sinh(\frac{\beta\omega}{2})). \tag{3.4}$$

Noting that

$$\begin{aligned} \log(2\sinh(\frac{\beta\omega}{2})) &= \frac{\beta\omega}{2} + \log(1 - e^{-\beta\omega}), \\ &= \frac{\beta\omega}{2} - \sum_n \frac{e^{-n\beta\omega}}{n}, \end{aligned} \tag{3.5}$$

the second term on the right is the Bose-Einstein integral function of order one. We refer the reader to the literature [7] and merely give the result here. In the notation of [7],

$$\begin{aligned} g_1(e^{-\beta\omega}) &= \sum_n \frac{e^{-\beta\omega}}{n} \\ &= -\log(\beta\omega) + \sum_{n=1}^{\infty} \frac{(-1)^n \zeta(1-n)(\beta\omega)^n}{n!}. \end{aligned} \tag{3.6}$$

Here $\zeta(z)$ is the Riemann zeta function. Since $\zeta(-2n) = 0$ only $\zeta(1-2n)$ and $\zeta(0)$ terms contribute and we have the expression [8] according to $\zeta(1-2n) = \frac{-1^n B_n}{2n}$ where

B_n are Bernoulli numbers and $\zeta(0) = -1/2$. As a result

$$g_1(e^{-\beta\omega}) = -\log(\beta\omega) + \sum_{n=1}^{\infty} \frac{(-1)^n B_n (\beta\omega)^{2n}}{(2n)!2n} + \frac{\beta\omega}{2}. \tag{3.7}$$

Therefore we have,

$$\log(2\sinh(\frac{\beta\omega}{2})) = -\sum_{n=1}^{\infty} \frac{(-1)^n B_n (\beta\omega)^{2n}}{(2n)!2n} + \log(\beta\omega). \tag{3.8}$$

3.2. Calculation of the Partition Function in 1-d

We will now separately calculate the contributions to the partition function from the first and second terms of Equation (3.8). Hence we set

$$-\log(Z) = I + K, \tag{3.9}$$

where

$$I = -\frac{L}{\pi a} \sum_{n=1}^{\infty} \frac{(-1)^n B_n \beta^{2n}}{(2n)!2n} \int_m^{\sqrt{m^2+\Delta^2}} \frac{\omega^{2n+1} d\omega}{\sqrt{(\omega^2 - m^2)(\Delta^2 + m^2 - \omega^2)}}, \tag{3.10}$$

and

$$K = \frac{L}{\pi a} \int_m^{\sqrt{m^2+\Delta^2}} \frac{\omega \log(\beta\omega) d\omega}{((\omega^2 - m^2)(\Delta^2 + m^2 - \omega^2))^{1/2}}. \tag{3.11}$$

Now, defining for the first term of Equation (3.8),

$$I_n = \int_m^{m'} \frac{\omega^{2n+1} d\omega}{\sqrt{(\omega^2 - m^2)(\Delta^2 + m^2 - \omega^2)}}, \tag{3.12}$$

where $m' = \sqrt{m^2 + \Delta^2}$, and we get

$$I = -\frac{L}{\pi a} \sum_{n=1}^{\infty} \frac{(-1)^n B_n}{(2n)!2n} \beta^{2n} I_n. \tag{3.13}$$

Setting $\omega^2 = m^2 + z$,

$$I_n = \frac{1}{2} \int_0^{\Delta^2} \frac{(m^2 + z)^n dz}{(z(\Delta^2 - z))^{1/2}}. \tag{3.14}$$

Now from [9], we have

$$I_n = \frac{1}{2} m^{2n} {}_2F_1(-n, 1/2; 1, -\Delta^2/m^2) B(1/2, 1/2), \tag{3.15}$$

where ${}_2F_1$ is the hypergeometric function of its arguments and B is the beta function. Now we use [10], and express the hypergeometric function in terms of Legendre polynomials. Thus we have

$${}_2F_1(-n, 1/2; 1, -\Delta^2/m^2) = (1 + \frac{\Delta^2}{m^2})^{n/2} P_{-n-1}\left(\frac{1 + \frac{\Delta^2}{2m^2}}{\left(1 + \frac{\Delta^2}{m^2}\right)^{1/2}}\right), \tag{3.16}$$

with $P_{-n-1} = P_n$ and $P_n(1) = 1$, making the approximation $\Delta/m \ll 1$ we see that

$$ {}_2F_1(-n, 1/2; 1, -\Delta^2/m^2) = (1 + \frac{\Delta^2}{m^2})^{n/2} \left(P(1) + \mathcal{O}\left(\frac{\Delta^4}{m^4}\right)\right). \tag{3.17} $$

Therefore we get,

$$ I = -\frac{L}{2a} \sum_{n=1}^{\infty} \left[\beta m \left(1 + \frac{\Delta^2}{m^2}\right)^{1/4} \right]^{2n} \frac{1}{(2n)!} \frac{1}{2n} (-1)^n B_n, \tag{3.18} $$

with $m \left(1 + \frac{\Delta^2}{m^2}\right)^{1/4} = \omega_0$,

$$ I = -\frac{L}{2a} \sum_{n=1}^{\infty} (\omega_0 \beta)^{2n} \frac{(-1)^n B_n}{(2n)!2n}, \tag{3.19} $$

with $x = i\beta\omega_0$,

$$ I = -\frac{L}{2a} \sum_{n=1}^{\infty} \frac{x^{2n}}{(2n)!} \frac{B_n}{2n}. \tag{3.20} $$

Taking the derivative with respect to x and multiplying with x; we get,

$$ x\frac{dI}{dx} = -\frac{L}{2a} \sum_{n=1}^{\infty} \frac{x^{2n}}{(2n)!} B_n, \tag{3.21} $$

from the identity in [8] page 125,

$$ \frac{x}{2} \cot(\frac{x}{2}) = 1 - \sum_{n=1}^{\infty} \frac{x^{2n}}{(2n)!} B_n, \tag{3.22} $$

with $x = iz$; we have,

$$ \frac{dI}{dz} = -\frac{L}{2a} \left[\frac{1}{z} - \frac{1}{2} \coth(\frac{z}{2}) \right]. \tag{3.23} $$

Integrating over z with $z = \omega_0$

$$ I = -\frac{L}{2a} \left[\log(z) - \log(\sinh(\frac{z}{2})) \right] + C_o, \tag{3.24} $$

where C_0 is the constant of integration. Since $I(0) = 0$,

$$ I(\beta) = -\frac{L}{2a} \left[\log(\beta\omega_0) - \log(2\sinh(\frac{\beta\omega_0}{2})) \right]. \tag{3.25} $$

We now calculate the contribution of the second term in Equation (3.8) to the series expansion. We have defined K such that given in the Equation (3.11),

$$ K = \frac{L}{\pi a} \int_m^{\sqrt{\Delta^2 + m^2}} \frac{\omega \log(\beta\omega) d\omega}{((\omega^2 - m^2)(\Delta^2 + m^2 - \omega^2))^{1/2}}. \tag{3.26} $$

Setting $\omega^2 = u$,

$$\begin{aligned} K =& \frac{L}{2\pi a}\left\{\int_{m^2}^{\Delta^2+m^2} \frac{\log(\beta)du}{\left[(u-m^2)(\Delta^2+m^2-u)\right]^{1/2}}\right. \\ &\left. +\frac{1}{2}\int_{m^2}^{\Delta^2+m^2} \frac{\log(u)du}{\left[(u-m^2)(\Delta^2+m^2-u)\right]^{1/2}}\right\}. \end{aligned} \tag{3.27}$$

We have therefore $K = K_1 + K_2$ where K_1 and K_2 are the first and second terms respectively in the above expression. For the first term, K_1 we refer the reader to [9]. $K_1 = \frac{L}{2a}\log(\beta)$. For the second term on the right (K_2), setting $u = m^2 + \Delta^2 - y$ we have

$$\begin{aligned} K_2 = \frac{L}{4\pi a}&\left\{\int_0^{\Delta^2} \frac{dy \log(m^2+\Delta^2)}{[y(\Delta^2-y)]^{1/2}}\right. , \\ &\left. + \int_0^{\Delta^2} \frac{dy \log(1-\frac{y}{m^2+\Delta^2})}{[y(\Delta^2-y)]^{1/2}}\right\}. \end{aligned} \tag{3.28}$$

The first term above again gives [8],

$$= \frac{L}{2a}\log((m^2+\Delta^2)^{1/2}). \tag{3.29}$$

Setting $y = \Delta^2 z^2$, the second term gives,

$$= \frac{L}{2\pi a}\int_0^1 \frac{dz \log(1-\frac{\Delta^2 z^2}{m^2+\Delta^2})}{[1-z^2]^{1/2}}. \tag{3.30}$$

From [9],

$$K_2 = \frac{L}{2a}\log(\frac{m+(\Delta^2+m^2)^{1/2}}{2(\Delta^2+m^2)^{1/2}}). \tag{3.31}$$

Finally, $K = K_1 + K_2$ equals to

$$K = \frac{L}{2a}\log(\frac{\beta((m^2+\Delta^2)^{1/2}+m)}{2}). \tag{3.32}$$

Collecting results from Equations (3.25) and (3.32), we have

$$\begin{aligned} \log(Z) = \frac{L}{2a}&\left\{\log(\frac{\omega_0}{kT}) - \log(2\sinh(\frac{\omega_0}{2kT}))\right. , \\ &\left. - \log(\frac{(m^2+\Delta^2)^{1/2}+m}{2kT})\right\}, \end{aligned} \tag{3.33}$$

with $\omega_0 = m(1+\frac{\Delta^2}{m^2})^{1/4}$. Up to order $\frac{\Delta^4}{m^4}$

$$\log(Z) = -\frac{L}{2a}\log(2\sinh(\frac{\omega_0}{2kT})). \tag{3.34}$$

3.3. Ground State Energy

Now we calculate the ground state energy for our system of BSHOs. We have

$$E_0 = \sum_{k=0} \frac{\omega_k}{2}, \tag{3.35}$$

setting $\hbar = 1$. Using the expression for the enumeration of the momentum states

$$= \frac{L}{2\pi a} \int_m^{(\Delta^2+m^2)^{1/2}} \frac{\omega^2 d\omega}{((\omega^2 - m^2)(\Delta^2 + m^2 - \omega^2))^{1/2}}. \tag{3.36}$$

Setting $\omega^2 = m^2 + y$ and $2\omega d\omega = dy$

$$E_0 = \int_0^{\Delta^2} \frac{L}{4\pi a} \frac{(m^2 + y)^{1/2} dy}{(y(\Delta^2 - y))^{1/2}}, \tag{3.37}$$

again using the result from [9],

$$E_0 = \frac{mL}{4a} \, {}_2F_1 \left[-1/2, 1/2; 1, -\Delta^2/m^2\right]. \tag{3.38}$$

Now, we use the result in [10] page 561,

$${}_2F_1 \left[-1/2, 1/2; 1, -\Delta^2/m^2\right] = \left(1 + \frac{\Delta^2}{m^2}\right)^{1/4} P_{-3/2} \left[\frac{(1 + \frac{\Delta^2}{2m^2})}{(1 + \frac{\Delta^2}{m^2})^{1/2}}\right], \tag{3.39}$$

with $P_{1/2} = P_{-3/2}$ and $\Delta^2/m^2 \ll 1$, and $P_n(1) = 1$ we have

$$E_0 = \frac{mL}{4a} \left(1 + \frac{\Delta^2}{m^2}\right)^{1/4}. \tag{3.40}$$

3.4. Thermodynamics of BSHO's in 1-d

We have for Z from Equation (3.34),

$$\log(Z) = -\frac{L}{2a} \log(2 \sinh(\frac{\omega_0}{2kT})), \tag{3.41}$$

due to the well known relationship $E = -\left(\frac{\partial \log(Z)}{\partial \beta}\right)_L$

$$E = \frac{\omega_0 L}{4a} \coth(\frac{\omega_0}{2kT}). \tag{3.42}$$

Now for $\frac{\omega_0}{2kT} \ll 1$,

$$E = \frac{L}{2a} kT, \tag{3.43}$$

and for $\frac{\omega_0}{2kT} \gg 1$,

$$E = \frac{\omega_0 L}{4a}, \tag{3.44}$$

we get the same result for the ground state energy as in Equation (3.40). Now we will calculate the entropy of our system of BSHO's. Again we have the order of $\frac{\Delta^4}{m^4} \ll 1$

$$A = \frac{L}{2a} kT \log(2\sinh(\frac{\omega_0}{kT})), \tag{3.45}$$

with

$$S = -\left(\frac{\partial A}{\partial T}\right)_L = \frac{L}{2a} k \left(\frac{\omega_0}{2kT}\coth(\frac{\omega_0}{2kT}) - \log(2\sinh(\frac{\omega_0}{2kT}))\right). \tag{3.46}$$

Now we consider the asymptotic behavior of entropy as $T \to 0$, and $T \to \infty$. As $T \to 0$, S also goes to zero. Thus, our expression for the entropy satisfies the third law of thermodynamics. As $T \to \infty$,

$$S = \frac{L}{2a} k \left(\log(\frac{kT}{\omega_0}) + 1\right). \tag{3.47}$$

We have obtained an expression for S, A, E in terms of T and L. We take the variable L for the volume of the system. Indeed in the case of 2d (3d) systems (work in progress), we have L^2 (L^3) respectively which is consistent with our choice. Also naturally $P = -\left(\frac{\partial A}{\partial L}\right)_T$ which follows from the expression given for the free energy. Also, we have $E + PL - TS = \mu N$. Since the number of phonons are not conserved $\mu = 0$, N is irrelevant, and $E + PL - TS = 0$. This is satisfied when the expressions for E, S, and P are substituted into this expression. Thus we have everything is as it should be.

