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Physics 731 HOMEWORK ASSIGNMENT #4 Due: Tuesday, Oct. 2, 2001

***NO CLASS on Thurs., Sept. 27*; make-up Wed., Oct. 3 (or Tues. Sept. 25??), 7:15-8:30pm.**

Read Ashcroft & Mermin (A&M), chap. 22. Skim chap. 21.

1. A&M 22–1 **2**. A&M 22–2 **3**. A&M 22–3

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 (7^{th}) 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 distances.

b) Using the general 1–D dispersion relation $\omega^2 = (2/M)\Sigma_{m\geq 1} K_m(1 - \cos mka)$ [eqn. (22.90)], show that the dispersion relation for this specific system can be written as

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

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

c) Show that ω^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 ζ is the Riemann zeta function].

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

6. Using http://dept.kent.edu/projects/ksuviz/leeviz/phonon/phonon.html (or analytically), consider a diatomic chain. Take ka = 0.5 and set the mass ratio to 4.

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)?

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Look carefully at A&M 22–4. The 3 results are interesting and important, but tedious to derive. Solutions will also be provided to the following problem, which you should not turn in but may find interesting: 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.