PH427 Periodic Systems – Review Topics

1. Coupled oscillators
   Eigenvalues (frequencies), normal modes (symmetric and anti-symmetric)

2. *N*-atom monatomic chain
   Equation of motion (Newton's 2^{nd}),
   Dispersion relation: $\omega(k) = 2\sqrt{\frac{\kappa}{m}}\sin\left(\frac{ka}{2}\right)$, periodicity in "*k*-space", Brillouin zone, existence and implication of maximum frequency, linear dispersion for *ka* << 1.

   Effect of boundary conditions: *k*-values of normal modes

   $$k_q = q\frac{\pi}{(N+1)a} \cong q\frac{\pi}{Na} \text{ for large } N,\ q = 1, 2, 3, \ldots,\ \omega(k_q) = 2\sqrt{\frac{\kappa}{m}}\sin\left(\frac{k_q a}{2}\right).$$

3. Diatomic chain

   Equations of motion (Newton's 2^{nd});
   Dispersion relation with two branches (optic and acoustic), halving of Brillouin zone compared with monatomic chain with same interatomic separation; energy gap, absorption of light by optic vibrations at $k \cong 0$, evanescent waves.

4. Density of states

   D(E) dE = dn = number of states in energy interval *dE* $\Rightarrow$ *D(E) = dn/dE* (in 1-dimension).
   $D(\omega)d\omega = dn$ = number of states in frequency interval $d\omega \Rightarrow D(\omega) = dn/d\omega$
   Calculate density of states for monatomic chain: $D(\omega) = \frac{2N}{\pi\omega_{\max}}\frac{1}{\sqrt{1-\left(\omega/\omega_{\max}\right)^2}}$.

5. Quantization of normal mode energies (amplitudes): phonons ("particles" with energy $E = \hbar\omega$ and momentum $p = \hbar k$); conservation of ω and *k* in physical processes

6. Thermal distribution function for phonons (Bose-Einstein distribution):

   $$f_{BE}(E,T) = \frac{1}{\exp\left(E/k_BT\right) - 1}.$$

7. Know how to set up integral calculations involving density of states and distribution function. For example, the total energy (for determining heat capacity):

$$E_{tot} = \int_0^{E_{\max}} E\, D(E)\, f_{BE}(E,T)\, dE\ ;$$

What approximations can be made at very low and very high temperature?

8. Electron in finite square well potential

Form of solutions to Schrodinger's equation (wave functions), i.e. oscillatory or exponentially decaying, even or odd solutions.

9. Band formation in linear chain of square well potentials

Observations from computer simulations, theoretical solution using Linear Combination of Atomic orbitals ($|\psi\rangle = \sum_1^N c_n |n\rangle$); derivation of band function in nearest neighbor approximation ($E(k) = \alpha + 2\beta \cos(ka)$).
Determination of quantized *k*-values for periodic boundary conditions ($k_q = q\frac{2\pi}{Na}\ \ q = 0,1,2,3,...$).

10. Interpretation of band structure: effective mass $m_{eff} = \hbar^2 \big/ \left(d^2E(k)/dk^2\right)$, meaning of negative effective mass, periodicity in *k*-space (Brillouin zone), electron (group) velocity $v_g = \frac{1}{\hbar}\frac{dE(k)}{dk}$.

11. Bloch theorem for a solution of Schrodinger's equation in a periodic potential:
$\psi_k(x+ma) = e^{imka}\psi_k(x)$. Example: $\psi_k(x) = \frac{1}{N^{1/2}}\sum_1^N e^{inka}\phi_n(x)$.

12. Metals, insulators and semiconductors

Fermi-Dirac distribution $f_{FD}(E,T)$ and relation of Fermi energy to energy bands (E_F in gap gives an insulator at $T = 0$; E_F in band gives a metal).

13. Density of states for free particle (useful for electrons in conduction band or holes and valence band of semiconductor).
In 3 dimensions (most important), density of states per unit volume is
$\overline{D}_{3D}(E) = \frac{\pi}{2}\left(\frac{8m}{h^2}\right)^{3/2}\sqrt{E}$. Know how to set up integrals to calculate carrier concentration, for example.

14. Semiconductor phenomena:
Doping with donors and acceptors, fundamental optical absorption and energy gap, direct and indirect gaps, p-n junctions (depletion layer, built-in field, recombination and generation currents, effective of applied potential, I-V characteristic of junction diode).