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Problem #2
Stat Therm
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2.1 n_i = number of interstial sites
n_ℓ = number of lattice sites
$n_a = N$ = number of atoms
n_s = number of schottky defects (# vacancies in lattice)
n_b = number of atoms in interstial sites

$n_i = n_\ell = 2n_a = 2N$
$n_s = n_b$ - given

the number of atoms in interstitial sites equals the number of vacancies in the lattice

$E_s = E_a + \epsilon$
$E_i = E_a + \epsilon$

E_a = energy of atom in lattice
E_s = energy of Schottky defect atom
E_i = energy of atom in interstitial site

$$\Omega(n_s) = \binom{N}{n_s} \qquad \Omega(n_i) = \binom{N}{n_i}$$

$$\Omega(n_s + n_i) = \binom{N}{n_s}\binom{N}{n_i} = \left[\binom{N}{n}\right]^2 = \Omega(n)$$

$E = n\epsilon = (n_i + n_s)\epsilon$ energy associated with Schottky defects + interstitical sites

entropy

$$S(n) = k \ln \Omega(n) = k \ln \Omega(n_s + n_i)$$

$$S(n) = k \ln \left(\frac{N!}{n_s!(N-n_s)!}\right)\left(\frac{N!}{n_i!(N-n_i)!}\right)$$

$$S(n) = k\left(\ln N!^2 - \ln n_s! - \ln(N-n_s)! - \ln n_i! - \ln(N-n_i)!\right)$$

$$S(n) = k\{2N \ln N - 2N - n_s \ln n_s + n_s - (N-n_s)\ln(N-n_s)$$
$$+ (N-n_s) - n_i \ln n_i + n_i - (N-n_i)\ln(N-n_i) - (N-n_i)\}$$

$$S(n) = k\{2N \ln N - n_i \ln n_i - n_s \ln n_s - (N-n_i)\ln(N-n_i) - (N-n_s)\ln(N-n_s)\}$$

for $n_i = n_s$

$$S(n) = k\{2N\ln N - 2n\ln n - 2(N-n)\ln(N-n)\}$$

$$\frac{n}{N} = \frac{1}{e^{\varepsilon/kT}+1}$$

$$S(n) = k\{2N\ln N - 2N(e^{\varepsilon/kT}+1)^{-1}(\ln N(e^{\varepsilon/kT}+1)^{-1})$$
$$- 2N(1-(e^{\varepsilon/kT}+1)^{-1})\ln N(1-(e^{\varepsilon/kT}+1)^{-1})\}$$

$T \to 0 \quad n \to 0$

$$S(n, T=0) = k\{2N\ln N - 0 - 2N\ln N\} = 0$$

as $kT \gg \varepsilon \qquad \frac{n}{N} \to \frac{1}{e^0+1} = \frac{1}{2}$

$$S(n, kT\gg\varepsilon) = k\{2N\ln N - 2N(\tfrac{1}{2})\ln(N/2)$$
$$- 2(N/2)\ln(N/2)\}$$
$$= k\{2N\ln N - 2N\ln(N/2)\} = 2Nk(\ln N - \ln(N/2))$$
$$= 2Nk\ln\left(\frac{N}{N/2}\right) = 2Nk\ln 2$$

for $\varepsilon = 1\text{eV}$ $\quad T = 300K \quad n/N \sim e^{-20}$ are in interstitial sites

$n/N \sim e^{-20}$

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2.2 N weakly interacting sys

$$\bar{E} = nE_1 + (N-n)E_2$$

$$= NE_1(e^{E_1/kT}+1)^{-1} + E_2 - E_2(e^{E_2/kT}+1)^{-1}$$

$E_2 \to 0$ convenience $E_1 \to \varepsilon$

$$\bar{E} = \frac{N\varepsilon}{e^{\beta\varepsilon}+1} = \frac{Nz}{\beta(e^z+1)} \qquad \frac{\partial \bar{E}}{\partial T} = \frac{\partial \bar{E}}{\partial z}\frac{\partial z}{\partial \beta}\frac{\partial \beta}{\partial T}$$

$$\frac{\partial \beta}{\partial T} = \frac{-1}{kT^2}$$

$$\frac{\partial z}{\partial \beta} = \varepsilon$$

$$C = \frac{\partial \bar{E}}{\partial T} = \frac{N k z^2 e^z}{(e^z+1)^2} \qquad z = \beta\varepsilon$$

$$\frac{\partial \bar{E}}{\partial z} = \frac{N}{\beta(e^z+1)} + \frac{Nz}{\beta(e^z+1)^2}$$

$$= \frac{N(e^z+1+z)}{\beta(e^z+1)^2}$$

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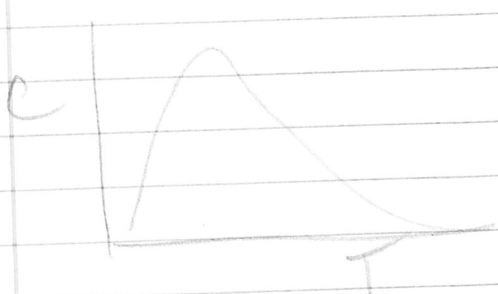

