

# **FYS3410 - Vår 2011 (Kondenserte fasers fysikk)**

<http://www.uio.no/studier/emner/matnat/fys/FYS3410/index-eng.xml>

Based on Introduction to Solid State Physics by Kittel

## **Course content**

- **Periodic structures, understanding of diffraction experiment and reciprocal lattice**
- **Imperfections in crystals: diffusion, point defects, dislocations**
- **Crystal vibrations: phonon heat capacity and thermal conductivity**
- **Free electron Fermi gas: density of states, Fermi level, and electrical conductivity**
- **Electrons in periodic potential: energy bands theory classification of metals, semiconductors and insulators**
- **Semiconductors: band gap, effective masses, charge carrier distributions, doping, pn-junctions**
- **Metals: Fermi surfaces, temperature dependence of electrical conductivity**

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## **FYS3410 lecture schedule and exams: Spring 2011**

<b>W/19/1/2011:</b>	<b>Introduction and motivation. Periodicity and lattices</b>	<b>1h</b>
<b>M/24/1/2011:</b>	<b>Index system for crystal planes. Crystal structures</b>	<b>2h</b>
<b>W/26/1/2011:</b>	<b>Reciprocal space, Laue condition and Ewald construction</b>	<b>1h</b>
<b>M/31/1/2011:</b>	<b>Brillouin Zones. Interpretation of a diffraction experiment</b>	<b>2h</b>
<b>W/02/2/2011:</b>	<b>Crystal binding, elastic strain and waves</b>	<b>1h</b>
<b>M/07/2/2011:</b>	<b>Elastic waves in cubic crystals; defects in crystals</b>	<b>2h</b>
<b>W/09/2/2011:</b>	<b>Defects in crystals; case study – vacancies; diffusion</b>	<b>2h</b>
<b>M/14/2/2011:</b>	<b>Crystal vibrations and phonons</b>	<b>2h</b>
<b>W/16/2/2011:</b>	<b>Lattice heat capacity: Dulong-Petit and Einstein models</b>	<b>2h</b>
<b>M/21/2/2011:</b>	<b>Phonon density of states (DOS) and Debye model</b>	<b>2h</b>
<b>W/23/2/2011:</b>	<b>General result for DOS; role of anharmonic interactions</b>	<b>2h</b>
<b>M/28/2/2011:</b>	<b>Thermal conductivity and repetition of crystal vibrations</b>	<b>2h</b>
<b>W/02/3/2011:</b>	<b>no lectures</b>	
<b>M/07/3/2011:</b>	<b>no lectures</b>	
<b>W/09/3/2011:</b>	<b>no lectures</b>	
<b>M/14/3/2011:</b>	<b>Free electron Fermi gas in 1D and 3D – ground state</b>	<b>2h</b>
<b>W/17/3/2011:</b>	<b>Density of states, effect of temperature – FD distribution</b>	<b>1h</b>
<b>M/21/3/2011:</b>	<b>Heat capacity of FEFG</b>	<b>2h</b>
<b>W/23/3/2011:</b>	<b>Repetition</b>	<b>1h</b>
<b>M/28/3/2011:</b>	<b>Mid-term exam</b>	

<b>M/04/4/2011:</b>	<b>Electrical and thermal conductivity in metals</b>	<b>2h</b>
<b>W/06/4/2011:</b>	<b>Bragg reflection of electron waves at the boundary of BZ</b>	<b>2h</b>
<b>M/11/4/2011:</b>	<b>Energy bands, Kronig - Penny model</b>	<b>2h</b>
<b>W/13/4/2011:</b>	<b>Empty lattice approximation; number of orbitals in a band</b>	<b>2h</b>

### **Påsk uppehåll**

**W/27/4/2011**      **no lectures**

**M/02/5/2011:**      **no lectures**

**W/04/5/2011:**      **no lectures**

<b>M/09/5/2010:</b>	<b>Semiconductors, effective mass method, intrinsic carriers</b>	<b>2h</b>
<b>W/11/4/2010:</b>	<b>Impurity states in semiconductors and carrier statistics</b>	<b>2h</b>
<b>M/16/5/2010:</b>	<b>p-n junctions, Schottky contacts and heterojunctions</b>	<b>2h</b>
<b>W/18/5/2010:</b>	<b>Metals and Fermi surfaces</b>	<b>1h</b>
<b>M/23/5/2010:</b>	<b>Repetition</b>	<b>2h</b>
<b>26-27/5/2010:</b>	<b>Final Exam (sensor:???)</b>	

