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**Physics 731** **HOMEWORK ASSIGNMENT #4** **Due: Oct. 3, 2006**
**deadline Oct. 5**

Read A&M, chap. 22. Skim chap. 21 and D&G 5.3.1 and 5.3.2.

**1**. A&M 22–1; you do not need to do part d, but note the result (and you will get the solution). Note that logarithms typically show up in borderline cases (marginality).

**2**. This problem shows how localized modes arise around defects. Calculate the eigenfrequency of a mass defect $M_0 \neq M$ in a linear chain at the position n=0 by invoking the ansatz

$$u(na) = u_0 \exp[-\kappa(\omega)\,|n|\,a - i\omega t]$$

for displacements; show that

$$\omega^2 = \omega_0^2/[(M_0/M)\{2-(M_0/M)\}],$$

where $\omega_0^2$ is defined in 5b. For $M_0 < M$, note that $\omega > \omega_0$, so above the band. This corresponds to localized vibrations. For $M_0 > M$, $\omega$ is in the band (and the formula suggests there is an unstable mode for $M_0 > 2M$ !?!).

**3**. A&M 22–3; to amplify and clarify the comments in class.

**4**. A&M 22–5, parts a, b, and c only. Hint for part a: Use the chain rule to show

$\partial\phi/\partial R_\mu = \phi' \partial R/\partial R_\mu = \phi' R_\mu/R$ etc. (where $R^2 = \Sigma_\mu R_\mu^2$),

and thence get $\phi_{\mu\nu} = \partial^2\phi/\partial R_\mu \partial R_\nu$ in eq. (22.11).

**5.** [Essentially Kittel (8th) 4–7]: Consider a simple model of soft phonon modes: Consider a line of ions of equal mass but alternating in charge, with $q_m = (-1)^m e$ as the charge on the m^th ion. Their interatomic potential is the sum of two contributions: 1) a short-range interaction of force constant $K_{1R} = \gamma$ that acts between nearest neighbors only, and 2) a Coulomb interaction between all ions.

a) Show that the contribution of the Coulomb interaction to the atomic force constants is $K_{mc} = 2\,(-1)^m e^2/m^3 a^3$, where $a$ is the equilibrium nearest-neighbor distance.

b) Using the general 1–D dispersion relation

$$\omega^2 = (2/M)\ \Sigma_{m\geq 1} K_m(1 - \cos mka)\ \text{[eqn. (22.90)]},$$

show that the dispersion relation for this specific system can be written as

$$\frac{\omega^2}{\omega_0^2} = \sin^2(ka/2) + \sigma\sum_{m=1}^{\infty}(-1)^m\left[1-\cos(mka)\right]/m^3,$$

where $\omega_0^2 = 4\gamma/M$ and $\sigma = e^2/\gamma a^3$.

c) Show that $\omega^2$ is negative (i.e. the mode is unstable, or "soft") at the zone boundary $ka = \pi$ if $\sigma > 0.475$ [i.e. $4/\{7\zeta(3)\}$, where $\zeta$ is the Riemann zeta function].

d) Show that the speed of sound at small ka is imaginary if $\sigma > 1/(2 \ln 2) \cong 0.721$.

**Problems 6-8 are NOT assigned this year!**

[6]. But you should play with this wonderful applet, shown in class!!
Using Phonon dispersion and display of TA and TO modes in 1D
`<http://dept.kent.edu/projects/ksuviz/leeviz/phonon/phonon.html>`
(or analytically), consider a diatomic chain. Set (on the applet screen) $ka = 0.5$ and set the mass ratio to 4. (Warning: the applet takes $a$ as the interatomic spacing, so half the lattice spacing $a$ used in class!)

a) Find the ratio of the amplitudes of the vibrations of the two atoms in i) the optical and ii) the acoustic branch.

b) What is the ratio of the period of the acoustic mode to that of the optical mode? For what value of $ka$ is this ratio about 2 (with mass ratio fixed at 4)?

[7]. A&M 22–2 is done succinctly in D&G, eqs. 5.3.11–5.3.13; β is the spring constant.

[8]. Solutions will also be provided to the following interesting classical problem: Consider a monatomic chain of N+1 atoms with interatomic separation $a$, as discussed in class. Supposed rather than periodic [B-vK] boundary conditions, we use fixed boundary conditions: $u(0) \equiv 0$ and $u(Na) \equiv 0$. What are the allowed independent values of $k$? How many are there? (Note that these solutions are standing waves rather than traveling waves.) Compare and reconcile your findings with those for periodic boundary conditions.

Look carefully at A&M 22–4. The 3 results are interesting and important, but tedious to derive