PHYS 4P70 Equations

Constants

$\hbar = 6.61 \times 10^{-16}$ eV-s	$h = 6.64 \times 10^{-34}$Js	$c = 2.998 \times 10^{8}$m/s
$\mu_B = 9.27 \times 10^{-24}$J/T	$hc = 1239$eV-nm	$m = 0.511$MeV/c^2
$k_B = 1.38 \times 10^{-23}$J/K	$k_B = 8.61 \times 10^{-5}$eV/K	$e = 1.602 \times 10^{-19}$C
$N_A = 6.02 \times 10^{23}$mol^{-1}	$N_A k_B = R$=8.314 J/mol K	
hc= 1239 eV-nm	$m_e c^2 = 0.511$ MeV	$m_p c^2 \approx m_n c^2 \approx 940$MeV

Quantum Mechanics

$p = \frac{h}{\lambda} \qquad E = \hbar\omega \qquad k = \frac{2\pi}{\lambda} \qquad v_g = \frac{d\omega}{dk} \qquad v = \omega/k$

$E^2 = (pc)^2 + (mc^2)^2 \qquad \vec{p} = \hbar\vec{k} \qquad g(\vec{k}) = 2 * \left(\frac{L}{2\pi}\right)^D \qquad E_k = \frac{\hbar^2 k^2}{2m}$

$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) + V(\vec{r})\psi(\vec{r}) = E\psi(\vec{r})$

$E_n = \frac{\hbar^2}{2m}(\frac{2\pi n}{L})^2 \qquad E_n = \hbar\omega_o(n + \frac{1}{2})$

Thermodynamics, Statistical Mechanics

$dU = đQ - đW \qquad dU = TdS - pdV \qquad H = U + PV \qquad PV = Nk_BT = nRT$

$C_v = \left(\frac{\partial U}{\partial T}\right)_V \qquad C_p = \left(\frac{\partial H}{\partial T}\right)_P$

$S = k_B \ln g \qquad Z = \sum_i g_i e^{-E_i/k_BT} \qquad Z = \frac{1}{h^3}\int\int\left[e^{-E(\vec{x},\vec{p})/k_BT}\right]d^3x d^3p$

$P(E) = \frac{g(E)e^{-E/k_BT}}{Z} \qquad < E >= \frac{k_BT^2}{Z}\left(\frac{\partial Z}{\partial T}\right)_V$

$f_{FD}(\epsilon,\mu,T) = \frac{1}{e^{\frac{(\epsilon-\mu)}{k_BT}}+1} \qquad f_{BE}(\epsilon,\mu,T) = \frac{1}{e^{\frac{(\epsilon-\mu)}{k_BT}}-1} \qquad f_{MB}(\epsilon,\mu,T) = e^{\frac{(\mu-\epsilon)}{k_BT}}$

$n_Q \approx 1/\lambda_T^3 \qquad \lambda_T = \sqrt{\frac{h^2}{3mk_BT}}$

Free Electron Gas

$g(\epsilon) = \frac{dN}{d\epsilon} = \frac{dN}{dk}\frac{dk}{d\epsilon} \qquad g(\vec{k}) = 2 * \left(\frac{L}{2\pi}\right)^D \qquad N = \int_0^\infty g(\epsilon)f(\epsilon)d\epsilon$

$N = \int\left(\frac{L}{2\pi}\right)^D d^Dk \qquad E = \int_0^\infty \epsilon g(\epsilon)f(\epsilon)d\epsilon \qquad E = \int 2\left(\frac{L}{2\pi}\right)^D \frac{\hbar^2k^2}{2m}d^Dk$

$\vec{J} = \sigma\vec{E} \qquad \vec{J} = ne\vec{v}_d \qquad \sigma = \frac{ne^2\tau}{m} = \frac{1}{\rho} \qquad R = \frac{\rho L}{A} \qquad R_H = \frac{1}{ne} \qquad V_H = \frac{IB}{nqt}$