## **Lecture 13: Debye model, general results for DOS, anharmonic interactions**

- **Repetition: Calculating phonon density of states – DOS – in 1-, 2- and 3-dimensions**
- **Debye model: explaining approximations and derivation of  $T^3$  temperature dependence for heat capacity**
- **Anharmonic crystal interactions**

## Lecture 13: Debye model, general results for DOS, anharmonic interactions

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## Calculating phonon density of states – DOS – in 1-D

Since atoms  $s$  and  $s+N$  have the same displacement, we can write:

$$u_s = u_{s+N} \longrightarrow ue^{i(ksa-\omega t)} = ue^{i(k(s+N)a-\omega t)} \longrightarrow 1 = e^{ikNa}$$

This sets a condition on allowed  $k$  values:

$$kNa = 2\pi n \rightarrow k = \frac{2\pi n}{Na} \quad n = 1, 2, 3, \dots$$

So the separation between allowed solutions ( $k$  values) is:

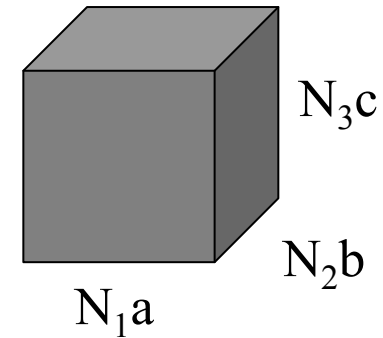
$$\Delta k = \frac{2\pi}{Na} \quad \Delta n = \frac{2\pi}{Na} \quad \text{independent of } k, \text{ so the density of modes in } k\text{-space is uniform}$$

Thus, in 1-D:

$$\frac{\# \text{ of modes}}{\text{interval of } k\text{-space}} = \frac{1}{\Delta k} = \frac{Na}{2\pi} = \frac{L}{2\pi}$$

## Calculating phonon density of states – DOS – in 3-D

Now for a 3-D lattice we can apply periodic boundary conditions to a sample of  $N_1 \times N_2 \times N_3$  atoms:



$$\frac{\text{\# of modes}}{\text{volume of } k\text{-space}} = \frac{N_1 a}{2\pi} \frac{N_2 b}{2\pi} \frac{N_3 c}{2\pi} = \frac{V}{8\pi^3} = N(k)$$

Now we know from before that we can write the differential # of modes as:

$$dN = N(\omega)d\omega = N(k)d^3\vec{k} = \frac{V}{8\pi^3} d^3\vec{k}$$

We carry out the integration in  $k$ -space by using a “volume” element made up of a constant  $\omega$  surface with thickness  $dk$ :

$$d^3\vec{k} = (\text{surface area}) dk = \left[ \int dS_\omega \right] dk$$

## Calculating phonon density of states – DOS – in 3-D

Rewriting the differential  
number of modes in an interval:

$$dN = N(\omega)d\omega = \frac{V}{8\pi^3} \int dS_\omega dk$$

We get the result:

$$N(\omega) = \frac{V}{8\pi^3} \int dS_\omega \frac{dk}{d\omega} = \frac{V}{8\pi^3} \int dS_\omega \frac{1}{\frac{\partial \omega}{\partial k}}$$

A very similar result holds for  $N(E)$  using constant energy surfaces for the density of electron states in a periodic lattice!

This equation gives the prescription for calculating the density of modes  $N(\omega)$  if we know the dispersion relation  $\omega(k)$ .

We can now set up the Debye's calculation of the heat capacity of a solid.



