Consider a 2-D metal. It has two distinct freedoms: the conduction electrons and the lattice vibrations, i.e. phonons. Assume that the particles are confined to move within the plane, so there are only two dimensions in which the phonons or electrons can propagate and there are only 2 possible phonon polarizations.

Answer the following questions.

1. **Partition Functions**

a.) What is the Partition Function of one of the electron states, in terms of e_{e-s} (electron state energy) m, and b (i.e. 1/kT)?

$$Z_{e-s} = \sum_{n=0}^{n=1} e^{-n(e_{e-s}-m)b} = e^{-0(e_{e-s}-m)b} + e^{-1(e_{e-s}-m)b} = 1 + e^{-(e_{e-s}-m)b}$$

b.) What is the Partition Function of one of the phonon states, in terms of e_{p-s} (phonon state energy) and b (i.e. 1/kT)? Recall, $\sum_{n=0}^{\infty} x^n = \frac{1}{1-x}$ for x < 1.

$$Z_{ph-s} = \sum_{n=0}^{n=\infty} e^{-n(e_{eh-s}-m)b} = \sum_{n=0}^{n=\infty}\left(e^{-(e_{eh-s}-m)b}\right)^n = \frac{1}{1-e^{-(e_{eh-s}-m)b}}$$

2. **Average Occupancy**

c.) What is the average occupancy of one of the electron states, in terms of e_{e-s} (electron state energy) m, and b (i.e. 1/kT)?

$$\bar{n}_{e-s} = \sum_{n=0}^{n=1} n_{e-s}\frac{e^{-n(e_{e-s}-m)b}}{Z_{e-s}} = \frac{\sum_{n=0}^{n=1} n_{e-s}e^{-n(e_{e-s}-m)b}}{1+e^{-(e_{e-s}-m)b}}$$

$$\bar{n}_{e-s} = \frac{0e^{-0(e_{e-s}-m)b} + 1e^{-1(e_{e-s}-m)b}}{1+e^{-(e_{e-s}-m)b}} = \frac{e^{-(e_{e-s}-m)b}}{1+e^{-(e_{e-s}-m)b}} = \frac{1}{e^{(e_{e-s}-m)b}+1}$$

d.) What is the average occupancy of one of the phonon states, in terms of e_{p-s} (phonon state energy) and b (i.e. 1/kT)?

$$\bar{n}_{ph-s} = \sum_{n=0}^{n=1} n\frac{e^{-n(e_{ph-s}-m)b}}{Z_{ph-s}} = -\frac{1}{Z_{ph-s}}\frac{\partial Z_{ph-s}}{\partial((e_{e-s}-m)b)} = \left(1-e^{-(e_{eh-s}-m)b}\right)\frac{e^{-(e_{eh-s}-m)b}}{\left(1-e^{-(e_{eh-s}-m)b}\right)^2}$$

$$\bar{n}_{ph-s} = \frac{1}{e^{(e_{eh-s}-m)b}-1} = \frac{1}{e^{e_{eh-s}b}-1}$$

But, for phonons, there is no chemical potential, μ=0.

3. **Density of States**

e.) What is the density of states for the electrons, $g_e(e)$, in terms of m, L, h and possibly e?

$$g_e(e) = \frac{n_{e-sw/e}}{de} = n_{spin}\frac{A_{p.w/e}\ /\Delta A_p}{de} = n_{spin}\frac{\frac{1}{4}2ppdp/(h/2L)^2}{de} = n_{spin}\frac{pdp^2/(h/L)^2}{de}$$

The area (since it's a 2-D system) in momentum space with the same energy is that with the same magnitude of momentum, i.e., the area of an annulus of width dp. Since I'm considering standing waves, I'm confined to the positive quadrant, thus the factor of ¼.

Given non-relativistic electrons, $p^2 = 2me$, also, being electrons, there are 2 spin options.

$$g_e(e) = 2\frac{p\,2mde\ /(h/L)^2}{de} = 4pm\left(\frac{L}{h}\right)^2$$

f.) What is the density of states for the phonons, $g_p(e)$, in terms of c_s (wave speed), *L*, *h* and possibly *e*?

$$g_{ph}(e) = \frac{n_{ph-sw/e}}{de} = n_{polarizations}\frac{A_{p.w/e}\ /\Delta A_p}{de} = n_{pol}\frac{\frac{1}{4}2ppdp/(h/2L)^2}{de}$$

Everything's the same as above, including there being 2 polarizations (analogous to spins for the electrons) but now the energy – momentum relationship is $e = pc_s$

$$g_{ph}(e) = 2\frac{2pede\ /(hc_s/L)^2}{de} = 4p\left(\frac{L}{hc_s}\right)^2 e$$