2.3 A system has $E_1 = \varepsilon$ $E_2 = 2\varepsilon$ $E_3 = 3\varepsilon$ $\Rightarrow E_1 = 0$ $E_2 = \varepsilon$ $E_3 = 2\varepsilon$

$g(E_1) = g(E_3) = 1$ $g(E_2) = 2$

find heat capacity

$$Z = \sum_{E_r} g(E_r) e^{-\beta E_r} = e^{0} + 2e^{-\beta\varepsilon} + e^{-2\beta\varepsilon}$$

$$\bar{E} = -\frac{\partial \ln Z}{\partial \beta} = \frac{1}{Z}\frac{\partial Z}{\partial \beta} = \frac{1}{Z}\overbrace{\left(-2\varepsilon e^{-\beta\varepsilon} - 2\varepsilon e^{-2\beta}\right)}^{dZ/d\beta}$$

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$$C_v = \left(\frac{\partial \bar{E}}{\partial T}\right)_v = \frac{\partial \bar{E}}{\partial \beta}\frac{\partial \beta}{\partial T} \qquad \frac{\partial \beta}{\partial T} = \frac{\partial}{\partial T}\frac{1}{KT} = \frac{-1}{KT^2}$$

2.29 $C_v = \frac{+1}{KT^2}\frac{\partial^2 \ln Z}{\partial \beta^2} =$

$$= \frac{1}{KT^2}\frac{\partial}{\partial \beta}\frac{1}{Z}\left(2\varepsilon e^{-\beta\varepsilon} + 2\varepsilon e^{-2\beta\varepsilon}\right) = \frac{2\varepsilon}{KT^2}\frac{\partial}{\partial \beta}\frac{1}{Z}\left(e^{-\beta\varepsilon} + e^{-2\beta\varepsilon}\right)$$

$$= \frac{2\varepsilon}{KT^2}\left\{\frac{-1}{Z^2}\left(e^{-\beta\varepsilon} + e^{-2\beta\varepsilon}\right) + \frac{2\varepsilon}{KT^2}\frac{1}{Z}\left(-\varepsilon e^{-\beta\varepsilon} - 2\varepsilon e^{-2\beta\varepsilon}\right)\right\}$$

$$= \frac{2\varepsilon}{KT Z^2}\left\{-e^{-\beta\varepsilon} + e^{-2\beta\varepsilon} + Z\left(-\varepsilon e^{-\beta\varepsilon} - 2\varepsilon e^{-2\beta\varepsilon}\right)\right\}$$

algebra ...

$$C = 2k\frac{x^2 e^x}{(e^x+1)^2} \qquad x = \beta\varepsilon$$

2.6 $E_1 = 19.82\,eV$

$$kT = \frac{1.38\cdot 10^{-23}\,J}{K}\left(\frac{1\,eV}{1.6\cdot 10^{-19}\,J}\right)10{,}000\,K = .8625\,eV$$

$$\frac{(3n)}{N} = 3\left(\frac{1}{e^{E/kT}+1}\right) = 3\left(\frac{1}{e^{22.9797}+1}\right) = 3.1\cdot 10^{-10}$$

2.5 $E_r = \hbar\omega(r+\tfrac{1}{2}) \quad r = 0, 1, 2, \ldots$

$\hbar\omega = .3\,eV$

$T = 1000\,K$

$$\frac{n_1}{n_0} = \frac{n_1/N}{n_0/N} = \frac{\varepsilon_1\left(e^{\varepsilon_1/kT}+1\right)^{-1}}{\varepsilon_0\left(e^{\varepsilon_0/kT}+1\right)^{-1}} = e^{-\beta\hbar\omega} = 0.03$$

Kittel + Kroemer

1. Entropy + Temperature   Given $g(U) = CU^{3N/2}$

a) Show that $U = 3/2\, N\tau$

$$\sigma(N,U) = \ln CU^{3N/2} = \ln C + \frac{3N}{2}\ln U$$

$$\tau^{-1}\left(\frac{\partial\sigma}{\partial U}\right)_N = \frac{3N}{2U} \Rightarrow U = \frac{3}{2}N\tau$$