Crystal Structure

$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3 \qquad V = \vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3$$

structure	lattice	basis
sc	$a\hat{x}, a\hat{y}, a\hat{z}$	
bcc	$\frac{a}{2}(-1,1,1);\ \frac{a}{2}(1,-1,1);\frac{a}{2}(1,1,-1)$	
bcc	sc	$(0,0,0); (\frac{1}{2},\frac{1}{2},\frac{1}{2})$
fcc	$\frac{a}{2}(0,1,1);\ \frac{a}{2}(1,0,1);\frac{a}{2}(1,1,0)$	
fcc	sc	$(0,0,0); (0,\frac{1}{2},\frac{1}{2}); (\frac{1}{2},0,\frac{1}{2}); (\frac{1}{2},\frac{1}{2},0)$
CsCl	sc	Cs (0,0,0); Cl $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
NaCl	fcc	Na (0,0,0); Cl $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
Diamond	fcc	C (0,0,0); C $(\frac{1}{4},\frac{1}{4},\frac{1}{4})$
ZnS (zincblende)	fcc	Zn (0,0,0); S $(\frac{1}{4},\frac{1}{4},\frac{1}{4})$
simple hexagonal (sh)	$\frac{a}{2}\hat{x} \pm \frac{\sqrt{3}a}{2}\hat{y}, c\hat{z}$	
hcp	sh	$(0,0,0); (a/2, a\sqrt{3}/6, c/2)$
simple tetragonal	$a\hat{x}, a\hat{y}, c\hat{z}$	
simple orthorhombic	$a\hat{x}, b\hat{y}, c\hat{z}$	

Reciprocal Lattice

$$\vec{b}_i = \left[\frac{2\pi}{\vec{a}_1\cdot\vec{a}_2\times\vec{a}_3}\right]\vec{a}_j\times\vec{a}_k \quad \vec{G} = h\vec{b}_1+k\vec{b}_2+l\vec{b}_3 \quad e^{\vec{G}\cdot\vec{R}} = 1 \quad \vec{a}_i\cdot\vec{b}_j = 2\pi\delta_{ij} \quad d = \frac{2\pi}{|\vec{G}|}$$

Diffraction

elastic: $2d\sin\theta = \lambda \qquad \vec{k}' = \vec{k} + \vec{G}$

$$S_{\vec{G}} = \sum_i f_i e^{-i\vec{G}\cdot\vec{r}_i} = S_{lattice} \times S_{basis} \qquad I_{hkl} \propto |S_{hkl}|^2 * multiplicity$$

xray : $f_i \approx Z_i \qquad E = hf = pc = \hbar kc$

neutron: $f_i \approx b_i \qquad E = \frac{p^2}{2m} = \frac{\hbar^2k^2}{2m}$

Lattice Vibrations

N2L for 1-D monatomic basis:

$$m\frac{d^2u[na]}{dt^2} = Cu[(n-1)a] - 2Cu[na] + Cu[(n+1)a]$$

$$u[na] = Ae^{i(kna-\omega t)}$$

$$\omega = \sqrt{\frac{4C}{L}}|\sin\frac{ka}{2}|$$

Inelastic Neutron Scattering:

$$\hbar\vec{q}' = \hbar\vec{q} \pm \hbar\vec{k} + \hbar\vec{G} \qquad \frac{\hbar^2 q'^2}{2m_n} = \frac{\hbar^2 q^2}{2m_n} \pm \hbar\omega(k)$$

Thermal Properties of vibrations:

$$E = (n+\frac{1}{2})\hbar\omega \qquad < n >= \frac{1}{e^{\frac{\hbar\omega}{kT}} - 1}$$

Einstein Model: $g(\omega) = 3N\delta(\omega - \omega_o)$

Density of k-values : $D_d = d\left(\frac{2\pi}{L}\right)^d$

$$g(\omega) = \frac{dN}{dk}\frac{dk}{d\omega}$$

Debye Model in 3D: $g(\omega) = \frac{3V}{2\pi^2}\frac{\omega^2}{v^3} \quad \theta_D = \frac{\hbar\omega_D}{k_B}$

$$E_{TOT} = \int_0^{\omega_D} g(\omega) < n > \hbar\omega \cdot d\omega$$