4. **Energy Scales**

g.) What is the Fermi Energy of the electrons, e_F?

$$N = \int_0^{e_F} g_e(e)de = 4pm\left(\frac{L}{h}\right)^2 e_F \Rightarrow e_F = \frac{N}{4pm}\left(\frac{h}{L}\right)^2$$

h.) What is the Debey Energy of the phonons, $e_D = kT_D$?

$$2N = \int_0^{e_D} g_{ph}(e)de = 2p\left(\frac{L}{hc_s}\right)^2 e_D^2 \Rightarrow e_D = \frac{hc_s}{L}\sqrt{pN}$$

i.) Re-express $g_e(e)$ and $g_p(e)$ in terms of e_F and e_D, respectively.

$$g_e(e) = \frac{N}{e_F} \qquad g_{ph}(e) = 4\frac{N}{e_D^2}e$$

5. **Thermal Energy**

j.) *Set up* the general integrals for the thermal energy of the Phonons and of the electrons, U_p and U_e. For the electrons, by making the substitution

$e = (e - m) + m$ in the numerator, you can rewrite your integral as two integrals. Now, you can get your integrals for U_p and U_e in terms of an appropriate variable of integration, x.

$$U_{ph} = \int_0^{e_D} e g_{ph}(e)\bar{n}_{ph} de = \int_0^{e_D} e 4\frac{N}{e_D^2} e \frac{1}{e^{eb}-1} de = 4\frac{N}{e_D^2}\int_0^{e_D} \frac{e^2}{e^{eb}-1} de = 4\frac{N}{e_D^2}\frac{1}{b^3}\int_0^{T_D/T}\frac{x^2}{e^x-1}dx$$

$$4\frac{N}{e_D^2}(kT)^3\int_0^{T_D/T}\frac{x^2}{e^x-1}dx$$

$$U_e = \int_0^{\infty} e g_e(e)\bar{n}_e de = \int_0^{\infty} e \frac{N}{e_F}\frac{1}{e^{(e-m)b}+1} de = \frac{N}{e_F}\int_0^{\infty}\frac{e}{e^{(e-m)b}+1} de$$

$$= \frac{N}{e_F}\left(\int_0^{\infty}\frac{e-m}{e^{(e-m)b}+1}de + \int_0^{\infty}\frac{m}{e^{(e-m)b}+1}de\right) = \frac{N}{e_F}\left(\frac{1}{b^2}\int_{-mb}^{\infty}\frac{x}{e^x+1}dx + \frac{m}{b}\int_{-mb}^{\infty}\frac{1}{e^x+1}dx\right)$$

$$= \frac{N}{e_F}\left((kT)^2\int_{-mb}^{\infty}\frac{x}{e^x+1}dx + mkT\int_{-mb}^{\infty}\frac{1}{e^x+1}dx\right)$$

For the next two parts, the following facts may be useful.

$$\int_{x_{min}}^{x_{max}}\frac{1}{e^x+1}dx = -\ln\left(1+e^{-x}\right)\Big|_{x_{min}}^{x_{max}}$$

$$\int_{x_{min}}^{x_{max}}\frac{x^n}{e^x+1}dx = \frac{1}{n+1}\frac{x^{n+1}}{e^x+1}\Bigg|_{x_{min}}^{x_{max}} + \frac{1}{n+1}\int_{x_{min}}^{x_{max}}\frac{x^{n+1}e^x}{\left(e^x+1\right)^2}dx = \frac{1}{n+1}\frac{x^{n+1}}{e^x+1}\Bigg|_{x_{min}}^{x_{max}} + \frac{1}{n+1}\int_{x_{min}}^{x_{max}}\frac{x^{n+1}}{\left(e^{x/2}+e^{-x/2}\right)^2}dx$$

$$\int_0^{\infty}\frac{x}{e^x+1}dx = \frac{p^2}{12} \qquad \int_0^{\infty}\frac{x}{e^x-1}dx = \frac{p^2}{6}$$

$$\int_0^{\infty}\frac{x^2}{e^x+1}dx = 1.803 \qquad \int_0^{\infty}\frac{x^2}{e^x-1}dx = 2.404$$

$$\int_0^{\infty}\frac{x^3}{e^x+1}dx = \frac{7}{8}\frac{p^4}{15} \qquad \int_0^{\infty}\frac{x^3}{e^x-1}dx = \frac{p^4}{15}$$

k.) Low T limit: Evaluate the thermal energies (U_p and U_e) in the low T limit. (not when T=0 mind you, just when it's small).