## **Lecture 13: Debye model, general results for DOS, anharmonic interactions**

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# Debye model

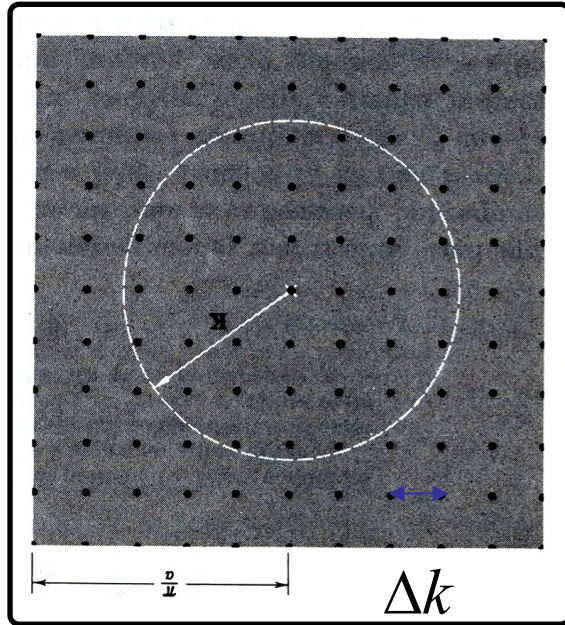
We know that we need to evaluate an upper limit for the heat capacity integral:

$$C_V(T) = \int_{\omega=0}^{\omega_{\max}} N(\omega) C_E(\omega, T) d\omega$$

If the dispersion relation is known, the upper limit will be the maximum  $\omega$  value. But Debye made several simple assumptions, consistent with a uniform, isotropic, elastic solid:

- 3 independent polarizations (L, T<sub>1</sub>, T<sub>2</sub>) with equal propagation speeds  $v_g$
- continuous, elastic solid:  $\omega = v_g k$
- $\omega_{\max}$  given by the value that gives the correct number of modes per polarization (N)

# Lattice heat capacity: Debye model



$$\Delta k = \frac{2\pi}{L}$$

$N_k$ : Allowed number of  $k$  points in a sphere with a radius  $k$

$$N_k = \left(\frac{L}{2\pi}\right)^3 \frac{4\pi}{3} k^3 = \left(\frac{L}{2\pi}\right)^3 \frac{4\pi\omega^3}{3v^3} = \frac{V\omega^3}{6\pi^2 v^3}$$

$$D(\omega) = \frac{dN_k}{d\omega} = \frac{V\omega^2}{2\pi^2 v^3} \quad \text{Density of states of acoustic phonons for 1 polarization}$$

$$\omega(k) = vk \quad \text{phonon dispersion relation}$$

## Debye temperature $\theta$

$$N = \frac{V\omega_D^3}{6\pi^2 v^3} \quad \rightarrow$$

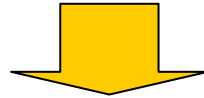
$$\hbar\omega_D = k_B\theta$$

$$\theta = \frac{\hbar v}{k_B} \left(\frac{6\pi^2 N}{V}\right)^{\frac{1}{3}}$$

$N$ : number of unit cell

## Thermal energy $U$ and lattice heat capacity $C_V$ : Debye model

3 polarizations for acoustic modes



$$U = 3 \int d\omega D(\omega) n(\omega) \hbar \omega = 3 \int_0^{\omega_D} d\omega \frac{V \omega^2}{2\pi^2 v^3} \frac{\hbar \omega}{\exp(\hbar \omega / k_B T) - 1}$$

$$C_V = \left( \frac{\partial U}{\partial T} \right) \Big|_V = \frac{3V \hbar^2}{2\pi^2 v^3 k_B T^2} \int_0^{\omega_D} d\omega \frac{\omega^4 \exp(\hbar \omega / k_B T)}{[\exp(\hbar \omega / k_B T) - 1]^2}$$

$$C_V = 9Nk_B \left( \frac{T}{\theta} \right)^3 \int_0^{x_D} dx \frac{x^4 e^x}{(e^x - 1)^2}$$

# Debye model

Better agreement than Einstein model at low T

Universal behavior for all solids!

