PHYSICS 555 FALL 2003

problem set 1
due Friday Sept. 19

1. a. In class, 6 “atoms” of mass $M$ connected by harmonic springs $K$ were studied, allowing only motions along the ring. Draw the curves for $\omega(k)$ for rings with 7 and 8 atoms, showing the discrete allowed values of $k$. What is the degeneracy of each level?

b. In class, the $\pi$ electron system of benzene ($C_6H_6$) was discussed. The single particle energy levels $\epsilon(k) = -2W \cos(ka)$ was derived. For cyclopentadiene ($C_5H_5$) draw the dispersion curve for $\epsilon(k)$, showing the discrete allowed values of $k$. What is the degeneracy and the ground state occupancy of each level?

2. Consider the benzene single-particle wavefunction

$$|\psi(t)\rangle = \alpha(t)|k = 2\pi/6a\rangle + \beta(t)|k = 4\pi/6a\rangle.$$  

This can be considered as a model for a partially-excited electron-hole pair state (try to explain what that means.)

a. This is not a stationary state. Given the $t = 0$ values $\alpha(0) = \beta(0) = 1/\sqrt{2}$, find $\alpha(t)$ and $\beta(t)$.

b. Plot $|\psi(t)|^2$ versus atom position at the two times $t = 0$ and $t = \pi \hbar/6W$.

c. The quantity $\partial\epsilon/\partial k$ is $\hbar v(k)$ where $v(k)$ is the group velocity. Compare this with the plots in part [b].

3. Bond alternation occurs naturally, a nice example being polyacetylene ($\left(CH\right)_n$) where the C-C bonds alternate between short and long. Consider 2N identical atoms on a ring. The atom displacement (along the ring is denoted by $u_i$. The numbering system is

$$|u\rangle = \begin{pmatrix} u_{a1} \\ u_{b1} \\ u_{a2} \\ \vdots \\ u_{bN} \end{pmatrix}$$

and the potential energy for atom displacement is

$$U_{\text{tot}} = \frac{1}{2}K_1 \sum_{n=1}^{N} (u_{a,n} - u_{b,n})^2 + \frac{1}{2}K_2 \sum_{n=1}^{N} (u_{b,n} - u_{a,n+1})^2$$

so that alternate pairs are connected by springs of differing spring constants $K_1$ and $K_2$. The equation of motion can be written as

$$M \frac{d^2}{dt^2} |u\rangle = -\mathbf{K}|u\rangle$$
a. Write out the form of the dynamical matrix $K$.

b. Note that there are $N$, not $2N$ translation symmetries. To each eigenvalue $\exp(ik\ell)$ of $\hat{T}(\ell)$ there are two eigenstates which can be chosen to be

$$|k\rangle = \sqrt{\frac{1}{N}} \begin{pmatrix} e^{ik} \\ 0 \\ 0 \\ \vdots \\ e^{iNk} \\ 0 \end{pmatrix}$$

$$|k\rangle = \sqrt{\frac{1}{N}} \begin{pmatrix} 0 \\ e^{ik} \\ 0 \\ \vdots \\ e^{iNk} \end{pmatrix}$$

Why must we choose $\exp(iNk) = 1$?

c. Show that a solution of Newton’s laws can be generated from eigenstates of translation

$$|u(t)\rangle = \alpha_k(t)|k\rangle + \beta_k(t)|k\rangle .$$

Write Newton’s laws as a $2 \times 2$ matrix equation for $\alpha_k(t)$ and $\beta_k(t)$.

d. Find the eigenfrequencies $\omega_s(k)$ of the two branches ($s = 1, 2$) of normal modes of oscillation. Plot $\omega_s(k)$ and indicate why you get exactly $2N$ such normal modes.