Following the discussion above we can define $L/2a$ to be the volume. Now we want to calculate explicitly the pressure of this model in this case. We have to order Δ^4/m^4 using the Maxwell's relationship, $P = -\left(\frac{\partial A}{\partial L}\right)_T$ as noted above,

$$P = -\frac{kT}{2a} \log(2\sinh(\frac{\omega_0}{2kT})). \tag{3.48}$$

We see that the pressure is a monotonically increasing function of temperature as naively expected. On the other hand as $T \to 0$, P goes to $-\frac{\omega_0}{4a}$. As $T \to \infty$, P goes to $\frac{kT}{2a}\log(\frac{kT}{\omega_0})$. Or more generally we have

$$P = -\frac{\omega_0}{4a} - \frac{kT}{2a}\log(1 - e^{-\frac{\omega_0}{kT}}). \tag{3.49}$$

We see that pressure can attain negative values. The temperature at $P = 0$, is such that $2\sinh(\frac{\omega_0}{2kT_0}) = 1$, or $\cosh(\frac{\omega_0}{2kT_0}) = \frac{\sqrt{5}}{2}$. We see that the pressure is a monotonically increasing function of temperature, as would be naively expected. Now we consider variations in pressure as a function of T_c, $\delta T = T - T_c$, $\delta P = P - P_c$. So, we have

$$\delta P = \frac{k}{4a}\left(\frac{\omega_0}{kT_c}\right)\sqrt{5}\,\delta T. \tag{3.50}$$

We see that there exists a remote possibility of considering this behavior as a phase transition such that δP is an order parameter with the critical exponent, say $\sigma = 1$, although the other thermodynamical functions are well defined and therefore lack examples of singular behavior to merit being called phase transitions. Now we calculate specific heat at constant volume and constant pressure. From above (3.42),

$$C_L = \left(\frac{\partial E}{\partial T}\right)_L = \frac{kL}{2a}\left(\frac{\omega_0}{2kT}\right)^2 (2)\left(\frac{\omega_0}{2kT}\right). \tag{3.51}$$

We observe the ideal gas behavior in this formula. As $T \to 0$ on the other hand we observe a Schottky type anomaly in the specific heat. Now, we use the result from [11]

$$C_P - C_L = \frac{TL\alpha^2}{K_T}, \tag{3.52}$$

where α is the coefficient of thermal expansion

$$\alpha = \frac{1}{L}\left(\frac{\partial L}{\partial T}\right)_P, \tag{3.53}$$

and K_T is the compressibility

$$K_T = \frac{1}{L}\left(\frac{\partial L}{\partial P}\right)_T. \tag{3.54}$$

Since P is independent of L we have, $\left(\frac{\partial P}{\partial L}\right)_T = 0$ and $\frac{1}{K_T} = 0$. Therefore from $P = P(T)$, constant pressure means constant temperature i.e. $\left(\frac{\partial L}{\partial T}\right)_P$ is not defined. Therefore, we make the conjecture $C_P = C_L$. We also see that the thermodynamical relationship $E - TS + PL = \mu N$ is obeyed with $\mu N = 0$ since the number of phonons are not conserved. Therefore, our calculation is self-consistent.

4. CALCULATION OF THE PARTITION FUNCTION OF FERMIONIC OSCILLATORS IN ONE DIMENSION

4.1. The Partition Function

In this section we consider the case of a system of Fermionic Simple Harmonic Oscillators (FSHO) with the same dispersion relationship as the previously given one. In analogy with the previous calculation, we make the passage from the discrete case to the continuous case. Our dispersion relationship reads the same as the previous case

$$\omega_k^2 = m^2 + \Delta^2 \sin[2](\frac{k\pi a}{L}), \tag{4.1}$$

for a single FSHO, we have from [12] the expression for the partition function,

$$Z_k = 2\cosh(\frac{\beta\omega_k}{2}), \tag{4.2}$$

and for a system of FSHOs we have

$$Z = \prod_k Z_k. \tag{4.3}$$

Now going explicitly to the continuum limit and enumerating the momentum states,

$$\Delta k = \frac{L}{\pi a}\frac{\omega\Delta\omega}{[(\omega^2 - m^2)(\Delta^2 + m^2 - \omega^2)]^{1/2}}. \tag{4.4}$$

In the continuum limit

$$\log(Z) = \frac{L}{\pi a}\int_m^{\sqrt{\Delta^2+m^2}} \frac{\omega d\omega}{[(\omega^2 - m^2)(\Delta^2 + m^2 - \omega^2)]^{1/2}} \log(2\cosh(\frac{\beta\omega}{2})), \tag{4.5}$$

and expanding log term, in power of $e^{-\beta\omega}$, we have

$$\begin{aligned} \log(2\cosh(\frac{\beta\omega}{2})) &= \frac{\beta\omega}{2} + \sum_{n=1}^{\infty}(-1)^{n+1}\frac{e^{-n\beta\omega}}{n}, \\ &= \frac{\beta\omega}{2} + f_1(e^{-\beta\omega}), \end{aligned} \tag{4.6}$$

where f_1 is the Fermi-Dirac integral function, of order 1, in direct analogy to the Bose-Einstein integral function.

We have, also from [7]

$$f_1(e^{-\beta\omega}) = g_1(e^{-\beta\omega}) - g_1(e^{-2\beta\omega}), \tag{4.7}$$

where $g_1(e^{-\beta\omega})$ is the Bose-Einstein integral function of order 1. For $g_1(e^{-\beta\omega})$ and $g_1(e^{-2\beta\omega})$, we have from [7],

$$g_1(e^{-\beta\omega}) = \left[-\log(\beta\omega) + \sum_{i=1}^{\infty} (-1)^i \frac{B_i(\beta\omega)^{2i}}{(2i)!(2i)} + \frac{\beta\omega}{2} \right], \tag{4.8}$$

$$g_1(e^{-2\beta\omega}) = \left[-\log(2\beta\omega) + \sum_{i=1}^{\infty} (-1)^i \frac{B_i(2\beta\omega)^{2i}}{(2i)!(2i)} + \frac{2\beta\omega}{2} \right], \tag{4.9}$$

$$f_1(e^{-\beta\omega}) + \frac{\beta\omega}{2} = \left[\log(2) + \sum_{i=1}^{\infty} (-1)^i \frac{B_i(1-2^{2i})(\beta\omega)^{2i}}{(2i)!(2i)} \right]. \tag{4.10}$$

Take the integral over ω with the density of states given above. Considering the first term in the parenthesis in Equation (4.10) and taking the integral over ω using our dispersion relationship, we have as in the first part of Equation (3.27), defining S_1,

$$S_1 = \frac{L}{\pi a} \log(2) \int_m^{\sqrt{\Delta^2+m^2}} \frac{\omega d\omega}{[(\omega^2 - m^2)(\Delta^2 + m^2 - \omega^2)]^{1/2}}, \tag{4.11}$$

from [9],

$$S_1 = \frac{L}{2a} \log(2). \tag{4.12}$$

For the second term on the other hand, defining S_2,

$$S_2 = \frac{L}{\pi a} \int_m^{\sqrt{\Delta^2+m^2}} \sum_{i=1}^{\infty} (-1)^i \frac{B_i(1-2^{2i})}{(2i)!2i} (\beta\omega)^{2i} \frac{\omega d\omega}{(m^2 - \omega^2)(\Delta^2 + m^2 - \omega^2))^{1/2}}. \tag{4.13}$$

As a result we have

$$S_2 = I(\beta\omega_0) - I(2\beta\omega_0), \tag{4.14}$$

where I is defined in (3.10) and in (3.25). Thus, $S = S_1 + S_2$ and

$$\begin{aligned} \log(Z) = \frac{L}{2a} \Big\{ & \left[\log(\beta\omega_0) - \log(2\sinh(\frac{\omega_0\beta}{2})) \right] \\ & - \left[\log(2\beta\omega_0) - \log(2\sinh(\omega_0\beta)) \right] + \log(2) \Big\}. \end{aligned} \tag{4.15}$$

Finally we have

$$\log(Z) = \frac{L}{2a} \log(2\cosh(\frac{\beta\omega_0}{2})). \tag{4.16}$$

4.2. Thermodynamical Quantities for FSHO's in One Dimension

Now, we consider the quantities S, P, E, L, A, C_L, C_P (entropy, pressure, energy, volume, Helmholtz free energy, specific heat at constant volume, specific heat at constant pressure respectively). From above, we have

$$\log(Z) = \frac{L}{2a}\log(2\cosh(\frac{\omega_0}{2kT})), \tag{4.17}$$

$$A = -kT\log(Z), \tag{4.18}$$

$$E = -\left(\frac{\partial \log(Z)}{\partial \beta}\right)_L = -\frac{L}{4a}\omega_0 \tanh(\frac{\omega_0}{2kT}), \tag{4.19}$$

with

$$C_L = \left(\frac{\partial E}{\partial T}\right)_L = \frac{L}{2a}\left(\frac{\omega_0}{2kT}\right)^2 \operatorname{sech}(2(\frac{\omega_0}{2kT})k). \tag{4.20}$$

And with the thermodynamical identity from [11], we have

$$C_P - C_L = \frac{TL\alpha^2}{K_T}, \tag{4.21}$$

again since $\left(\frac{\partial P}{\partial L}\right)_T = 0$, $1/K_T = 0$, α is not defined, so we say that $C_P = C_L$. We now give the expression for S, the entropy as

$$S = -\left(\frac{\partial A}{\partial T}\right)_L = \frac{L}{2a}k\log(2\cosh(\frac{\omega_0}{2kT})) - \frac{\omega_0}{2kT}\tanh(\frac{\omega_0}{2kT}). \tag{4.22}$$

Next, we consider the asymptotic behavior as $T \to 0$ and $T \to \infty$ for the thermodynamical quantities above. First, we consider E when temperature goes to zero, as

$$E = -\frac{L}{4a}(T), \tag{4.23}$$

and as the temperature goes to infinity, we have

$$E = \frac{L}{2a}\left(\frac{\omega_0}{2kT}\right)\frac{\omega_0}{2}. \tag{4.24}$$

Now consider the behavior of specific heat at constant volume

$$\text{as} \quad T \to 0^+ \qquad C_L = \frac{L}{2a}\left(\frac{\omega_0}{2kT}\right)^2 e^{-\left(\frac{\omega_0}{2kT}\right)}, \tag{4.25}$$

$$\text{as} \quad T \to 0^- \qquad C_L = \frac{L}{2a}\left(\frac{\omega_0}{2kT}\right)^2 e^{\left(\frac{\omega_0}{2kT}\right)}. \tag{4.26}$$

Now we have for S, the asymptotic behavior as $T \to \pm\infty$ as given below,

$$S = k\frac{L}{2a}\left[\log(2) - \left(\frac{\omega_0}{2kT}\right)^2\right]. \tag{4.27}$$

As $T \to 0$ on the other hand,

$$S = 0. \tag{4.28}$$

We see that our equation for entropy satisfies the third law of thermodynamics. Also, for T goes to infinity or minus infinity, the entropy goes as $\log(2)$ which is the entropy of a system of paramagnetic material as T goes to infinity or minus infinity. From above we see immediately that T can attain negative values as a result of the dependence of A, S, E on temperature as given by for example [7]. Indeed the thermodynamical quantities for a system of FSHOs, A, E, S are exactly the same as the ones given in the case of a paramagnetic system of spin one half dipoles in the presence of a magnetic field, with $\frac{L}{2a}$ exchanged with N. Since the paramagnetic system can attain negative values of temperature, our system can also do so. The reason for the paramagnetic system to obtain negative values is that the energy is bounded from above. Bosonic systems similar to the one which is considered in this paper are not bounded from above and therefore do not attain negative temperatures.