$$U_{ph} = 4\frac{N}{e_D^2}(kT)^3\int_0^{T_D/T}\frac{x^2}{e^x-1}dx$$

In this limit, the upper limit of integration, T_D/T>>1, but the denominator of the integrand will kill of the integrand well before it reaches T_D/T, so I am free to extend the integration up to infinity without much changing the outcome.

$$U_{ph_{lowT}} \approx 4\frac{N}{e_D^2}(kT)^3\int_0^\infty \frac{x^2}{e^x-1}dx = 4\frac{N}{e_D^2}(kT)^3 2.404 = 4.808\frac{N}{e_D^2}(kT)^3$$

$$U_e = \frac{N}{e_F}\left((kT)^2\int_{-mb}^{\infty}\frac{x}{e^x+1}dx + mkT\int_{-mb}^{\infty}\frac{1}{e^x+1}dx\right)$$

The second integral can be done without any approximation, using

$$\int_{-mb}^{\infty}\frac{1}{e^x+1}dx = -\ln\left(1+e^{-x}\right)\Big|_{-mb}^{\infty} = \ln\left(1+e^{mb}\right)$$

The first integral must be approximated. Integrating the first integral by parts, $\left(\int udv = uv\big| - \int vdu\right)$ where $u = \frac{1}{e^x+1} \Rightarrow du = -\frac{e^x}{\left(e^x+1\right)^2}dx$ and $dv = xdx \Rightarrow v = \frac{1}{2}x^2$ so,

by parts gives

$$\int_{-mb}^{\infty}\frac{x}{e^x+1}dx = \frac{1}{2}\frac{x^2}{e^x+1}\Big|_{-mb}^{\infty} + \frac{1}{2}\int_{-mb}^{\infty}\frac{x^2e^x}{\left(e^x+1\right)^2}dx = -\frac{1}{2}\frac{(mb)^2}{e^{-mb}+1} + \frac{1}{2}\int_{-mb}^{\infty}\frac{x^2e^x}{\left(e^x+1\right)^2}dx.$$

In the low temperature limit, $mb >> 1$, furthermore, the integrand dies off very quickly for x far from 1, so, we can set the lower limit of integration equal to –infinity without significantly changing the result.

$$\int_{-mb}^{\infty}\frac{x}{e^x+1}dx \approx -\frac{1}{2}\frac{(mb)^2}{e^{-mb}+1} + \frac{1}{2}\int_{-\infty}^{\infty}\frac{x^2e^x}{\left(e^x+1\right)^2}dx$$

Now, this is an even integral running over symmetric limits, so

$$\int_{-mb}^{\infty}\frac{x}{e^x+1}dx \approx -\frac{1}{2}\frac{(mb)^2}{e^{-mb}+1} + \int_0^{\infty}\frac{x^2e^x}{\left(e^x+1\right)^2}dx$$

Finally, integrating by parts *back* again gives

$$\int_{-mb}^{\infty}\frac{x}{e^x+1}dx \approx -\frac{1}{2}\frac{(mb)^2}{e^{-mb}+1} + 2\int_0^{\infty}\frac{x}{e^x+1}dx - \frac{x^2}{e^x+1}\Big|_0^{\infty} = -\frac{1}{2}\frac{(mb)^2}{e^{-mb}+1} + 2\frac{p^2}{12} + 0$$

Putting these all together gives

$$U_e = \frac{N}{e_F}\left((kT)^2\left(-\frac{1}{2}\frac{(mb)^2}{e^{-mb}+1} + 2\frac{p^2}{12}\right) + mkT\ln\left(1+e^{mb}\right)\right)$$

$$U_e = \frac{N}{e_F}\left(-\frac{1}{2}\frac{(m)^2}{e^{-mb}+1} + (kT)^2\frac{p^2}{6} + mkT\ln\left(1+e^{mb}\right)\right)$$

Substituting $m = kT\ln\left(e^{e_F/kT}-1\right)$

$$U_e = \frac{N}{e_F}\left(-\frac{1}{2}(kT)^2\left(1-e^{-e_Fb}\right)\left(\ln\left(e^{e_Fb}-1\right)\right)^2 + (kT)^2\frac{p^2}{6} + e_FkT\ln\left(e^{e_Fb}-1\right)\right)$$

at low T, $U_e \approx \frac{N}{e_F}\left(\frac{1}{2}\left(1+e^{-e_Fb}\right)(e_F)^2 + (kT)^2\frac{p^2}{6}\right)$

l.) One of the two integrals in your U_e expression can be analytically solved. This is evident if you do a second change of variables $y = e^{-x}$ Low T Limit: Evaluate the integrals in the low temperature limitWithout actually evaluating these integrals, take the appropriate derivative to get the integrals for heat capacity.