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b) Show that $(\partial^2\sigma/\partial U^2)_N$ is negative

$$\left(\frac{\partial^2\sigma}{\partial U^2}\right)_N = \frac{\partial}{\partial U}\left(\frac{1}{\tau}\right) = \frac{\partial}{\partial U}\left(\frac{3N}{2U}\right) = -\frac{3N}{2U^2}$$

Since $N > 0$ and $U^2 > 0$, $\frac{3N}{2U^2} < 0$ $\therefore \left(\frac{\partial^2\sigma}{\partial U^2}\right)_N < 0$

2.3 Quantum Harmonic Oscillator

a) Find entropy of a set of N oscillators of frequency ω as a function of the total quantum number n.

Start with the multiplicity function of Ch. 1:

$$g(N,n) = \frac{(N+n+1)!}{n!(N-1)!} \sim \frac{(N+n)!}{n!N!}$$

find entropy

$$\sigma(N,n) = \ln(g(N,n)) \sim \ln(N+n)! - \ln n! - \ln N!$$

Use Stirling's approximation

$$\sigma(N,n) \sim (N+n)\ln(N+n) - (N+n) - n\ln n + n - N\ln N + N$$

$$\sigma(N,n) \sim (n+N)\ln(N+n) - n\ln n - N\ln N$$

b) Let $U = n\hbar\omega$ the total energy of the N oscillators

$$\sigma(N,U) = (N + U/\hbar\omega)\ln(N + U/\hbar\omega) - \frac{U}{\hbar\omega}\ln(U/\hbar\omega) - N\ln N$$

Solve for total energy U at temperature τ

$$\tau^{-1} = (\partial\sigma/\partial U)_N = \frac{1}{\hbar\omega}\ln(N + U/\hbar\omega) + \left(\frac{N+U/\hbar\omega}{N+U/\hbar\omega}\right)1/\hbar\omega - \frac{1}{\hbar\omega}\ln U/\hbar\omega - \left(\frac{U/\hbar\omega}{U/\hbar\omega}\right)\frac{1}{\hbar\omega}$$

$$\tau^{-1} = \frac{1}{\hbar\omega}\ln(N + U/\hbar\omega) - \frac{1}{\hbar\omega}\ln U/\hbar\omega$$

$$\hbar\omega\tau^{-1} = \ln(\hbar\omega N/U + 1)$$

$$e^{\hbar\omega/\tau} = \hbar\omega N/U + 1 \Rightarrow \hbar\omega N/U = e^{\hbar\omega/\tau} - 1$$

$$\Rightarrow U = \hbar\omega N(e^{\hbar\omega/\tau} - 1)^{-1}$$ (the Planck result)

4 The meaning of "never"

10^{18} s = age of universe

Suppose 10^{10} monkeys type 10 keys per second for 10^{18} s

typewriters have 44 keys

Hamlet has 10^5 characters

a) Probability of any sequence of $m = 10^5$ char

$P(\text{sequence } 10^m) = (1/x)(1/x)\cdots(1/x) = (1/x)^m$

independent probabilities are product of x keys

$P(\text{sequence}) = (1/x)^m = 10^{\log_{10}(1/x)^m} = 10^{\log_{10} x^{-m}} = 10^{-m \log_{10} x}$

$$P = \left(\frac{1}{44}\right)^{10^5} = \left(\frac{1}{44}\right)^{100{,}000} = 10^{-10^5 \log 44} = 10^{-164{,}345}$$

because $\log_{10}(44) = 1.64345$

b) Show that the probability that a monkey-Hamlet will be typed in the age of the universe is approximately $10^{-164316}$

total number of possible books $= 44^m = 44^{10^5} = 10^{164345}$

books 10^{10} monkeys can type in 10^{18} s at 10^5 char / 10 char^{-1} $= 10^4$ s per book is

$$\left(\frac{N_{book}}{monkey}\right) = 10^5 \frac{10^8}{(10^4 \text{ s per book})} = 10^{19} \text{ unique sequences of } 10^5 \text{ char}$$

the factor is because the sequence of Hamlet can start at any character, not just at an integral book

$$N_{books} = N_{monkey}\left(\frac{N_{book}}{monkey}\right) = 10^{10} \text{ monkey} \left(\frac{10^{9} \text{ book}}{monkey}\right) = 10^{29} \text{ books}$$

$$\text{Probability} = \frac{\#\text{ books produced}}{\#\text{ possible books}} = \frac{10^{29} \text{ books}}{10^{164345} \text{ books}} = 10^{-164316}$$