Finally, we will calculate the pressure in terms of L and T. We have for our system of FSHO's a well known expression for the Helmholtz free energy and derivative with respect to L. First, we let $\frac{L}{2a}$ to stand for volume. Then, with

$$A = -kT\frac{L}{2a}\log(2\cosh(\frac{\omega_0}{2kT})), \tag{4.29}$$

$$P = -\left(\frac{\partial A}{\partial L}\right)_T = \frac{kT}{2a}\log(2\cosh(\frac{\omega_0}{2kT})). \tag{4.30}$$

Also, we obtain the result that the pressure attains negative values for negative temperatures. Now, we consider the asymptotic behavior of the pressure P, as T goes to zero and as T goes to plus or minus infinity. As T goes to zero,

$$P = \frac{\omega_0}{4a}(T) \quad \text{where} \quad (T) = \theta(T) - \theta(-T). \tag{4.31}$$

We observe discontinuous behavior of pressure as T goes to zero from above and from below. And now, as T goes to infinity,

$$P = \frac{kT}{2a}\left(\log(2) + \frac{1}{2}\left(\frac{\omega_0}{2kT}\right)^2\right). \tag{4.32}$$

4.3. Conclusion and Summary for 1-d SHO's

We have shown that for our one dimensional systems of BSHO's and FSHO's energy and specific heat as a function of the temperature T, lattice size L, lattice spacing a are given by

$$\text{FSHO's} \quad E = -\frac{L}{4a}\omega_0 \tanh\left(\frac{\omega_0}{kT}\right) \quad C_L = \frac{L}{2a}\left(\frac{\omega_0}{2kT}\right)^2 [2]\left(\frac{\omega_0}{2kT}\right), \tag{4.33}$$

$$\text{BSHO's} \quad E = -\frac{L}{4a}\omega_0 \coth\left(\frac{\omega_0}{kT}\right) \quad C_L = \frac{L}{2a}\left(\frac{\omega_0}{2kT}\right)^2 [2]\left(\frac{\omega_0}{2kT}\right). \tag{4.34}$$

We note that for the FSHO's we see that there is a discontinuity in E as a function of temperature i.e.

$$T \to 0^+ \qquad E = -\frac{L}{4a}\omega_0, \tag{4.35}$$

$$T \to 0^- \qquad E = \frac{L}{4a}\omega_0. \tag{4.36}$$

We discussed the behavior of pressure for FSHO's which is given by Equation (4.30) and as T goes to zero, we have

$$P = \frac{\omega_0}{4a}(T). \tag{4.37}$$

Thus we see that in the case where L stands for the volume of the system there is a discontinuity in E and P at $T = 0$. This does not pose any problem however since the real thermodynamical parameter is $1/T$ and not T. Therefore $T = 0^-$ and $T = 0^+$ are infinitely apart from each other. Hence there is no real discontinuity. Also we see that as T drops below zero the pressure attains negative values for FSHO's. For the bosonic simple harmonic case with the Equation (3.48) we see that for $P = 0$, we have, for T_C

$$kT_C = \frac{\omega_o}{\log(\frac{5}{4})}, \tag{4.38}$$

for $T < T_C$, $P < 0$; it (only) looks like a phase transition. Because there are no singularities.

Finally, as far as entropy is concerned

$$S = \frac{L}{2a}k\left(\left(\frac{\omega_0}{2kT}\coth(\frac{\omega_0}{2kT})\right) - \log(2\sinh(\frac{\omega_0}{2kT}))\right), \tag{4.39}$$

for BSHO's and

$$S = \frac{L}{2a}k\left(\log(2\cosh(\frac{\omega_0}{2kT})) - \frac{\omega_0}{2kT}\tanh(\frac{\omega_0}{2kT})\right), \tag{4.40}$$

for FSHO's. We see immediately that S is a continuous function of T and L for both FSHO's and BSHO's. For T goes to 0_+

$$S = \frac{L}{2a}k\log(2), \tag{4.41}$$

(which is identically the same as the paramagnetic system of spin 1/2 dipoles in the presence of a magnetic field). As noted above while attempting to calculate C_P, there is a problem with the well known equation [11]

$$C_P - C_L = \frac{\alpha^2}{K_T T}, \tag{4.42}$$

where α is the coefficient of thermal expansion given in Equation (3.53) and K_T is the compressibility given in Equation (3.54).
Since $\left(\frac{\partial P}{\partial L}\right)_T$ vanishes, $\frac{1}{K_T}$ equals to zero. On the other hand, since P is a function of temperature only and because when we take derivative with respect to temperature, we have to keep P fixed, so, α is not defined.

Another thing which comes up is that for a single oscillator is

$$Z = \log(2\sinh(\frac{\omega}{2kT}))\left(\log(2\cosh(\frac{\omega}{2kT}))\right), \tag{4.43}$$

for BSHO (FSHO) where ω is the eigenfrequency of the Hamiltonian. For our case however, we have a collection of BSHO's (FSHO's) and the total result after summing over eigenmodes is that

$$Z = -\frac{L}{2a}\log(2\sinh(\frac{\omega_0}{2kT}))\left(\log(2\cosh(\frac{\omega_0}{2kT}))\right). \tag{4.44}$$

For bosonic and fermionic cases separately, we also have

$$\omega_0 = m\left(1 + \frac{\Delta^2}{m^2}\right)^{1/4}, \tag{4.45}$$

and if L is taken to be the number of oscillators, we have that ω_0 is something like the average of frequencies summed over with modes.

Apart from the discontinuity in E and P as T goes to zero for FSHO's and from the behavior of BSHO's such that $P < 0$ for $T < T_C$, all the physical quantities are well behaved functions of temperature and volume. Thus we can tentatively state that we will not observe a traditional phase transition. We have only made one approximation (i.e. $\Delta/m \ll 1$), otherwise our results are valid for all T and L. Universality demands that no phase transition is possible for $\Delta/m \simeq 1$ or $\Delta/m \gg 1$, if there is no phase transition for $\Delta/m \ll 1$, since the form of the Hamiltonian remains the same.

One amusing thing which comes up above is that with the standard relationship for the thermodynamical quantities, we have the formula

$$E - TS + PV = \mu N. \tag{4.46}$$

However, for our system, we are making calculations with phonons, the numbers of which are not conserved so N is not a parameter and μ is defined to be zero. In the two cases which we have studied above this relation is satisfied for the case $L/2a$ stands for the volume and P is thus defined.

5. BOSONIC SIMPLE HARMONIC OSCILLATORS IN N-DIMENSIONS

5.1. n-Dimensional Problem

The ultimate aim of the present section is to calculate the partition function for a system of n-dimensional bosonic simple harmonic oscillator (BSHO's) with a particular but different dispersion relationship where instead of the previous paper [13] with $\omega^2 = m^2 + \Delta^2 \sin^2(k\pi a/L)$, we have

$$\omega^2 = m^2 + \sum_{i=1}^{n} \Delta_i^2 \sin^2(k_i \pi a/L). \tag{5.1}$$

We have calculated the partition function of the one dimensional problem in the previous paper [13]. We will now calculate it explicitly for arbitrary n using the method of induction. The standard result for the partition function of a system of uncoupled BSHO's is given in terms of the summation of individual frequencies by

$$\log(Z) = \sum_k \log(Z_k), \tag{5.2}$$

$$Z_k = -\log(2\sinh(\beta\omega_k/2)), \tag{5.3}$$

$$Z_k = -\beta\omega_k/2 + \sum_j e^{-j\beta\omega}/j. \tag{5.4}$$

We have from [2, 7],

$$g_1(e^{-\beta\omega}) = \sum_n e^{-j\beta\omega}/j, \tag{5.5}$$

where $g_1(e^{-\beta\omega})$ is the Bose-Einstein function of order one and the argument $e^{-\beta\omega}$, such that

$$g_1(e^{-\beta\omega}) = -\log(\beta\omega) + \sum_{j=1}^{\infty} (-1)^j (\beta\omega)^j \zeta(1-j)/(j)!, \tag{5.6}$$

where $\zeta(z)$ is the Riemann zeta function. Since $\zeta(-2j) = 0$ only $\zeta(1-2j)$ and $\zeta(0) = -1/2$ terms remain.

For the complete partition function we have

$$\log(Z) = \sum_k \log(Z_k) = -\sum_k \left(\log(\beta\omega_k) - \sum_j \frac{1}{(2j)!} (\beta\omega_k)^{2j} \zeta(1-2j) \right), \tag{5.7}$$

where we define the first term of the last equality as K and the second term as I. Now, we go to the continuous case and convert the sum over discrete ω_k to the integral of the continuous case. First, we have enumerating the density of states as

$$u_i = \varDelta_i \sin(\pi k_i a/L), \tag{5.8}$$

$$dk_i = \frac{L}{\pi\, a} \frac{1}{\varDelta_i} \frac{1}{(1-(u_i^2/\varDelta_i^2))^{1/2}}\, du_i. \tag{5.9}$$

Since $\int \prod_i dk_i = Nn$, i.e. $(L/2a)^n = Nn$ where N is the total number of oscillators and n is the dimension of the system and writing $\omega_k^2 = m^2 + \sum_i \varDelta_i^2 \sin^2(k_i\pi a/L)$, by defining[1] the following

$$I_j = \left(\frac{L}{\pi a}\right)^j \int_0^1 \cdots \int_0^1 \prod_{i=1}^{j} \frac{du_i}{(1-u_i^2)^{1/2}} \left(\beta^2 \left(m^2 + \sum_{i=1}^{j} \varDelta_i^2 u_i^2 \right) \right)^j \tag{5.10}$$

such that

$$I = \sum_j \frac{1}{(2j)!} \zeta(1-2j) I_j.$$

Now we set $u_i^2 = z_i$ and we take the integral over z_j first. The result is by [9],

$$I_j = \left(\frac{L}{2\pi a}\right)^n \left(m^2 + \sum_{i=1}^{n-1} \varDelta_i^2 z_i \right)^j B(1/2, 1/2)\ {}_2F_1(-j, 1/2; 1, -1/\varGamma), \tag{5.11}$$

where

$$\varGamma = \left(\frac{m^2}{\varDelta_n^2} + \sum_{i=1}^{n-1} \frac{\varDelta_i^2}{\varDelta_n^2} \right). \tag{5.12}$$

Now, use [10] and express the hypergeometric function in terms of the Legendre polynomials. Thus we have

$${}_2F_1(-n, 1/2; 1, -\varGamma) = (1+\varGamma^{-1})^{n/2}\, P_{-n-1}\left(\frac{1+\varGamma^{-1}/2}{(1+\varGamma^{-1})^{1/2}} \right), \tag{5.13}$$

and

$$P_{-n-1}(z) = P_n(z), \tag{5.14}$$

where $\varGamma$ is defined by 5.12 and $\varDelta_i^2/m^2 \ll 1$.

[1] For the details of this calculation, consult [13]

In light of our approximation which is the only approximation we make in this section, and since we have $P_n(1) \simeq$ for the first integration, we get

$$\Gamma^{-1} = \frac{\Delta_n^2}{m^2}. \tag{5.15}$$

Thus we obtain the result that

$$I_j = \left(\frac{L}{2\pi a}\right)^n \int_0^1 ... \int_0^1 \prod_{i=1}^{n-1} \frac{du_i}{(1-z_i)^{1/2} z_i^{1/2}} \left(1 + \frac{\Delta_j^2}{m^2}\right)^{j/2} \left(\beta^2 \left(m^2 + \sum_{i=1}^{n-1} \Delta_i^2 z_i\right)\right)^j, \tag{5.16}$$

going through the same procedure as above we continue to take the integrals of u_i. Every time we take the integral over u_i a term of $(1 + \Delta_i^2/m^2)^{1/2}$ comes up. Finally a term of $(m^2 + \Delta_1^2 z_1)^n$ remains which brings up the term $m^{2n}(1 + \Delta_1^2/m^2)^{1/2}$. The final result is

$$I = \left(\frac{L}{2a}\right)^n \sum_{j=1}^{\infty} \left(\prod_{i=1}^{n} \left(1 + \Delta_i^2/m^2\right)^{j/2}\right) (m\beta)^{2j} \left(1/(2j)!\right) \zeta(1-2j). \tag{5.17}$$

Noting that $\zeta(-2n) = 0$ and $\zeta(0) = -1/2$, we use the identity from [**?**] that $\zeta(1-2n) = (2/(2\pi)^{2n})\Gamma(2n)\zeta(2n)\cos(n\pi)$ to get the final result that is

$$I(\beta\omega_0) = \left(\frac{L}{2a}\right)^n \sum_{j=1}^{\infty} \frac{2(-1)^j}{(2j)!} \left(\frac{(\beta\omega_0)}{2\pi}\right)^{2j} \Gamma(2j)\zeta(2j), \tag{5.18}$$

after defining

$$\omega_0 = m \prod_{i=1}^{n} (1 + \Delta_i^2/m^2)^{1/4}. \tag{5.19}$$

Now use the integral representation for the Riemann-Zeta function, along with the Gamma function, then we have

$$\zeta(2n) = \frac{1}{\Gamma(2n)} \int_0^\infty dt\, \frac{t^{2n-1}}{e^t - 1}. \tag{5.20}$$

As a result, we have

$$I = 2\left(\frac{L}{2a}\right)^n \sum_{j=1}^{\infty} \frac{(-1)^j}{(2j)!} \left(\frac{\beta\omega_0}{2\pi}\right)^{2j} \int_0^\infty dt\, \frac{t^{2j-1}}{e^t - 1}. \tag{5.21}$$

Setting $z = \beta\omega_0/2\pi$, differentiating with respect to z, taking the dummy index j to $j+1$, and using the series expansion for the sin function, we have

$$\frac{dI}{dz} = -2\left(\frac{L}{2a}\right)^n \int_0^\infty dt\, \frac{\sin(zt)}{e^t - 1}. \tag{5.22}$$