$$C_{ph} = \frac{\partial U_{ph}}{\partial T} = \frac{\partial}{\partial T}\left(4\frac{N}{e_D^2}\int_0^{e_D} \frac{e^2}{e^{eb}-1} de \right) = 4\frac{N}{e_D^2}\int_0^{e_D} \frac{\partial}{\partial T}\left(\frac{e^2}{e^{eb}-1}\right) de = 4\frac{N}{e_D^2}\frac{1}{kT^2}\int_0^{e_D} \frac{e^3 e^{eb}}{\left(e^{eb}-1\right)^2} de$$

$$C_e = \frac{\partial U_e}{\partial T} = \frac{\partial}{\partial T}\left(\frac{N}{e_F}\int_0^{\infty} \frac{e}{e^{(e-m)b}+1} de \right) = \frac{N}{e_F}\int_0^{\infty} \frac{\partial}{\partial T}\left(\frac{e}{e^{(e-m)b}+1}\right) de = \frac{N}{e_F}\frac{1}{kT^2}\int_0^{\infty} \frac{e(e-m)e^{(e-m)b}}{\left(e^{(e-m)b}+1\right)^2} de$$

a. Use $e = (e-m)+m$, rewrite the $C_{v\text{-}e}$ integral first as two integrals, and then change variables to $x = (e-m)b$. Similarly, change variables for the phonons' integral.

$$C_{ph} = 4\frac{N}{e_D^2}\frac{1}{kT^2}\frac{1}{b^4}\int_0^{T_D/T} \frac{x^3 e^x}{\left(e^x-1\right)^2} dx = 4\frac{N}{e_D^2}k^3T^2\int_0^{T_D/T} \frac{x^3 e^x}{\left(e^x-1\right)^2} dx$$

$$C_e = \frac{N}{e_F}\frac{1}{kT^2}\int_0^{\infty} \frac{e(e-m)e^{(e-m)b}}{\left(e^{(e-m)b}+1\right)^2} de =$$

$$C_e = \frac{N}{e_F}\frac{1}{kT^2}\left(\int_0^{\infty} \frac{(e-m)(e-m)e^{(e-m)b}}{\left(e^{(e-m)b}+1\right)^2} de + \int_0^{\infty} \frac{(m)(e-m)e^{(e-m)b}}{\left(e^{(e-m)b}+1\right)^2} de \right)$$

$$C_e = \frac{N}{e_F}\frac{1}{kT^2}\left(\frac{1}{b^3}\int_{-mb}^{\infty} \frac{x^2 e^x}{\left(e^x+1\right)^2} dx + \frac{1}{b^2} m \int_{-mb}^{\infty} \frac{x e^x}{\left(e^x+1\right)^2} dx \right)$$

$$C_e = \frac{N}{e_F}k\left(kT\int_{-mb}^{\infty} \frac{x^2 e^x}{\left(e^x+1\right)^2} dx + m\int_{-mb}^{\infty} \frac{x e^x}{\left(e^x+1\right)^2} dx \right)$$

$$U = \frac{N}{e_F}\int_0^{\infty} \frac{e\,de}{e^{(e-m)b}+1}$$

$$C_V = \frac{1}{kT^2}\frac{N}{e_F}\int_0^{\infty} \frac{e(e-m)e^{(e-m)b}de}{\left(e^{(e-m)b}+1\right)^2} = \frac{1}{kT^2}\frac{N}{e_F}\left(\int_0^{\infty} \frac{(e-m)^2 e^{(e-m)b}de}{\left(e^{(e-m)b}+1\right)^2} + m\int_0^{\infty} \frac{(e-m)e^{(e-m)b}de}{\left(e^{(e-m)b}+1\right)^2} \right)$$

$$= \frac{1}{kT^2}\frac{N}{e_F}\left((kT)^3 \int_{-mb}^{\infty} \frac{x^2 e^x dx}{\left(e^x+1\right)^2} + (kT)^2 m \int_{-mb}^{\infty} \frac{x e^x dx}{\left(e^x+1\right)^2} \right)$$

$$= \frac{1}{kT^2}\frac{N}{e_F}\left((kT)^3 \left(\left.\frac{-\frac{1}{2}x^2}{\left(e^x+1\right)}\right|_{-mb}^{\infty} + \int_{-mb}^{\infty} \frac{x\,dx}{\left(e^x+1\right)} \right) + (kT)^2 m \left(\left.\frac{-\frac{1}{2}x}{\left(e^x+1\right)}\right|_{-mb}^{\infty} + \frac{1}{2}\int_{-mb}^{\infty} \frac{dx}{\left(e^x+1\right)} \right) \right)$$