Debye temperature is related to “stiffness” of solid, as expected

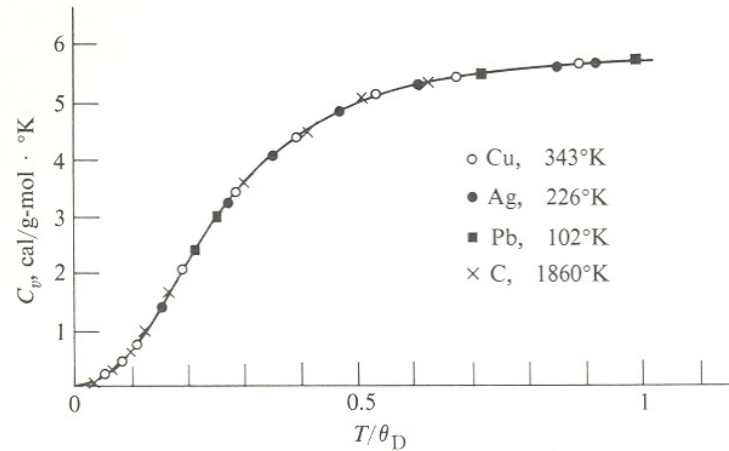


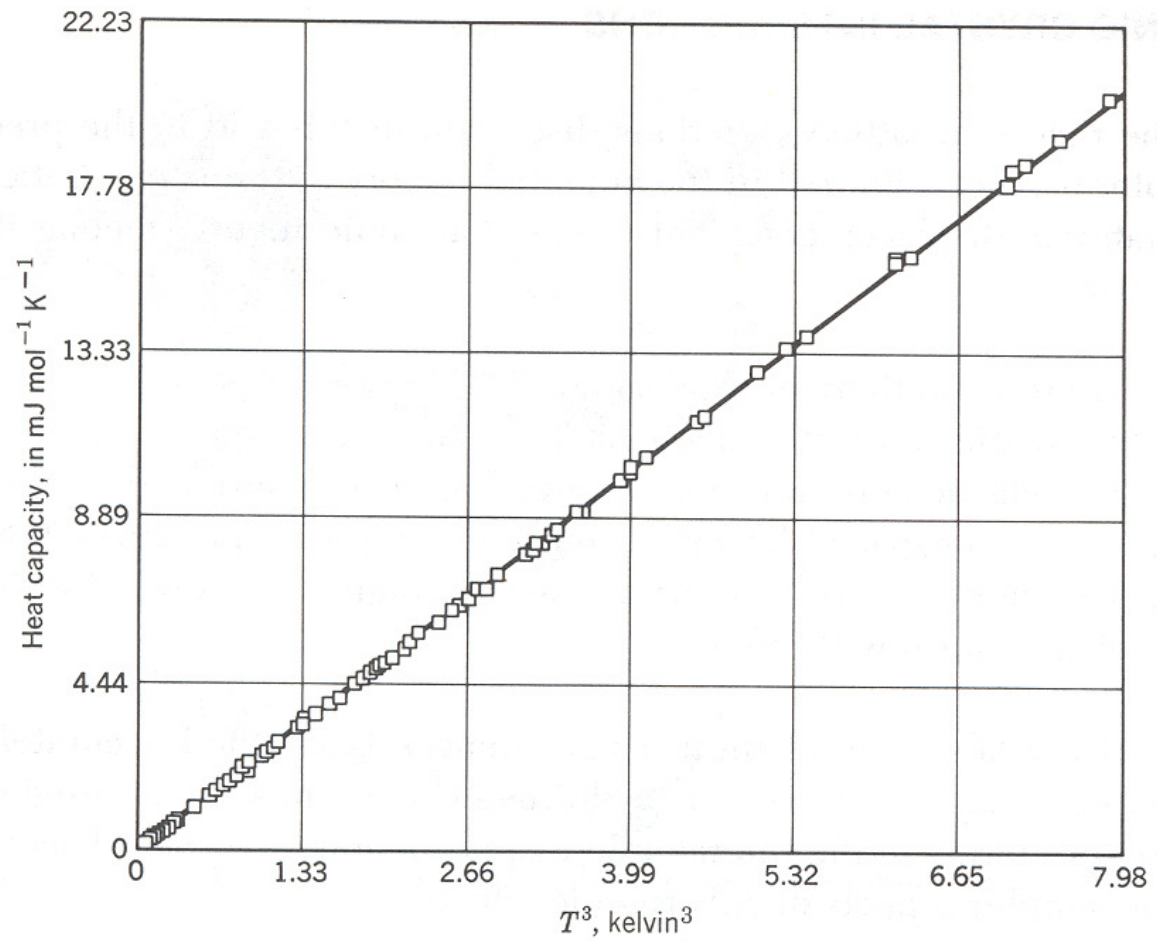
Fig. 3.13 Specific heats versus reduced temperature for four substances. Numbers refer to Debye temperatures. Note the high Debye temperature for diamond.