Now from [9], for the integral with $(L/2a)^n = Nn$,

$$-\frac{dI}{dz} = \left(\pi \coth(z\pi) - \frac{1}{z}\right)(Nn). \tag{5.23}$$

With $z = \beta\omega_0/2\pi$ and $I(0) = 0$ from the integral of Equation (5.23),

$$I = -Nn\left(\log(\sinh(\frac{\omega_0}{2kT})) - \log(\frac{\omega_0}{2kT})\right). \tag{5.24}$$

Having obtained an expression for I, now we calculate the K term of Equation (5.7). We have

$$K = \left(\frac{L}{\pi a}\right)^n \left(\int_0^1 ... \int_0^1 \prod_{i=1}^{n} \frac{du_i}{(1-u_i^2)^{1/2}} \log[\beta m\left(1 + \sum_{j=1}^{n} \frac{\Delta_j^2 u_j^2}{m^2}\right)^{1/2}]\right). \tag{5.25}$$

Since again, $\Delta_i^2/m^2 \ll 1$, we have

$$\log(1 + \sum_{j=1}^{n} \frac{\Delta_j^2 u_j^2}{m^2}) = \sum_{i=1}^{n} \log(1 + \frac{\Delta_i^2 u_i^2}{m^2}). \tag{5.26}$$

Taking the integrals, by [9], we have

$$\int_0^1 \frac{du_i}{(1-u_i^2)^{1/2}} \log(1 + \frac{\Delta_i^2 u_i^2}{m^2}) = \pi \log(\frac{1 + \left(1 + \frac{\Delta_i^2}{m^2}\right)^{1/2}}{2}). \tag{5.27}$$

Taking the multiple integral, we have

$$K = \left(\frac{L}{2a}\right)^n \left(\sum_{i=1}^{n} \log(\frac{1 + \left(1 + \frac{\Delta_i^2}{m^2}\right)^{1/2}}{2}) + \log(\beta m)\right). \tag{5.28}$$

5.2. Thermodynamics of n-dimensional BSHO's

We have from above, for the Helmholtz free energy (since we are working in the canonical ensemble),

$$A = -kT \log Z = nNkT \log(2\sinh(\omega_0/2kT)) \tag{5.29}$$

with A given, we can obtain the relevant thermodynamical quantities such as $E, S, c_v, c_p, P, \alpha$, i.e. energy, entropy, specific heat at constant volume and pressure, coefficient of thermal expansion, and pressure respectively given in [13]. We merely give the final results as follows

$$E = -\frac{\partial \log Z}{\partial \beta} = \frac{nN\omega_0}{2} \coth\left(\frac{\omega_0}{2kT}\right) = nN\omega_0\left(\frac{1}{2} + \frac{1}{e^{\omega_0/kT} - 1}\right) \tag{5.30}$$

$$S = -\left(\frac{\partial A}{\partial T}\right)_V = nNk\left(\frac{\omega_0}{2kT}\coth\left(\frac{\omega_0}{2kT}\right) - \log\left(2\sinh\left(\frac{\omega_0}{2kT}\right)\right)\right) \tag{5.31}$$

$$C_V = nNk\left(\frac{\omega_0}{2kT}\right)^2\left(\frac{\omega_0}{2kT}\right). \tag{5.32}$$

The asymptotic behavior of the thermodynamical quantities as $\omega/kT \to \infty$, $(T \to 0)$ are given by, for the energy

$$E = \frac{nN\omega_0}{2}, \tag{5.33}$$

and for the entropy of the system which means that the third law of thermodynamics is obeyed,

$$S \to 0, \tag{5.34}$$

and

$$C_V = nN\left(\frac{\omega_0}{2kT}\right)^2 e^{-\omega_0/kT}, \tag{5.35}$$

which gives a Schottky type anomaly, and as $\omega_0/kT \to 0$, $T \to \infty$;

$$\begin{aligned} E &= nNkT, \\ S &= nNk\left(1 + \log(kT/\omega_0)\right), \\ C_V &= nNk. \end{aligned} \tag{5.36}$$

We see that energy and specific heat obey the law of equipartition of energy. Now regarding the pressure of the system, we state that contrary to what is sometimes erroneously assumed, since the factor $L/2a$ appears in the expression for the Helmholtz free energy and $L/2a = N$, the number of oscillators, pressure depends on volume only through the volume dependence of the effective frequency of vibration, $\omega_0 = m\prod_{i=1}^{n}\left(1 + \mathit{\Delta}_i^2/m^2\right)^{1/4}$. For the pressure now, we go to [1] and write it as follows for our system

$$P = -\frac{\partial U_{\text{eq}}}{\partial V} - kT\frac{\partial \log Q}{\partial V}, \tag{5.37}$$

with $-kT\log Q = A$ where $\log Q$ is calculated above and A is the Helmholtz free energy where

$$A = nNkT\log(2\sinh(\omega_0/2kT)). \tag{5.38}$$

Here U_{eq} is the cohesive energy of the solid, i.e. it is related to potential energy at the equilibrium position of the atoms of the solid. Now for exact harmonic oscillators eigenfrequencies are independent of volume. Therefore taking the derivative with respect to volume of terms on the right hand side we have,

$$P = -\left(\frac{\partial \omega}{\partial V}\right)\frac{nNk}{2}\coth(\frac{\omega_0}{2kT}) - \frac{\partial U_{\text{eq}}}{\partial V}, \tag{5.39}$$

that is

$$P = -\frac{\partial \log(\omega_0)}{\partial \log(V)} \frac{U_{\text{osc}}}{V} - \frac{\partial U_{\text{eq}}}{\partial V}, \tag{5.40}$$

where U_{osc} is the energy of the oscillations of the atoms in the solid.
On the other hand, a rigorously harmonic oscillator $\partial \omega_0 / \partial V$ equals to zero, therefore for the pressure we have

$$P = -\frac{\partial U}{\partial V}, \tag{5.41}$$

i.e. pressure is a function only of volume when the crystal is rigorously harmonic. Now we have the identity below such that

$$\left(\frac{\partial V}{\partial T} \right)_P = -\frac{(\partial P / \partial T)_V}{(\partial P / \partial V)_T}. \tag{5.42}$$

Since $(\partial P / \partial T)_V = 0$ from above and $(\partial P / \partial V)_T$ is non-zero (and of large magnitude) the coefficient of the thermal expansion where $\alpha = \frac{1}{V} \left(\frac{\partial V}{\partial T} \right)_P$ equals to zero for a rigorously harmonic oscillator. Now for the specific heat at constant pressure we have the relation

$$C_P - C_V = \frac{T V \alpha^2}{K_T}, \tag{5.43}$$

where $K_T = -V(\partial P / \partial V)$ is the bulk modulus, and α is the coefficient of thermal expansion as above. Thus for rigorously harmonic oscillator specific heat at constant volume equals to that in constant pressure. If the crystal is not rigorously harmonic one can refer to the expressions above to calculate the α (keeping P constant) and then C_P and pressure. We see that energy and specific heat obey the law of equipartition of energy.

Passing to the realm of anharmonic physics we have from [1], $\alpha = \frac{1}{3B} \left(\frac{\partial P}{\partial T} \right)_V$, where B is the bulk modulus with

$$B = -V \left(\frac{\partial P}{\partial V} \right)_T. \tag{5.44}$$

Therefore from above, using $(\partial P / \partial T)_V$ that we have calculated above

$$\alpha = -\frac{1}{3B} \left(\frac{\partial \log \omega_0}{\partial \log V} \right) \left(\frac{\partial U_{\text{osc}}}{\partial T} \right)_V \frac{1}{V}, \tag{5.45}$$

where U_{osc} is the energy due to the oscillations of the crystal with

$$C_V = \left(\frac{\partial U_{\text{osc}}}{\partial T}\right)_V, \tag{5.46}$$

thus,

$$\alpha = -\frac{1}{3B}\left(\frac{\partial \log \omega_0}{\partial \log V}\right)\frac{C_V}{V}. \tag{5.47}$$

Thus with the introduction of a parameter $\gamma = -\left(\partial \log \omega_0 / \partial \log V\right)$, we have

$$\alpha = \frac{1}{3B}\gamma\frac{C_V}{V} \tag{5.48}$$

where γ is the Grüneisen parameter, which equals to $\gamma = -\left(\partial \log \omega_0 / \partial \log V\right)$ in our special case. We note in passing that in the general case γ is given by

$$\gamma = \frac{\sum_{k,s} \gamma_{ks} C_{Vs}(\vec{k})}{\sum_{k,s} C_{Vs}(\vec{k})}, \tag{5.49}$$

where $\gamma_{ks} = -(\partial \log \omega_s \vec{k} / \partial \log V)$, and C_{Vs} given by is the contribution of the normal mode given by $\vec{k}, s$ to the total specific heat. Thus, it depends on the detail of the dispersion relationship as well as on the temperature.

The bulk modulus given above depends only weakly on temperature. Thus our theory (as well as our particular model) with constant γ_{ks} predicts that the coefficient of thermal expansion should have the same temperature dependence as the specific heat. Thus, it should approach a constant value as temperature is increased to infinity, and approach zero as T goes to zero.

6. FERMIONIC SIMPLE HARMONIC OSCILLATORS IN N-DIMENSION

6.1. n-Dimensional Problem

In this section, we will consider the case of a system of FSHO's as in the previous case for n-dimensions, n being arbitrary.

In analogy with the previous calculations, we will make the passage from the discrete case to the continuous case. Now, our dispersion relation reads from the Equation (5.1) with $1 \leq k \leq L/a$ and for a single FSHO, we have from [12] the expression for the partition function for a single oscillator as

$$Z_k = \log(2\cosh(\frac{\beta\omega_k}{2})) \tag{6.1}$$

where $\beta = 1/kT$ and ω_k are the relevant frequencies of vibration. For a system of uncoupled FSHO's, after expressing the Hamiltonian in terms of the normal modes of oscillation, we have $\log(Z) = \sum_k \log(Z_k)$.

We now formulate our problem again starting from the Equation (5.1) where m, Δ are the parameters of dispersion relationship, a is the lattice spacing, L is the length (volume) of the lattice and k_i is an integer analogous to the wave vector and n is the dimension of the lattice. We see for $g(\omega)$, the density of states, after making the variable transformation is

$$u_i = \Delta_i \sin(\frac{k_i \pi a}{L}) \tag{6.2}$$

then, we have

$$g(\omega) = \prod_1^n \Delta k_i = \prod_i^n \frac{L}{\pi a} \frac{du_i/\Delta_i}{(1 - u_i^2/\Delta_i^2)^{1/2}}. \tag{6.3}$$

Therefore, from $\log(Z) = \sum_k \log(Z_k)$, we have

$$\log(Z_k) = \left(\frac{L}{\pi a}\right)^n \int_0^1 ... \int_0^1 \prod_{i=1}^n \frac{du_i/\Delta_i}{(1 - z_i/\Delta_i^2)^{1/2}} \log(2\cosh(\beta\omega_k/2)), \tag{6.4}$$

where ω_k is given in the Equation (5.1). Also, we have

$$\log(2\cosh(\beta\omega_k/2)) = \frac{\beta\omega}{2} + \sum_{j=1}^{\infty}(-1)^{j+1}\frac{e^{-j\beta\omega}}{j} = \frac{\beta\omega}{2} + f_1(e^{-\beta\omega}), \tag{6.5}$$

where f_1 is the Fermi-Dirac function of degree 1 and argument $e^{-\beta\omega}$ [7]. We also use the result

$$f_1(e^{-\beta\omega}) = g_1(e^{-\beta\omega}) - g_1(e^{-2\beta\omega}). \tag{6.6}$$

For $g_1(e^{-\beta\omega})$ and $g_1(e^{-2\beta\omega})$, we see that

$$g_1(e^{-\beta\omega}) = -\log(\beta\omega) + \sum_{i=1}^{\infty}\frac{\zeta(1-2i)}{(2i)!}(\beta\omega)^{2i} + \frac{\beta\omega}{2}, \tag{6.7}$$

and

$$g_1(e^{-2\beta\omega}) = -\log(2\beta\omega) + \sum_{i=1}^{\infty}\frac{\zeta(1-2i)}{(2i)!}(2\beta\omega)^{2i} + \beta\omega. \tag{6.8}$$

We have the result as

$$f_1(e{-}\beta\omega) + \frac{\beta\omega}{2} = \log(2) + \sum_{i=1}^{\infty}\frac{\zeta(1-2i)}{(2i)!}(\beta\omega)^{2i}(1-2^{2i}). \tag{6.9}$$

For the first term on the right (we define as K), integrating over u_i [9] gives

$$K = Nn\log(2). \tag{6.10}$$

For I we have,

$$I = \int_0^1 \dots \int_0^1 \prod_{j=1}^{n}\frac{du_j}{(1-u_j^2)1/2} Nn \sum_{i=1}^{\infty}\left(\frac{2}{\pi}\right)^n \frac{(\beta\omega)^{2i}}{(2i)!}\zeta(1-2i)(1-2^{2i}). \tag{6.11}$$

The term above is exactly of the same form as the Equation 5.17 in Section 3. In fact it is the difference of two such integrals different from each other in the exchange of the factor $2\beta\omega$ for $\beta\omega$. Thus, we can write the result as

$$-\log Z = nN\left(\log(2\sinh(\beta\omega_0/2)) - \log(\beta\omega)\right) - nN\left(\log(2\sinh(\beta\omega_0)) - \log(2\beta\omega)\right). \tag{6.12}$$

Adding I and K as above, we have

$$\log Z = nN\log(2\cosh(\beta\omega_0/2)), \tag{6.13}$$

with $\omega_0 = m\prod_{i=1}^{n}(1+\Delta_i^2/m^2)^{1/4}$ and N being the total number of oscillators and n is the number of dimensions.

