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EXPRESSION OF ENTROPY FOR SINGLE <111> TUNNELING MODEL

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Abstract

We study the many body localization aspects a single-particle mobility edges in fermionic systems. We investigate incommensurate lattices and random disorder Anderson models. Many body localization and quantum nonergodic properties are studied by comparing entanglement and internal entropy and by calculating the scaling of subsystem particle number fluctuations respectively. Every crystalline structure shows some deviations or the other from the regular atomic arrangement, as prescribed by the symmetry and structure of the respective unit cell. These deviations from the ideal crystal structure are called imperfections. The translational symmetry in a crystal is consistent with laws of thermodynamics, since these laws are applied to describe the growth of crystals all of which have some imperfections. Any increase in the defect concentration raises the entropy, which in term lowers the free energy at a finite temperature. In the equilibrium state there is a finite concentration of imperfection in the crystal.

The concentration of a particular type of imperfection depends on the type of the crystal lattice, the binding energy of the lattice and structure of the imperfection itself. Entropy is the measure of the disorder of a system, the greater the disorder, the higher is the entropy. In the magnetic field the moments will be partially ordered, so that the entropy is lowered by the field. The relatively small heat capacity associated with the lattice vibrations of solids at temperature near and below 1°K makes this region interesting in connection with an evaluation of contribution of the conduction electrons to the heat capacity of the metals. In the present study we limit ourselves to find out expression of entropy for <111> tunneling model. For this purpose we have developed first the defect contribution to the specific heat for <111> tunneling model.

Introduction

Single molecules are nanoscale thermodynamic systems with few degrees of freedom. The thermodynamic concept of entropy is key to the understanding of many chemical processes, including electron transfer reaction and quantum mechanical phenomenon. Tunneling is a quantum mechanical phenomenon when a particle is able to penetrate through a potential energy barrier that is higher in energy than the particle's kinetic energy. This

amagizing property of microscopic particles plays important roles in explaining several physical phenomena including radioactive decay.

It is a well-established fact that there exist no perfect crystals. Every crystalline structure shows some deviations or the other from the regular atomic arrangement, as prescribed by the symmetry and structure of the respective unit cell. These deviations from the ideal crystal structure are called imperfections. Imperfections could be of several types. The presence of defect is not accounted by the translational symmetry of the perfect crystal though it forms the basis of most of the interpretation in perfect crystals. We may obviously be curious to know how the translational symmetry in a crystal is consistent with laws of thermodynamics, since these laws are applied to describe the growth of crystals all of which have some imperfections, we know that the Halmholtz free energy

$$F = U - TS \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(i)}$$

must be minimum in the state of equilibrium at a certain temperature, U stands for the internal energy and S for the entropy. We take the advantage of the following statistical statements of entropy

$$S = K_B \text{ In } W \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(ii)}$$

Where W is the number of possible ways in which elements of system may be distributed.

Theory

In a perfect crystal there can be only one way (W = 1) to arrange atoms at different sites and therefore the entropy in this case will be zero. On the other hand a defect at a stie within a unit cell makes the unit cell look different from others. In this case there can be as many ways of arranging the defects as the number of sites within the unit cell, the entropy is given by

$$S = K_B \text{ In } N \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(iii)}$$

Where N is the number of sites in unit cells.

The above relation expresses the contribution of the defect to the entropy of the crystal. Thus any increase in the defect concentration raises the entropy, which in term lowers the free energy at a finite temperature. In the equilibrium state there is a finite concentration of imperfection in the crystal. In above example we considered only one type of defect, but as a necessary consequence of the inherent disorder associated with the finite temperature all kind of imperfections (one can imagine) could be present; though some of them might be very small in number. The concentration of a particular type of imperfection depends on the type of the crystal lattice, the binding energy of the lattice and structure of the imperfection itself. The imperfections are crucial to the interpretation of several properties of crystals that are not accounted by the transitional symmetry, to name a few; colour of crystals enhancement of conductivity of pure semiconductors, plasticity, strength of crystals luminescence and diffusion of atoms in solids are some such significant example [1].

Entropy is the measure of the disorder of a system, the greater the disorder, the higher is the entropy. In the magnetic field the moments will be partially ordered, so that the entropy is lowered by the field. The entropy is also lowered if the temperature is lowered, as more of the momen's line up.

If the magnetic field can then be removed without changing the entropy of the spin system. The order of the spin system will look like a lower temperature than the same degree of order in the presence of field. When the specimen is demagnetized adiabatically, entropy can flow into the spin system, only from the system of lattice vibrations [2]. At the temperature of interest the entropy of the lattice vibrations is usually negligible, thus the entropy of the spin systems will be essentially constant during adiabatic demagnetization of the specimen. Magnetic cooling is a one shot operation, not cyclic [3].

The relatively small heat capacity associated with the lattice vibrations of solids at temperature near and below 1ºK makes this region interesting in connection with an evaluation of contribution of the conduction electrons to the heat capacity of the metals. There have been many heat capacity measurements of both normal and superconducting metals in the temperature range 1ºK to 4ºK which is accessible with liquid helium techniques, but until recently no measurement in adiabatic demagnetization range had been made. Heat capacity measurements on superconducting aluminium at temperatures below 1ºK were undertaken because they would make available data covering an usually wide range of reduced temperatures. Normal state measurements were also made and the measurements were extended through the liquid helium range to permit a more careful study of the transition region near 1.2ºK and to obtain a more accurate evaluation of the normal state parameters that was possible from the measurements below 1ºK. Preliminary results of this investigation have already been presented [4] and similar measurements on the super conducting state have been reported by Goodman [5].