Table 3.1  
Debye Temperatures

Element	$\theta_D, ^\circ\text{K}$	Compound	$\theta_D, ^\circ\text{K}$
Li	335	NaCl	280
Na	156	KCl	230
K	91.1	CaF <sub>2</sub>	470
Cu	343	LiF	680
Ag	226	SiO <sub>2</sub> (quartz)	255
Au	162		
Al	428		
Ga	325		
Pb	102		
Ge	378		
Si	647		
C	1860		

# Debye model

Quite impressive agreement with predicted  $C_V \propto T^3$  dependence for Ar! (noble gas solid)



**Figure 11** Low temperature heat capacity of solid argon, plotted against  $T^3$ . In this temperature region the experimental results are in excellent agreement with the Debye  $T^3$  law with  $\theta_0 = 92.0$  K. (Courtesy of L. Finegold and N. E. Phillips.)

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# I

## Anharmonic Properties of Solids

Two important physical properties that ONLY occur because of anharmonicity in the potential energy function:

1. Thermal expansion
2. Thermal resistivity (or finite thermal conductivity)

### Thermal expansion

In a 1-D lattice where each atom experiences the same potential energy function  $U(x)$ , we can calculate the average displacement of an atom from its  $T=0$  equilibrium position:

$$\langle x \rangle = \frac{\int_{-\infty}^{+\infty} x e^{-U(x)/kT} dx}{\int_{-\infty}^{+\infty} e^{-U(x)/kT} dx}$$



## Thermal Expansion in 1-D

Evaluating this for the harmonic potential energy function  $U(x) = cx^2$  gives:

$$\langle x \rangle = \frac{\int_{-\infty}^{+\infty} x e^{-cx^2/kT} dx}{\int_{-\infty}^{+\infty} e^{-cx^2/kT} dx}$$

Now examine the numerator carefully...what can you conclude?

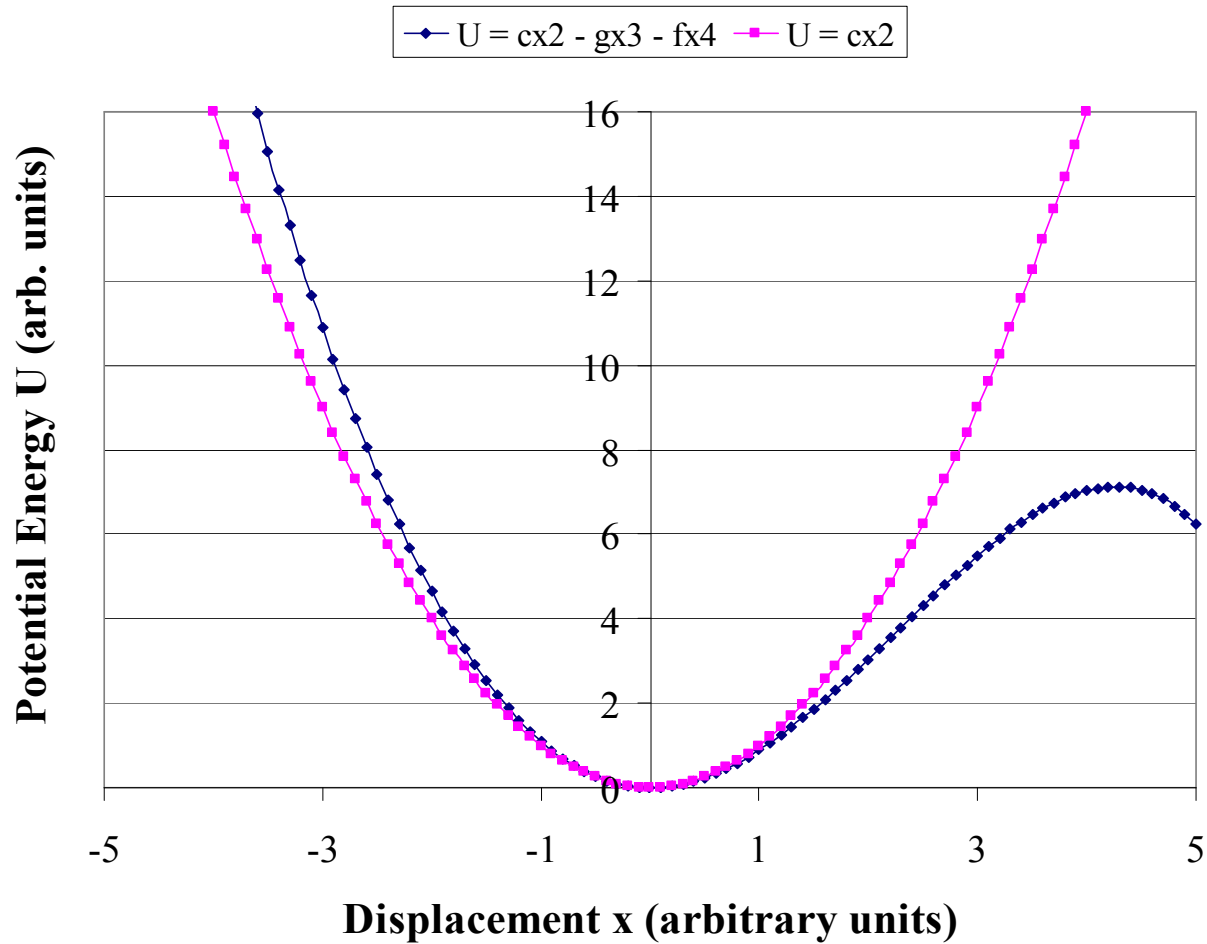
$$\langle x \rangle = 0! \quad \text{independent of } T!$$