6.2. Thermodynamical Quantities for the FSHO's

We consider in this subsection the thermodynamical quantities S, E, A, C_V, entropy, energy, Helmholtz free energy, specific heat at constant volume respectively, for the system of FSHOs we investigate in this section. A behavior we notice is that the energy of our particular system in question is bounded from above and below. The behavior for the limit below is a standard behavior for quantum systems. The fact that it is bounded from above, brings about the possibility of the attainment of negative temperatures for the system in question. The reason for this lies in the behavior of the Boltzmann factor. Since the energy is bounded from above our Boltzmann factor is limited in magnitude, i.e. it cannot blow up as E goes to infinity for $T < 0$. Now we also make the assumption that our system is in thermodynamical equilibrium in itself and also the system in question must be thermally isolated from the systems not satisfying the above properties.

We note that for the first condition there must be a residual interaction within the particles of the system such that transition among the eigenstates of the main (zeroth order) Hamiltonian is possible. The second condition is self-explanatory. We also note that the partition function and the relevant thermodynamical quantities thereof for our system are identical to those of the paramagnetic system consisting of magnetic dipoles in an external magnetic field. We only exchange the variables (ω_0) and (μB_0) where μ is the magnetic dipole and B_0 is the external magnetic field, and then the behavior of our system of FSHOs is identical to the paramagnetic system in a constant magnetic field. For a more comprehensive treatment of the behavior of systems with negative temperatures one can consult [7] and [14]. Now we only note that the behavior of the system with a negative temperature can be obtained by inserting $-T$ wherever $+T$ appears for any particular value of T.

Now, we go on to explicitly calculate the thermodynamical quantities we have from standard thermodynamical quantities

$$\log(Z) = nN \log\left(2\cosh\left(\frac{\omega_0}{2kT}\right)\right) \tag{6.14}$$

$$A = -kT\log(Z), \tag{6.15}$$

$$S = -\left(\frac{\partial A}{\partial T}\right)_V = nNk\left(\log\left(2\cosh\left(\frac{\omega_0}{2kT}\right)\right) - \frac{\omega_0}{2kT}\tanh\left(\frac{\omega_0}{2kT}\right)\right), \tag{6.16}$$

$$E = -\frac{\partial\log(Z)}{\partial\beta} = -\frac{nN}{2}\omega_0\tanh\left(\frac{\omega_0}{2kT}\right), \tag{6.17}$$

$$C_V = \left(\frac{\partial E}{\partial T}\right)_V = nNk\left(\frac{\omega_0}{2kT}\right)^2\left(\frac{\omega_0}{2kT}\right). \tag{6.18}$$

Now consider the asymptotic behavior as $T \to 0$ and as $T \to \infty$. First consider $\omega_0/2kT \to 0$, $(T \to \infty)$,

$$\begin{aligned} E &= -nN\left(\frac{\omega_0}{2kT}\right)\frac{\omega_0}{2}, \\ C_V &= nN\left(\frac{\omega_0}{2kT}\right)^2, \\ S &= nNk\left(\log(2) - \left(\frac{\omega_0}{2kT}\right)^2\right). \end{aligned} \tag{6.19}$$

Now let $\omega_0/2kT \to \infty$, $(T \to 0)$,

$$E = \frac{nN}{2}\left(T\omega_0\right) \tag{6.20}$$

$$C_V = nN\left(\frac{\omega_0}{2kT}\right)^2 e^{-\omega_0/kT} \tag{6.21}$$

$$S = 0 \tag{6.22}$$

The above relationships are valid for T greater than or less than zero. We note that the behavior of our FSHO's is reduced to the behavior of N-particle FSHO with a single frequency of vibration. We also see that the equipartition principle for the specific heat and the energy is not obeyed. Thus, as T increases with $kT/\omega_0 >> 1$, both E and C_V decreases to zero. In the relationship for S, we see that a factor of $\log(2)$ appears for $T \to \pm\infty$. The reason for which is that the degeneracy of each mode is 2. For $T \to 0$ we have the ground state energy with a sign $+(-)$ for $+T(-T)$. Again we observe a Schottky type of anomaly in the specific heat. Finally we see that $S \to 0$ as $T \to 0$.

6.3. Summary and Conclusion for SHO's in n-dimensions

In this final section, we present the reader a brief summary of the results obtained for our particular cases of BSHO's and FSHO's upon considering the generalization of the previous paper [13] to n-dimensions. First we consider BSHO's. After going through the calculations, we obtain a description of our system such that the behavior of our system is identical to that of a system so that there is a single frequency of vibration ω_0 with n-atoms. Here $\omega_0 = m \prod_{k=1}^{n} (1 + \Delta_k^2/m^2)^{1/4}$. This is exactly equal in form to the result obtained in the previous paper [13]. We also observe that this is exactly the same as that of the Einstein solid. Thus, we have justification for the Einstein solid such that the collection of the optical harmonic oscillators as above can behave as a system of oscillators with a single frequency of vibration.

We also find that the equipartition of energy holds for E and C_V that are energy and specific heat respectively. The ground state energy is given by, $E_0 = (1/2)Nn\omega_0$, which is the ground state energy of N-oscillators in n-dimensions with a single frequency of vibration ω_0. As T goes to zero, we have $C_V = nN(\omega_0/2kT)^2 e^{-\omega_0/kT}$, i.e. we observe a Schottky type anomaly in the specific heat the latter dropping to zero as T goes to zero. Also for temperatures small in magnitude the contribution of the optical mode to the specific heat goes to zero exponentially, so that we will not observe an appreciable contribution to the total specific heat. Finally we have that the entropy goes to zero as T goes to zero, i.e. the third law of thermodynamics is conserved.

In this thesis, for BSHO's, we have also calculated the pressure as a function of volume and temperature. We have shown that pressure is a function of volume only for a rigorously harmonic oscillator and have calculated pressure as functions of volume and temperature otherwise. We have also obtained an expression for the coefficient of thermal expansion in terms of the bulk modulus, a specific heat at constant volume and a parameter called the Grüneisen parameter. Following the treatment given in the reference [1]. This is so whenever we have only optical modes and when we consider only our particular dispersion relationship.

Now we consider the case of FSHO's. Again we have that the system is described by a single frequency of vibration with N-oscillators. As T goes to zero and T goes to infinity, specific heat goes to zero. We thus see that equipartition of energy and specific heat are not obeyed as $\omega_0/2kT$ goes to zero. For small T on the other hand we observe a Schottky type of anomaly in the specific heat. The ground state energy as $1/T \to \pm\infty$ goes as $\pm nN\omega_0/2$ as expected.

The most novel feature of our system of FSHO's is the attainment of negative temperature. Now the essential requirements for a system to be able to attain negative temperatures are as follows [14]:

(i) The system must be able to reach thermodynamical equilibrium when left to itself, so that it can be described by a temperature.

(ii) There must be an upper limit to the energy of the system so that upon taking the sum over energy eigenstates in the partition function the Boltzmann factor does not diverge.

(iii) The system must be thermally isolated from all other systems which do not satisfy the above requirements.

For our system we assume that requirements 1 and 3 are satisfied. Requirement 2 is shown to be true. Thus our system can attain negative temperatures whenever the relationship $(\partial S/\partial E)_V = 1/T < 0$. For such cases the system is said to attain negative temperatures.

7. CALCULATION OF THE PARTITION FUNCTION FOR 1-D ACOUSTICAL PHONONS

In this section, we are going to investigate the case of acoustical phonons, in direct analogy to the case of optical modes.

7.1. A Method of Calculation of the Partition Function for 1-d BSHO's

We are going to present the reader with several different methods for calculating the partition function and the thermodynamical quantities. In some of these methods, we are going to reach the same results in others, we use a different approach. We have as our dispersion relationship,

$$\omega = \mathit{\Delta} \sin(ka/2), \tag{7.1}$$

where $\mathit{\Delta}$ is our interacting parameter, which is related to the spring constant of the Simple Harmonic Oscillator (SHO), a is the lattice spacing, and k is the wavevector. We have for the partition function,

$$-\log Q = -\sum_k \log[Q_k] = \sum_{k=1}^{\infty} \log 2 \sinh \frac{\omega_k}{2kT}, \tag{7.2}$$

where Q_k is the partition function of a single (decoupled) eigenmode, ω_k being the eigenfrequency corresponding to this particular mode, and the summation is over all modes.

Again, we have, as in the optical modes,

$$-\log Q = \sum_k \frac{\beta\omega_k}{2} - \sum_k \sum_{n=1}^{\infty} \frac{e^{-n\beta\omega_k}}{n}, \tag{7.3}$$

with $g_1(\beta\omega) = \sum_n \frac{e^{-n-\beta\omega}}{n}$, being equal to the Bose-Einstein function of order 1, which is closely related to the Riemann-Zeta function $\zeta(n) = \sum_{k=1}^{\infty} \frac{1}{k^n}$. We have [2], [7],

$$g_1(\beta\omega) = -\log \beta\omega + \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \zeta(1-n)(\beta\omega)^n \tag{7.4}$$

which is valid for $\beta\omega < 1$.

Using the relation $\zeta(-2n) = 0$, where n is a positive integer, $\zeta(0) = \frac{-1}{2}$, and the relation below due to Riemann,

$$\zeta(1-2n) = \frac{2}{(2\pi)^{2n}}\zeta(2n)\Gamma(2n)(-1)^n. \tag{7.5}$$

We finally have,

$$-\log Q_k = \log\beta\omega_k - 2\sum_{n=1}^{\infty}(-1)^n(\frac{\beta\omega_k}{2\pi})^{2n}\frac{\Gamma(2n)}{(2n)!}\zeta(2n). \tag{7.6}$$

Now, we pass to the continuum case and using the enumeration of states for our dispersion relationship, we get

$$dn = \frac{L}{\pi a}\frac{d\omega}{\Delta(1-\frac{\omega^2}{\Delta^2})} = \frac{2N}{\pi}\frac{d\omega}{\Delta(1-\frac{\omega^2}{D^2})^{\frac{1}{2}}}, \tag{7.7}$$

where we used the relation above, and employed periodic boundary conditions, i.e. $kL = 2n\pi$ $(1 < n < N)$ where N is the number of particles, and where dn is the the number of eigenstates in the frequency interval $d\omega$ at the frequency ω, and finally summing and integrating over eigenfrequencies, and a summation index, where we equated the number of modes to the number of particles

$$-\log Q = -\sum_k \log Q_k \tag{7.8}$$

$$= (2N/\pi)\int_0 \frac{\frac{d\omega}{\Delta}}{(1-\frac{\omega^2}{D^2})^{\frac{1}{2}}}\log(\beta\omega) \tag{7.9}$$

$$-2(2N/\pi)\sum_{n=1}^{\infty}(\frac{\beta\Delta}{2\pi})^{2n}\frac{(-1)^n}{(2n)!}\Gamma(2n)\zeta(2n)\int\frac{\frac{d\omega}{\Delta}}{(1-\frac{\omega^2}{\Delta^2})^{\frac{1}{2}}}(\frac{\omega}{\Delta})^{2m}, \tag{7.10}$$

where I(κ) stands for the first (second) term on the right. Now, for I, we have

$$I = N\log(\frac{\beta\Delta}{2}). \tag{7.11}$$

For κ, we set $\omega^2 = u$, and using Beta functions.

$$K = -2N\sum_{n=1}^{\infty}(\frac{\beta\Delta}{2\pi})^{2n}\frac{\Gamma(2n)\zeta(2n)}{(n!)^2}(-1)^n. \tag{7.12}$$

We remark again that, for the validity of this result, we need to have $\frac{\beta\Delta}{2\pi} < 1$. Now, we use a standard integral relationship for the product of the Riemann-Zeta function and the Gamma function

$$\zeta(2n)\Gamma(2n) = \int_0^{\infty} dt\frac{t^{2n-1}}{e^{t-1}}. \tag{7.13}$$

We insert this relationship into the expression above and write the result in terms of the Bessel function of order zero, the series expansion of which is given below

$$J_0(t) = \sum_{k=0}^{\infty}(-1)^k \frac{(\frac{t}{2})^{2k}}{(k!)^2}. \tag{7.14}$$

As a result, we have

$$K = -2N \int_0^{\infty} \frac{dt}{e^t - 1} \frac{1}{t}(J_0(\frac{t\beta\Delta}{2\pi}) - 1), \tag{7.15}$$

where we first summed and then integrated. Next, we use another integral representation, this time for the Bessel function i.e.

$$J_0(t) - 1 = \frac{2}{\pi} \int_0^1 dz \frac{\cos tz - 1}{(1 - z^2)^{\frac{1}{2}}}. \tag{7.16}$$

Thus, finally we have for k

$$K = -\frac{4N}{\pi} \int_0^1 \frac{dz}{(1 - z^2)^{\frac{1}{2}}} \int_0^{\infty} \frac{dt}{t(e^t - 1)}(\cos(\frac{t\beta\Delta z}{2\pi}) - 1)). \tag{7.17}$$

Integrals are convergent, their orders can be interchanged.