At sufficiently low temperatures the normal state heat capacity C_n is generally considered to be the sum of an electronic and a lattice heat capacity, which are proportional to the first and third power of temperature respectively[6].

$$C_n = \gamma T + \frac{12}{5}\pi^4 R\left(\frac{T}{\theta}\right) \qquad \text{..... (iv)}$$

Where R is the gas constant, T is the temperature, θ is the Debye characteristic temperature of the lattice vibrations and γ is constant which is proportional to the density of states at the Fermi surface and which may depend on electron correlations [6] and the electron phonon interactions [7].

The electronic heat capacity of superconductor can be expected to yield information on the nature of the superconducting state; in particular, its temperature dependence should be related to the energy gap, which is feature of current theories [8]. The treatment of Bardeen, Cooper and Schrieffer [9] give an electronic superconducting state heat capacity C_{es}, which is for temperatures well below the critical temperature T_c, an exponential function of temperature is

$$\frac{C_{es}}{\gamma T_C} = a \exp\left(-b\frac{T_c}{T}\right) \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(v)}$$

In which the constants a and b are the same for all superconductors, measurements at temperatures below 1ºK are of particular interest as a test of this relation because those metals which show the properties associated with the ideal superconducting state, the soft superconductors and which have transition temperatures appreciably greater than 1ºK, also have relatively large lattice heat capacities. For example, for tin indium, thallium and lead with transitions at 3.7, 3.4, 2.4 and 7.2ºK the lattice heat capacity in superconducting state at the transition temperature amount to 45%, 77%, 83% and 94% of respective total heat capacities, on the other hand some of the soft superconductors with lower transition temperatures have relatively small lattice heat capacities the corresponding ratios for Aluminum, Zinc and Cadmium with transition temperatures 1.2, 0.8 and 0.5ºK are 1% and 3% and 3% respectively.

In ionic crystals specific heat varies as T^3 at very low temperature. But presence of paraelectric impurity even in small concentration have marked effect on the specific heat of ionic crystals. The variation with temperature shows an increase in specific heat at low temperature. If the presence of impurity splits the states into energy levels at separation Δ then the impurity contribution to the specific heat shows a peak at temperature Δ /k. Such type of

peaks in the specific heat called Schottky anomaly. This anomaly observed for most of the impurity systems can be explained within the frame work of the single multiplet tunneling model [10, 11].

In the present study we limit ourselves to find out expression of entropy for <111> tunneling model [12, 13]. For this purpose we have developed first the defect contribution to the specific heat for <111> tunneling model as follow:

Let the ground state tunneling multiplet is split into P levels then average energy to N impurity per unit volume at temperature T is given by:

$$E = \frac{N\sum_{i=1}^{p} g_i E_i Exp\left(-\frac{E_1}{kT}\right)}{\sum_{i=1}^{p} g_i Exp\left(-\frac{E_1}{kT}\right)} \quad \text{..... (vi)}$$

Where g_i is the degeneracy of the level and E_i is the energy splitting between the 1st and i^{th} level.

Expression for Specific Heat

The specific heat is given by the following expression

$$C_v = \frac{\partial < E >}{\partial T} \quad \text{..... (vii)}$$

Thus the impurity contributions to the specific heat for single multiplet <111> tunneling models have been already find out by the Raj Kumar *et al*. [12] which is given as follows:

$$C_v = 6Nky^2\left[\frac{e^{-y} + 4e^{-2y} + 6e^{-3y} + 4e^{-4y} + e^{-5y}}{\left(1 + 3e^{-y} + 3e^{-2y} + e^{-3y}\right)^2}\right] \quad \text{..... (viii)}$$

Where y = E/kT

Expression of Entropy for <111> model

Since the equation of the entropy is given as:

$$S = \int \frac{1}{T} C v dT \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(ix)}$$

Hence the equation of the entropy [11] for the <111> tunneling model will be:

$$S = \int \frac{1}{T} 6Nky^2 \left[\frac{e^{-y} + 4e^{-2y} + 6e^{-3y} + 4e^{-4y} + e^{-5y}}{\left(1 + 3e^{-y} + 3e^{-2y} + e^{-3y}\right)^2} \right] dT$$

$$= -6Nkye^{y} \frac{e^{4y} + 4e^{3y} + 6e^{2y} + 4e^{2y} + 4e^{y} + 1}{\left(1 + 3e^{y} + 3e^{2y} + e^{3y}\right)^2} dy$$

$$= -6Nk \int ye^{y} \frac{\left(1 + e^{y}\right)}{\left\{\left(1 + e^{y}\right)^3\right\}^2} dy$$

Thus after simplification we finally obtained expression for entropy given below:

$$S = -6Nk \left[\log\left(1 + e^{y}\right) - \frac{ye^{y}}{\left(1 + e^{y}\right)} \right] \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(x)}$$

Where N is impurity concentration, k is Boltzsman Constant and y = E/kT.

Results and Discussions

The result of present theoretical investigation for <111> tunneling model are given by equation (x) for entropy. This result can be used for future theoretical investigation to explain anomalous results of various experimentally as well as theoretically available systems. Our investigation revealed tautomerization in single prophycene molecules such as Cu (111), Ag (111) and Au (111) surface by a combination of low temperature scanning tunneling microscopy (STM) experiments and density functional theory (DFT) [14]. It is revealed that the trans configuration is the thermodynamically stable form of propylene on Cu (III) and Ag (III) where as the cis configuration occurs as a metastable form [15].

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