Thus any nonzero  $\langle x \rangle$  must come from terms in  $U(x)$  that go beyond  $x^2$ . For HW you will evaluate the approximate value of  $\langle x \rangle$  for the model function

$$U(x) = cx^2 - gx^3 - fx^4 \quad (c, g, f > 0 \quad \text{and} \quad gx^3, fx^4 \ll kT)$$

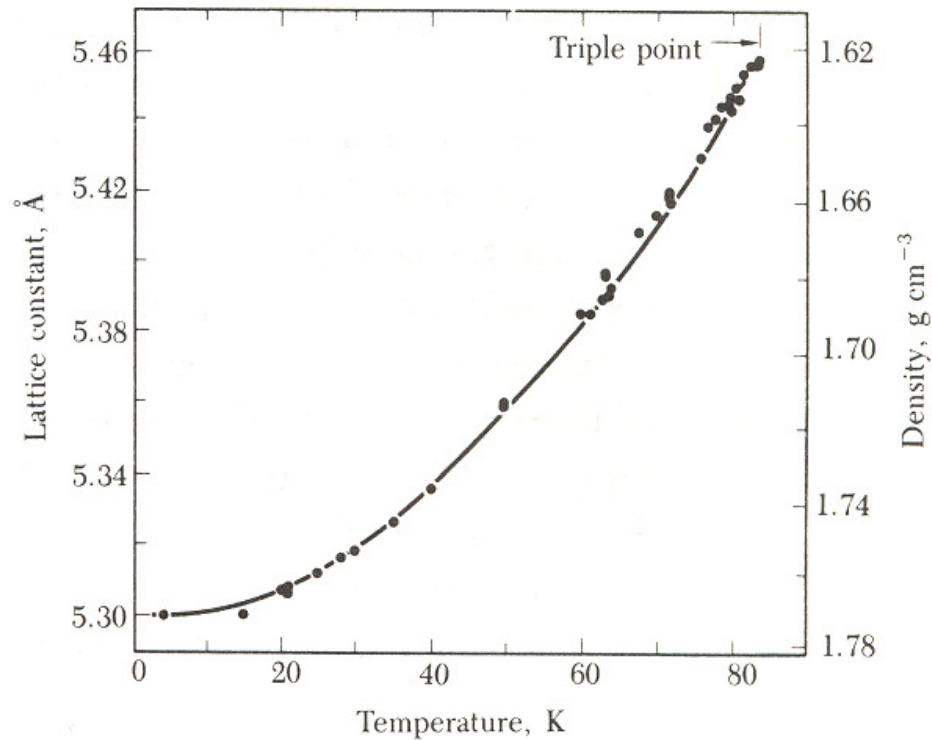
Why this form? On the next slide you can see that this function is a reasonable model for the kind of  $U(r)$  we have discussed for molecules and solids.

**Potential Energy of Anharmonic Oscillator**  
**( $c = 1$   $g = c/10$   $f = c/100$ )**



Do you know what  
form to expect for  
 $\langle x \rangle$  based on  
experiment?

# Lattice Constant of Ar Crystal vs. Temperature



Above about 40 K, we see:  $a(T) - a(0) \propto \langle x \rangle \propto T$

Usually we write:  $L = L_0(1 + \alpha[T - T_0])$   $\alpha$  = thermal expansion coefficient