Now, we expand $\frac{1}{e^t-1}$ into a geometric series in $\frac{1}{e^t-1} = \sum_{s=1}^{\infty} e^{-st}$, and differentiate with respect to s, upon which we get

$$\frac{\partial K}{\partial s} = \frac{4N}{\pi} \int_0^1 \frac{dz}{(1 - z^2)^{\frac{1}{2}}} \int_0^{\infty} dt(\sum_s e^{-st})(\cos \frac{t\beta\Delta z}{2\pi} - 1) \tag{7.18}$$

carrying out the integral with respect to t, and then integrating with respect to s, we obtain

$$K = \frac{2N}{\pi} \sum_{s=1}^{\infty} \int_0^1 \frac{dz}{(1 - z^2)^{\frac{1}{2}}} \log(1 + (\frac{\beta\Delta z}{2\pi s})^2). \tag{7.19}$$

Interchanging the orders of summation and integration,

$$K = \frac{2N}{\pi} \int_0^1 \frac{dz}{(1 - z^2)^{\frac{1}{2}}} \log \prod_{s=1}^{\infty}(1 + (\frac{\beta\Delta z}{2\pi s})^2), \tag{7.20}$$

from the well known identity, we have

$$\frac{\sinh \frac{\beta\Delta z}{2}}{\frac{\beta\Delta z}{2}} = \prod_{s=1}^{\infty}(1 + (\frac{\beta\Delta z}{2\pi s})^2), \tag{7.21}$$

$$K = -N \log \frac{\beta\Delta}{4} + 2N\frac{\beta\Delta}{2\pi} - \frac{2N}{\pi} \sum_{n=1}^{\infty} \int \frac{dz}{(1 - z^2)^{\frac{1}{2}}} \frac{e^{-n\beta\Delta z}}{n}, \tag{7.22}$$

and from [9], (page 322), we have

$$\int_0^1 \frac{dz}{(1 - z^2)^{\frac{1}{2}}} e^{-n\beta\Delta z} = \frac{\pi}{2}[L_0(n\beta\Delta) - I_0(n\beta\Delta)], \tag{7.23}$$

where $I_0(z)$ is the modified Bessel function of order zero, and $L_0(z)$ is the modified

Struve function of order zero with

$$I_0(z) = \sum_{n=0}^{\infty} \frac{(z/2)^{2n}}{(n!)^2}, \tag{7.24}$$

$$L_0(z) = \sum_{n=0}^{\infty} \frac{(z/2)^{2n+1}}{(\Gamma(n+\frac{3}{2}))^2}. \tag{7.25}$$

After adding I from above, we have

$$-\log Q = 2N\frac{\Delta\beta}{2\pi} + N\sum_{n=1}^{\infty}\frac{1}{n}[L_0(n\beta\Delta) - I_0(n\beta\Delta)]. \tag{7.26}$$

7.2. A Simpler Method for the Same Problem

Now, we are going to present the reader with another, much simpler method of reaching the same result. We have

$$-\log Q = \frac{\beta}{2}\frac{2N}{\pi}\int_0^{\Delta}\frac{\omega\frac{d\omega}{\Delta}}{(1-\frac{\omega^2}{\Delta^2})^{\frac{1}{2}}} - \frac{2N}{\pi}\sum_n\int\frac{\frac{d\omega}{\Delta}}{(1-\frac{\omega^2}{\Delta^2})^{\frac{1}{2}}}\frac{e^{-n\beta\omega}}{n}. \tag{7.27}$$

We see that we need not have $\frac{\beta\Delta}{2\pi} < 1$, for this result to be valid. Therefore with [9], we have that, for all z,

$$-\log Q = 2N\frac{\beta\Delta}{2\pi} + N\sum_{n=1}^{\infty}\frac{1}{n}[L_0(n\beta\Delta) - I_0(n\beta\Delta)]. \tag{7.28}$$

7.3. A Still Different Method

Now, we are going use another, more involved way of reaching the same result. We have, from above

$$K = \frac{2N}{\pi}\sum_{s=1}^{\infty}\int\frac{dz}{(1-z^2)^{\frac{1}{2}}}\log[1+(\frac{\beta\Delta z}{2\pi s})^2]. \tag{7.29}$$

Carrying out the integrals, after interchanging the orders of summation and integration, we get

$$K = \frac{2N}{\pi}\sum_{k=1}^{\infty}\frac{\log(1+(1+\frac{z^2}{k^2})^{\frac{1}{2}})}{2}. \tag{7.30}$$

To evaluate this sum, we use a summation formula due to Euler [5]. According to this formula, we have

$$\sum_{k=1}^{n} f(k) = \int_1^n dx f(x) + \frac{1}{2}f(1) + \frac{1}{2}f(n) + \int_1^n dx P(x) f(x). \tag{7.31}$$

For our case, n goes to infinity. For the theorem to be valid, $f(x)$ should be a monotonically decreasing positive function of x. Also, we have $P(x) = x - [x] - \frac{1}{2}$, where x is the largest integer less than or equal to x.

Thus, we have, expanding $P(x)$ in a Fourier series, such that we get

$$P(x) = x - \frac{3}{2} \tag{7.32}$$

for $1 < x < 2$. For our series, we have

$$P(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} [a_n \cos(2\pi n x) + b_n \sin(2\pi n x)]. \tag{7.33}$$

We immediately obtain $a_0 = a_n = 0$, $b_n = -\frac{1}{n}$. Also, we have

$$f'(x) = -\frac{\frac{z^2}{x}}{x + (x^2 + z^2)^{\frac{1}{2}}} \frac{1}{(x^2 + z^2)^{\frac{1}{2}}}. \tag{7.34}$$

Thus, we have for the integral above

$$R = \frac{2N}{\pi} \int_1^{\infty} \frac{dx}{(x^2 + z^2)^{\frac{1}{2}}} \frac{\frac{z^2}{x}}{(x^2 + z^2)^{\frac{1}{2}}} \sum_n \frac{\sin(2n\pi x)}{n}. \tag{7.35}$$

Since the sum and integral converge separately, we can exchange the orders of summation and integration.

Now, we obtain for the integral R

$$R = \frac{2N}{\pi} \sum_n \frac{1}{n} \int_0^{\infty} \frac{dx}{(x^2 + z^2)^{\frac{1}{2}}} \frac{\frac{z^2}{x}}{x + (x^2 + z^2)^{1/2}} \sin(2\pi n x) - \int_0^1 (\text{same integrand})], \tag{7.36}$$

where the first (second) term on the right is labeled as S(T). Now, set $\omega = 2\pi n$, we differentiate S with respect to ω, which is problematic since the Fourier series in question is discontinuous at discrete values of x.

Now, we get from [9],

$$\frac{\partial S}{\partial \omega} = \int_0^{\infty} \frac{dx}{x + (x^2 + z^2)^{\frac{1}{2}}} \frac{\cos \omega x}{(x^2 + z^2)^{\frac{1}{2}}} z^2 \frac{2N}{\pi}, \tag{7.37}$$

$$= \pi z \frac{2N}{\pi} \lim_{\nu \to 1} \frac{1}{\sin \nu\pi} [\frac{1}{2}\tilde{J}_{s_1}(i\omega z) + \frac{1}{2}\tilde{J}_{s_1}(-i\omega z)] - \cos\frac{\nu\pi}{2} I_{s_2}(\omega z), \tag{7.38}$$

where we eventually will take the limit $\nu \to 0$. Here, $\tilde{J}_1(z)$ is the Anger function of order one, and $I_1(z)$ is the modified Bessel function of order one, from grad.Rhyz we have

$$\tilde{J}_1(i\omega z) = \cos\frac{\nu\pi}{2}\sum_{n=0}^{\infty}\frac{(\frac{\omega z}{2})^{2n}}{\Gamma(n+\frac{3}{2})\Gamma(n+\frac{1}{2})} + i\sin\frac{\nu\pi}{2}\sum_{n=0}^{\infty}\frac{(\frac{\omega z}{2})^{2n+1}}{\Gamma(n+2)^{\Gamma(n+1)}}. \tag{7.39}$$

Thus

$$\frac{1}{2}[\tilde{J}(i\omega z) + \tilde{J}(-i\omega z)] = \cos\frac{\nu\pi}{2}\sum_{n=0}^{\infty}\frac{(\frac{\omega z}{2})^{2n}}{\Gamma(n+\frac{1}{2})\Gamma(n+\frac{3}{2})}. \tag{7.40}$$

Dividing by $\sin v\pi$, taking the limit v goes to zero (using L'hospital's) rule, after taking the integral with respect to ω, we obtain the following

$$S_1 = 2N\sum_{n=0}^{\infty}\frac{(N\frac{z}{2})^{2n}}{\Gamma(n+\frac{3}{2})\Gamma(n+\frac{1}{2})}. \tag{7.41}$$

Thus, we have for S

$$S = N\sum_{n=1}^{\infty}\frac{1}{n}L_0(n\beta\Delta), \tag{7.42}$$

where $L_0(z)$ is the modified struve function of order zero. Now calculate S_2. We have

$$\frac{\partial S_2}{\partial\omega} = -z\sum_{n=1}^{\infty}\frac{I_1(\omega z)}{n}, \tag{7.43}$$

$$S_2 = -N\sum_{n=1}^{\infty}\frac{I_0(n\beta\Delta)}{n}, \tag{7.44}$$

and finally,

$$S_k = N\sum_{n=1}^{\infty}\frac{1}{n}[L_0(n\beta\Delta) - I_0(n\beta\Delta)]. \tag{7.45}$$

Now, we go on to calculate T, where

$$T = -\frac{2N}{\pi}\sum_{n=1}^{\infty}\frac{1}{n}\int_0^1 dz\frac{\sin\pi nx}{x+(x^2+z^2)^{\frac{1}{2}}}\frac{z^2}{(x^2+z^2)^{\frac{1}{2}}}, \tag{7.46}$$

which is convergent. Integrating by parts gives

$$T = \frac{2N}{\pi}\sum_{n=1}^{\infty}\frac{1}{n}\log\frac{1+(1+\frac{z^2}{x^2})^{1/2}}{2}\sin(2\pi nx)|_{x=0}^{x=1} \tag{7.47}$$

$$-4N\sum_{n=1}^{\infty}\int dx\cos(2\pi nx)\log\frac{1+(1+\frac{z^2}{x^2})^{1/2}}{2}. \tag{7.48}$$

The first term vanishes upon using L'Hopital's rule, for the second term we have, by using the relationship

$$1 + 2\sum_{n=1}^{\infty} \cos 2\pi n x = \sum_{n=-\infty}^{+\infty} \zeta(x-n), \tag{7.49}$$

and noting only the $x = 0$, and $x = 1$ contribute with a factor of $\frac{1}{2}$, we have

$$T = -N \log \frac{1 + (1+z^2)^{\frac{1}{2}}}{2} - N \log \frac{z}{2x} + 2N \int_0^1 dx \log \frac{1 + (1+\frac{z^2}{x^2})^{\frac{1}{2}}}{2}. \tag{7.50}$$

Now inserting the x results into the Euler's formula

$$2N \sum_{k=1}^{\infty} \frac{\log(1 + (1+\frac{z^2}{x^2})^{\frac{1}{2}})}{2} = N \log \frac{1 + (1+z^2)^{\frac{1}{2}}}{2} - N \log \frac{1 + (1+z^2)^{\frac{1}{2}}}{2} \tag{7.51}$$

$$- N \lim_{x\to\infty} \log \frac{z}{2x} + 2N \int_0^{\infty} dx \log \frac{1 + (1+\frac{z^2}{x^2})^{\frac{1}{2}}}{2} \tag{7.52}$$

$$+ \sum_{n=1}^{\infty} \frac{1}{n}[L(n\beta\varDelta) - I_0(n\beta\varDelta)]. \tag{7.53}$$

Adding the term $N \log(\frac{\beta\varDelta}{2})$ to this expression, we have

$$-\log Q = 2N \int_0^{\infty} dx \log \frac{1 + (1+\frac{z^2}{x^2})^{\frac{1}{2}}}{2} + \lim_{x\to 0} \log(2\pi x) + N \sum_{n=1}^{\infty} \frac{1}{n}[L(n\beta\varDelta) - I_0(n\beta\varDelta)]. \tag{7.54}$$

Now take the integral over x after disregarding the $\log(2\pi x)$ term, we finally have

$$-\log \psi = 2N \frac{\varDelta\beta}{2\pi} + N \sum_{n=1}^{\infty} \frac{1}{n}[L_0(n\beta\varDelta) - I_0(n\beta\varDelta)]. \tag{7.55}$$

7.4. Thermodynamical Properties for 1-Dimensional Acoustical Phonons Using Melling Tranforms

7.4.1. Mellin Transforms and Thermodynamics

In this section, in contrast to the case for the optical mode in the two previous papers before [13] and [15], we have for our dispersion relationship

$$\omega = \varDelta \sin \frac{ka}{2}, \tag{7.56}$$

for the relevant partition function, we have

$$-\log Q = -\sum_k \log Q_k = \sum_{k=1}^{\infty} \log(2 \sinh \frac{\omega}{2kT}), \tag{7.57}$$

where Q_k stands for the partition function for a single eigen mode (decoupled from the rest of the oscillators) with ω_k being the eigen frequencies corresponding to this particular mode and the summation is made over all modes. We have as in the optical modes

$$-\log Q = \sum_k \frac{\beta\omega_k}{2} - \sum_k \sum_{n=1}^{\infty} \frac{e^{-\beta\omega_k n}}{n}. \tag{7.58}$$

We have $g_1(\beta\omega) = \sum_n \frac{e^{-n\beta\omega}}{n}$, $G_1(\beta\omega)$ being the Bose-Einstein function of order one, which is obviously closely related to the Riemann-Zeta function, $\zeta(n) = \sum_{k=1}^{\nu} \frac{1}{k^n}$. Now, we pass to the continuum case, using the enumaration of states for our dispersion relationship, we get

$$dn = \frac{L}{\pi a} \frac{d\omega}{(1 - \frac{\omega^2}{\Delta^2})^{1/2}} = \frac{2N}{\pi} \frac{d\omega}{\Delta(1 - \frac{\omega^2}{\Delta^2})^{1/2}}, \tag{7.59}$$

where we used the relation above, and employed periodic boundary conditions i.e. $kL = 2n\pi$ $(1 \leq n \leq N)$, and where dn is the number of eigenstates in the frequency interval $d\omega$ at the frequency ω.

We equated the total number of modes to the number of particles, and finally summing over a dummy index and integrating over eigenfrequencies we have.

$$-\log Q = \frac{\beta}{2} \frac{2N}{\pi} \int_0^{\Delta} \frac{\frac{d\omega}{\Delta}}{(1 - \frac{\omega^2}{\Delta^2})^{1/2}} - \frac{2N}{\pi} \sum_n \int \frac{d\omega}{(1 - \frac{\omega^2}{\Delta^2})^{1/2}} \frac{e^{-n\beta\omega}}{n}, \tag{7.60}$$

where in the second term above on the right, the sum and integral are separately convergent and thus it is permissible to reverse the order of summation and integration. The first term on the right gives after integration, $2N(\frac{\Delta\beta}{2\pi})$. The second term gives after using the relation in [9]

$$I = N \sum_{n=1}^{\infty} [L_0(n\beta\Delta) - I_0(n\beta\Delta)], \tag{7.61}$$

where $I_0(z)$ is the modified Bessel function of the first kind and order zero, and $L_0(z)$ is the modified Struve function of order zero, with the series expansion below (around z=0),

$$I_0(z) = \sum_{n=0}^{\infty} \frac{(\frac{z}{2})^{2n}}{(n!)^2}, \tag{7.62}$$

$$L_0(z) = \sum_{n=0}^{\infty} \frac{(\frac{z}{2})^{(2n+1)}}{\Gamma(\frac{(n+3)}{2})}^2 \tag{7.63}$$

7.4.2. Usage of the Mellin Transformation

Reproducing the result for the sum above, we have

$$G(x) = \sum_{k=1}^{\infty} \frac{1}{k}[L_0(k\beta\Delta) - I_0(k\beta\Delta)]. \tag{7.64}$$

We write this sum as below, for the case

$$G(x) = \sum_{k} \lambda_k g(\mu_k x), \tag{7.65}$$

where $\lambda_k = \frac{1}{k}$, $\mu_k = k$, $g(x) = L_0(x) - I_0(x)$. Taking the Mellin transformation of both sides we obtain

$$G^*(s) = \int dx x^{s-1} G(x) = \sum_k \int dx \frac{x^{s-1}}{k} g(kx) = \sum_k \frac{1}{k^{(1+s)}} g^*(s). \tag{7.66}$$

Thus

$$G^*(s) = \Lambda(s) g^*(s), \tag{7.67}$$

where $\Lambda(s) = \zeta(1+s)$. And for $g^*(s)$, the Mellin transformation of the base function we have, from [6] page 133,

$$g^*(s) = \frac{-1}{2}(\frac{\beta\Delta}{2})^{-s} \sec(\frac{s\pi}{2}) \frac{\Gamma(\frac{s}{2})}{\Gamma(1-\frac{s}{2})}. \tag{7.68}$$

Now, from [10] we have

$$g(x) = L_0(x) - I_0(x) \sim \frac{1}{\pi} \sum_{k=0}^{\infty} -1^{k+1} \frac{\Gamma(k+\frac{1}{2})}{\Gamma(-k+\frac{1}{2})} (\frac{2}{x})^{2k+1}. \tag{7.69}$$

Thus we obtain

$$g(x) \to (\frac{\beta\Delta}{2})^v, v = 0, \tag{7.70}$$

as x $\to 0$ and

$$g(x) \to (\frac{\beta\Delta}{2})^u, u = -1, \tag{7.71}$$

as x $\to \infty$. Since $v > u$, this sum called the (Harmonic sum), is defined over all x in $(0, \infty)$ [6] with the fundamental strip $0 < s < 1$. We have in this paper used the paper of [6] for Mellin transforms.

We will now consider the singular behaviour of this transform. First we investigate the behaviour of the poles to the right of the fundamental strip. By the nature of the Mellin Transform, this corresponds to the case $\beta\Delta > 1$. First, take the inverse transform of the function $G^*(s)$. Thus we obtain the asymptotic behaviour of $G(x)$ as $x \to \infty$

$$G(x) = -\frac{1}{2}\int_{c-i\infty}^{c+i\infty} dsx^{-s}(\frac{\beta\Delta}{2})^{-s}\sec(\frac{s\pi}{2})\frac{\Gamma\frac{s}{2}\zeta(1+s)}{\Gamma(1-\frac{s}{2})}, \tag{7.72}$$

where $0 < c < 1$, and the contour of integration is over the right half side (and we thus obtain a relative (-) sign. The poles are at $s = 2k+1$. Expanding $\sec(\frac{s\pi}{2})$ in terms of poles (for $k \geq 0$), we get, [8],

$$\sec\frac{s\pi}{2} = \frac{1}{2} + \frac{2}{\pi}\sum_{n=0}^{\infty}\frac{(-1)^{n+1}}{s-(2n+1)}. \tag{7.73}$$

The constant term does not contribute to the integral because, we have

$$\frac{\Gamma(\frac{s}{2})\zeta(1+s)}{\Gamma(1-\frac{s}{2})}, \tag{7.74}$$

where $\Gamma(s)$ does not have any zeroes, and it is an analytical function of s in the region integration, and the term $(\frac{x\beta\Delta}{2})^{-s}$ is also analytic in the region of integration. Now, taking the contour integral, upon evaluating the residue at $s = (2k+1)$, we have

$$G(x) = \frac{1}{\pi}\sum_{k=0}^{\infty}(-1)^{k+1}(\frac{\beta\Delta x}{2})^{(-2k-1)}\frac{\Gamma(k+\frac{1}{2})}{\Gamma(-k+\frac{1}{2})}\zeta(2k+2). \tag{7.75}$$

Now, consider the transform for $\beta\Delta < 1$, for this we find the poles for $s < 0$. (to the left of the fundamental strip). We have upon reproducing the relation

$$G^*(s) = \frac{-1}{2}(\frac{\beta\Delta}{2})^{-s}\sec(\frac{s\pi}{2})\frac{\Gamma(\frac{s}{2})}{\Gamma(1-\frac{s}{2})}\zeta(1+s). \tag{7.76}$$

The possible poles are $s = -(2k+1)$, s=0 (double pole) and $s = -2n$, $n \geq 1$. First, consider the case where s = 0. Using the identity due to Riemann, we have

$$\zeta(1+s) = 2(2\pi)^s\cos\frac{s\pi}{2}\zeta(-s)\Gamma(-s). \tag{7.77}$$

Near the vicinity of $s = 0$, we get with $\Gamma(s) = \frac{1}{s}$ (a second order pole)

$$G^*(s) = (\frac{\beta\Delta}{4\pi})^{-s}\frac{\zeta(-s)}{\Gamma(1-\frac{s}{2})}(\frac{2}{s^2}), \tag{7.78}$$

which gives the result, as the contribution from

$$G(x) = \log\frac{\beta\Delta}{2} + \gamma, \tag{7.79}$$

where γ is the Euler's constant, and we have used the relation, $\frac{\zeta'(0)}{\zeta(0)} = \log 2\pi$.

Now, consider the case $s = -(2k+1)$ $(k \geq 0)$. We have the term $\sec(\frac{s\pi}{2})\zeta(1+s)$. At $s = -(2k+1)$, we obtain $\sec\frac{s\pi}{2}\zeta(-2k)$. Now $\zeta(-2k)$ has a zero of order one for integer k. On the other hand $\sec{(k+\frac{1}{2})2\pi}$ has a pole of order one. Thus their product gives a constant, i.e there are not any poles. Now, consider $s = (-2n)$ $(m \geq 1)$. We have for the gamma-function

$$\Gamma(\frac{s}{2}) = \sum_{m=1}^{\infty} \frac{(-1)^m}{\frac{s}{2}+m} \frac{1}{m!}. \tag{7.80}$$

For the residue of s=-2n, we have

$$= \frac{-1}{2}(\frac{\beta\Delta}{2})^{2m}(-1)^m \frac{\zeta(1-2m)}{(\Gamma(m+1))^2} 2(-1)^m, \tag{7.81}$$

with Riemann's identity above, we finally have, for $\frac{\beta\Delta}{2} < 1$,

$$-\log Q = 2N\frac{\beta\Delta}{2\pi} + N\log\frac{\beta\Delta}{2} + N(\gamma) + N2\sum_{n=1}^{\infty}(-1)^{m+1}(\frac{\beta\Delta}{4\pi})^{2m}\frac{\zeta(2m)\Gamma(2m)}{\Gamma(m+1)^2}. \tag{7.82}$$

Now, we have from Equation (7.75) (for $\frac{\beta\Delta}{2} > 1$)

$$-\log Q = \frac{1}{\pi}\sum_{k=0}^{\infty}(-1)^{k+1}(\frac{\beta\Delta}{2})^{(-2k-1)}\frac{\Gamma(k+\frac{1}{2})}{\Gamma(-k+\frac{1}{2})}\zeta(2k+2) + 2N\frac{\beta\Delta}{2\pi}, \tag{7.83}$$

on the other hand, we have

$$-\log Q = 2N\frac{\Delta\beta}{2\pi} + \sum_n \frac{1}{n}[L_0(n\beta\Delta) - I_0(n\beta\Delta)]. \tag{7.84}$$

We have from [10],

$$L_0(z) - I_0(z) \sim \frac{1}{\pi}\sum_{k=0}^{\infty}(-1)^{k+1}\frac{\Gamma(k+\frac{1}{2})}{\Gamma(-k+\frac{1}{2})}(\frac{2}{z})^{2k+1}. \tag{7.85}$$

Thus, we have asymptotically

$$\sum_n \frac{1}{n}[L_0(n\beta\Delta) - I_0(n\beta\Delta)] = \sum_{k=0}^{\infty}\frac{1}{\pi}(\frac{\beta\Delta}{2})^{-2k-1}\frac{\Gamma(k+\frac{1}{2})}{\Gamma(-k+\frac{1}{2})}\zeta(2k+2), \tag{7.86}$$

when we set $\zeta(2k+2) \approx 1$, we have

$$S(x) = L_0(x) - I_0(x). \tag{7.87}$$

Thus, we have that in affect only a single term contributes to the sum over eigenfrequency which is similar to the optical mode case, in the previous papers [13] and [15].

7.4.3. Thermodynamics

For $\beta\Delta > 1$, we have, for the partition function,

$$-\log Q = 2N\frac{\Delta\beta}{2\pi} - \frac{4}{\pi}\sum_{k=0}^{\infty}(\frac{(2k)!}{k!})^2\frac{\zeta(2k+2)}{(2\beta\Delta)^{2k+1}}. \tag{7.88}$$

With $E = -\frac{\partial \log Q}{\partial \beta}$, we obtain,

$$E = 2N\frac{\Delta}{2\pi} + \frac{4}{\pi}kT\sum_{k=0}^{\infty}(\frac{(2k)!}{k!})^2\frac{(2k+1)\zeta(2k+2)}{(2\beta\Delta)^{2k+1}}. \tag{7.89}$$

We see that c_v is always greater than zero. For the first few terms, we have

$$E = 2N\frac{\Delta}{2\pi} + \frac{\pi}{3}\frac{N(kT)^2}{\Delta} + \frac{\pi^3}{15}\frac{kT^4}{\Delta^3}, \tag{7.90}$$

and

$$c_v = (\frac{\partial E}{\partial T})_v = \frac{2\pi}{3}Nk(\frac{kT}{\Delta}) + \frac{4\pi^3}{15}(\frac{kT}{\pi})^3 kN. \tag{7.91}$$

We now make three remarks.

(i) As $T \to 0$, the correct ground state energy is obtained.

(ii) As $T \to 0$, $c_v \propto (T)$ ($c_v \propto T^d$ in d dimensions) for a dispersion relation linear in k as $k \to 0$.

(iii) We have at our hands on asymptotic series in $(\beta\Delta)^{-2k-1}$. We assumed that it was legitimate to differentiate these series.

Now, let us calculate the entropy with the relation $S = -(\frac{\partial A}{\partial T})_v$ where $A = -kT\log Q$ and alternatively $S = \frac{E}{T} - \frac{A}{T}$. We obtain the same result

$$S = \frac{8N}{\pi}\sum_{k=0}^{\infty}(\frac{(2k)!}{k!})^2\frac{\zeta(2n+2)(n+1)}{(2\beta\Delta)^{2n+1}}. \tag{7.92}$$

The first two terms are

$$S = \frac{2\pi}{3}N\frac{kT}{\Delta} + \frac{4}{45}\pi^3(\frac{kT}{\Delta})^3. \tag{7.93}$$

We see that as $T \to 0$, $S \to 0$. Thus the third law of thermodynamics is seen to be obeyed.

Now consider the case $\frac{\Delta B}{2\pi} \ll 1$ (high temperature limit). Again employing the same relations

$$E = 2N\frac{\Delta}{2\pi} + NkT + 2N\sum_{n=1}^{\infty}(-1)^{n+1}(\frac{\beta\Delta}{4\pi})^{2n}\frac{\zeta(2n)\Gamma(2n)}{(n!)^2}. \tag{7.94}$$

The first two terms are

$$E = 2N\frac{\Delta}{2\pi} + NkT[1 + \frac{1}{48}(\frac{\Delta}{kT})^2 - 1]. \tag{7.95}$$

For c_v, we have

$$c_v = Nk[1 - \frac{1}{48}(\frac{1}{kT})^2]. \tag{7.96}$$

We see that as $T \to \infty$, the equipartition energy holds. Now let us calculate the entropy as $\beta\Delta \to 0$ for our system

$$S = Nk[1 + \log\frac{2kT}{\Delta}] + 2Nk\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{(\Gamma(k+1))^2}\zeta(2k)\Gamma(2k)(\frac{\beta\Delta}{4\pi})^{2k}2k. \tag{7.97}$$

The first term on the right is the standard term for the entropy of a system of harmonic oscillators as $T \to \infty$. The second term goes to zero as $\beta \to 0$ ($T \to 0$).

8. TWO OTHER METHODS FOR CALCULATION OF THE PARTITION FUNCTION FOR ACOUSTIC PHONONS

8.1. A Closed Form for the Partition Function

Above we have obtained an exact solution albeit in the form of a series. Now we will find an approximate but closed form for the partition function and the physical quantities in question. We now have

$$-\log Q_k = N \log \beta\omega_k - \frac{2N}{\pi}\sum_{k=1}^{\infty}(-1)^k(\frac{\beta\omega_k}{2\pi})^{2k}\frac{\Gamma(2k)\zeta(2k)}{(2k)!}. \tag{8.1}$$

Now set $\zeta(2n) = 1$, which is an excellent approximation for $n > 3$. Now for $\frac{\beta\Delta}{2\pi} < 1$, we have

$$-\log Q_k = N\log(\beta\omega_k) + \log[1 + (\frac{\beta\omega_k}{2\pi})^2]. \tag{8.2}$$

Now, sum (integrate) over ω_k. We obtain for the second term on the right as

$$= \frac{2N}{\pi}\int\frac{d\omega}{(1-\frac{\omega^2}{\Delta^2})^{\frac{1}{2}}}\log(1+(\frac{\omega\beta\Delta}{\Delta 2\pi})^2) = 2N\log(\frac{1+(1+z^2)^{\frac{1}{2}}}{2}) \tag{8.3}$$

where $z = \frac{\Delta\beta}{2\pi}$. Thus, we have for the full partition function,

$$\log Q = N\log\frac{\beta\Delta}{2} + 2N\log\frac{1+(1+z^2)^{\frac{1}{2}}}{2}. \tag{8.4}$$

We remind the reader that $z < 1$, and the only approximation we made was that $\zeta(2n) \sim 1$.

Before we proceed, we are going to derive this expression using another method. For this, we refer the reader to [4], (page 412),

$$\int\frac{dz}{(a+bx^2)^{n+1}} = \frac{1}{2^{n+1}}\frac{1}{b^{\frac{1}{2}}}\pi\frac{(2n-1)!}{n!}\frac{1}{a^{\frac{(2n+1)}{2}}}. \tag{8.5}$$

Now, set $a = \frac{1}{z}$, $b = 1$,

$$K = -2N \sum_{k=1}^{\infty} \frac{(\frac{z}{2})^{2k}}{(k!)^2} (-1)^k \Gamma(2k) \zeta(2k) = -\frac{2N}{z} \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{(-1)^n}{2n} \int \frac{dx}{(x^2 + \frac{1}{z^2})^{n+1}}. \tag{8.6}$$

where we set $\zeta(2k)$ as -1. For $z < 1$, $\frac{1}{x^2+\frac{1}{x^2}} < 1$ (for real x), and we can safely sum the series. Reversing the order of summation and integration above, we have

$$K = \frac{2N}{\pi z} \int_0^{\infty} \frac{dx}{(x^2 + \frac{1}{z^2})} \log (1 + \frac{1}{x^2 + \frac{1}{z^2}}). \tag{8.7}$$

Taking the integral, we obtain the same result i.e.

$$-\log \psi = N \log \frac{\beta \Delta}{2} + 2N \log \frac{[1 + (1 + z^2)^{1/2}]}{2} \tag{8.8}$$

where again, we used only the approximation that $\zeta(2k) \approx 1$, for all K.

Now, consider the thermodynamical properties as calculated from this relation for the partition function. We have (for $z < 1$)

$$E = \frac{-\partial logQ}{\partial \beta} \tag{8.9}$$

with $u = (1 + z^2)^{1/2}$, we obtain for E

$$E = NkT[3 - \frac{2}{u}] \tag{8.10}$$

and for the specific heat. We have

$$c_v = \frac{2Nk}{u^3}(u^3 - \frac{4u^2}{3} + \frac{2}{3}). \tag{8.11}$$

Finally, we obtain an expression for the entropy for $z < -1$. Thus,

$$S = \frac{1}{T}(E - A) = -(\frac{\partial A}{\partial T})_V = Nk[3 - \frac{2}{u} + \log \frac{2kT}{\Delta} - 2 \log (\frac{1+u}{2})]. \tag{8.12}$$

Here we remind the reader that, for these expressions to be valid, z must be less than or equal to one. Now, we immediately see that with $z < 1$, since $u > 1$ (and nonzero) the equations above are analytical functions of T, therefore there are no phase transitions for this range, i.e. $0 < z < 1$. Now consider the asymptotic behavior of this partition function as $T \to \infty$. We have

$$E = NkT[1 + (\frac{\Delta}{2\pi kT})^2 + ..], \tag{8.13}$$

$$c_v = NkT[1 - (\frac{\Delta}{2\pi kT})^2 + ..], \tag{8.14}$$

and

$$S = Nk[1 + \log \frac{2kT}{\Delta} + \frac{1}{2}(\frac{\Delta}{2\pi kT})^2 + ...]. \tag{8.15}$$

We see that the proper asymptotic behavior as $T \to \infty$ of a system of BSHO's is obtained, i.e $c_v = Nk$,

$$S = Nk[1 + \log(\frac{2kT}{\Delta})]. \tag{8.16}$$

8.2. Fermi-Dirac Function for BSHO's

Here we obtain still another expression for the partition function of our particular system of BSHO's, and compare in the next section with the result obtained there. Reproducing the result above as

$$-\log Q = N \log \frac{\beta\Delta}{2} + 2N \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{(k!)^2} (\frac{\beta\Delta}{4\pi})^{2k} \Gamma(2k)\zeta(2k). \tag{8.17}$$

Using the relation [10], we have

$$\Gamma(az + b) = (2\pi)^{(1/2)} e^{-az} (az)^{az+b-1/2}. \tag{8.18}$$

We immediately obtain the expression

$$-\log Q = N \log \frac{\beta\Delta}{2} + \frac{N}{\sqrt{\pi}} \tilde{f}_{3/2}(z^2), \tag{8.19}$$

where $\tilde{f}_{3/2}(z^2) = \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^{3/2}} z^{2k} \zeta(2k)$. We call $\tilde{f}_{3/2}(z^2)$ the modified Fermi-Dirac function at argument z^2 and order 3/2. Now, we make the approximation $\zeta(2k) \simeq 1$ which is an excellent approximation $(\tilde{\zeta}(s)10^{-4})$ $k > 3$. Thus we have, after replacing $\tilde{f}_{3/2}(z^2)$ with $f_{3/2}(z^2)$ (the regular Fermi-Dirac function) in this limit, now with

$$A = -kT = -kT \left[\log \frac{\beta\Delta}{2} f_{3/2}\left(z^2\right) \right], \tag{8.20}$$

for the Helmholtz free energy, using the relation $E = -\frac{\partial \log Q}{\partial \beta}$, we have

$$E = NkT[1 + \frac{2}{\sqrt{\pi}} f_{1/2}(z^2)], \tag{8.21}$$

where we used the relation

$$z\frac{d\tilde{f}_{3/2}(z)}{dz} = f_{1/2}(z). \tag{8.22}$$

For the specified heat,

$$c_N = \left(\frac{\partial E}{\partial T}\right)_v = Nk + \frac{2Nk}{\sqrt{\pi}} \left[f_{3/2}\left(z^2\right) - 2f_{-1/2}\left(z^2\right)\right]. \tag{8.23}$$

And finally we have for the entropy

$$S = -\left(\frac{\partial \Delta}{\partial T}\right)_V = Nk \left[\log \frac{2kT}{\Delta} + 1\right] + \frac{2Nk}{\sqrt{\pi}} \left[2f_{1/2}\left(z^2\right) - f_{3/2}\left(z^2\right)\right]. \tag{8.24}$$

For the case where $z << 1$, we have,

$$E = NkT[1 + \frac{2}{\sqrt{\pi}}\frac{\varDelta}{2\pi kT}^{2} + O(1/T4)], \tag{8.25}$$

$$c_v = Nk[1 - \frac{2}{\sqrt{\pi}}\frac{\varDelta}{2\pi kT}^{2} + O(1/T4)], \tag{8.26}$$

$$S = Nk[\log(\frac{2kT}{\varDelta}) + 1] + \frac{Nk}{\sqrt{\pi}}(\frac{1}{2\pi kT})^2. \tag{8.27}$$

Thus, after making the approximation that $S(2n) \simeq 1$, we obtain the proper asymptotic behavior as $T \to \infty$. The expression above are valid for $0 < z < 1$. If not for the Fermi–Dirac equation must be analytically continued to $t > 1$, something which we did not do.

8.3. Comparison of the Two Expressions Given Above

In this subsection, we compare the two expressions given in Section 8.1 and 8.2 above. We again remind the reader that these expressions are valid only for $z < 1$. In subsection 8.1, the only approximation we made was that $\zeta(2) \approx 1$. This is an excellent approximation for $k > 3$, on the other hand, for the solution in 8.2, we made the same approximation. In addition, we also used an asymptotical expressing for the Gamma Function.

Now, we have for the Fermi-Dirac case of Section 8.2, the following expression after expanding the Fermi-Dirac function and accepting only the first four terms

$$-\log Q = N\log(\beta\varDelta) + N(0.564z^2 - 0.139z^4 + 0.103z^6 - 0.0705z^8). \tag{8.28}$$

On the other hand for the closed form of section 8.1, we have after expanding for the partition function in a Taylor's series

$$-\log Q = N\log(\beta\varDelta) + N(0.5 - 0.187z^4 + 0.104z^6 - 0.0640z^8). \tag{8.29}$$

In both equations $z < \varDelta\beta/2\pi$. The similarity of the two expression is obvious. So at least the results of these two expressions are internally consistent.

9. CONCLUSION

In this thesis, we have elaborated on the conclusion of thermodynamical quantities of systems of harmonic oscillators. We have calculated the internal energy, specific heat at constant volume, entropy, and obtained results that are consistent with the $T \to 0$ and $T \to \infty$ asymptotic behaviour of general systems of harmonic oscillators. Our calculations are similar to those pertaining to the Debye theory and Einstein theory. Another result we obtained was that our theory of FSHO's admitted negative temperatures. Another interacting feature coming out of our calculations was that, for the optical modes, the system behaved exactly as a single harmonic oscillator with a particular frequency of vibration regardless of the dimension of our system.

We have made also a pet calculation relating the pressure, temperature, volume specific heats, the coefficient of thermal expansion and the Gruncisen constant to each other. We conclude by saying that the theory calls for calculations involving acoustical phonons in 2 and 3-dimensions.

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