Corrections:

second last sentense: \omega(\alpha) should be \omega^2(\alpha)

picture added after page 1 should be in page 1.

Physics 361 Solutions to Problem Set 2

October 25, 2002

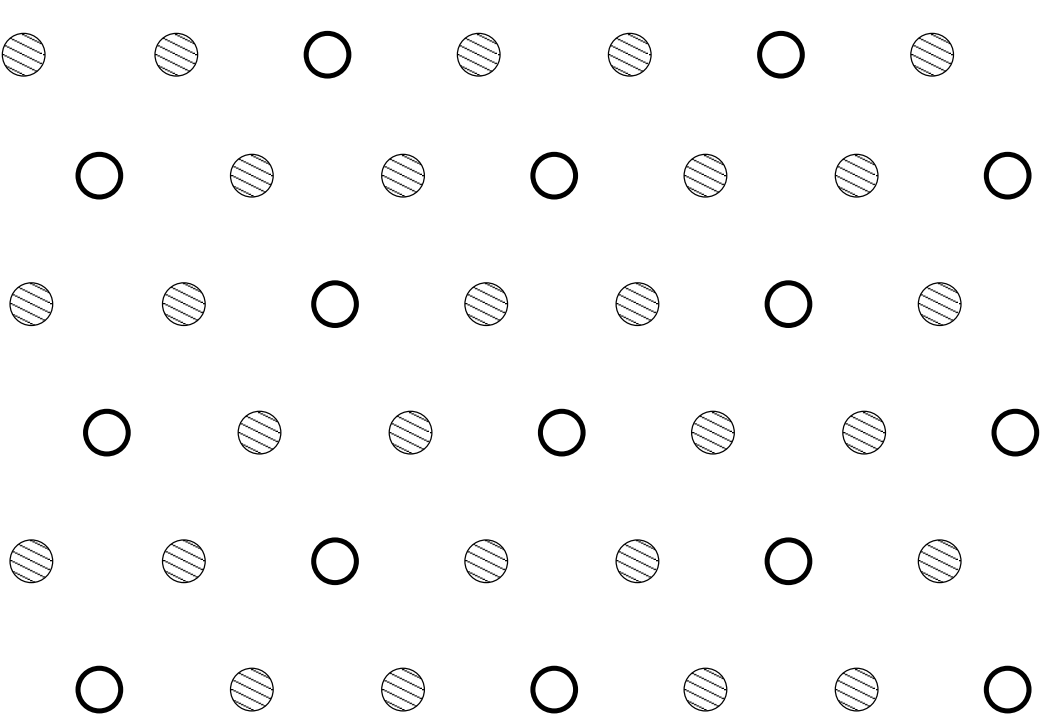
1 Scattering from a honeycomb lattice

The honeycomb lattice with hexagonal cells of side b is a Bravais lattice with basis. The Bravais lattice is generated by primitive vectors $(b/2)\{3\hat{\mathbf{x}} + \sqrt{3}\hat{\mathbf{y}}, 3\hat{\mathbf{x}} - \sqrt{3}\hat{\mathbf{y}}\}$, and a possible basis is $\{0, (b/2)(\hat{\mathbf{x}} + \sqrt{3}\hat{\mathbf{y}})\}$. The reciprocal lattice is generated by $(2\pi/3b)\{(\hat{\mathbf{x}} + \sqrt{3}\hat{\mathbf{y}}), (\hat{\mathbf{x}} - \sqrt{3}\hat{\mathbf{y}})$.

The relative intensity of scattering for each reciprocal lattice wavevector is given by the symmetry factor $S(k) = |\exp(ik \cdot d_1) + \exp(ik \cdot d_2)|^2$ where d_1 and d_2 are the vectors of the basis. A vector in the reciprocal lattice is given by $k = n_1\mathbf{b}_1 + n_2\mathbf{b}_2$ where n_i are integers and $\mathbf{b}_1$, $\mathbf{b}_2$ generate the reciprocal lattice. For the basis and generating vectors given above,

$$\begin{aligned} S &= 2[1 + \cos\frac{2}{3}\pi(2n_1 - n_2)] \\ &= \begin{cases} 4; & (2n_1 - n_2) \mod 3 = 0 \\ 1; & (2n_1 - n_2) \mod 3 = 1, 2 \end{cases} \end{aligned}$$

The scattering pattern is shown above with intense peaks in white.



2 Exchange repulsion

Single potential well. The Hamiltonian for a single potential well of width b and depth u is $H = -\partial_x^2 + V(x)$, with

$$V(x) = \begin{cases} 0 & ; \quad x < 0 \\ -u & ; \quad 0 < x < b \\ 0 & ; \quad b < x \end{cases}$$

The bound state wavefunction must be a decaying exponential outside the well and a sinusoid inside the well.

$$\Psi(x) = \begin{cases} Ae^{kx} & ; \quad x < 0 \\ B_+ e^{ik'x} + B_- e^{-ik'x} & ; \quad 0 < x < b \\ Ce^{-kx} & ; \quad b < x \end{cases}$$

If ϵ is the binding energy, then the eigenvalue equation for the bound state is $H\Psi(x) = -\epsilon\Psi(x)$ which gives $k'^2 = u - \epsilon$ and $k^2 = \epsilon$. The continuity of Ψ and its first derivative at 0 and b requires

$$\begin{aligned} \Psi(0) &= A = B_+ + B_- \\ \Psi(b) &= B_+ e^{ikb} + B_- e^{-ikb} = Ce^{-kb} \\ \Psi'(0) &= kA = ik'B_+ - ik'B_- \\ \Psi'(b) &= ik'B_+ e^{ik'b} - ik'B_- e^{-ik'b} = -kCe^{-kb} \end{aligned}$$

This leads to the equation for the bound state energy:

$$\tan(k'b) = \frac{2kk'}{k'^2 - k^2}$$

We are interested in the limit $b \to 0$ and $u \to \infty$ with ϵ held fixed. This means $kb \ll 1$ and $\epsilon \ll u$, but if we assume also that $k'b \ll 1$ so that $\tan(k'b) \approx k'b$ this equation yields

$$\epsilon^{1/2} = bu/2$$

To check our assumption, note that this solution implies $k'b \to \sqrt{2b}\epsilon^{1/4} \ll 1$ in this limit.

The wavefunction is $\Psi(x) = C\exp(-k|x|)$ with normalization constant $C = k^{1/2} = \epsilon^{1/4}$.

Two Atoms. If such a potential well is located at positions X and $-X$, then we assume that at large distances X one can define wavefunctions corresponding to a bound state in the "left" and "right" wells as

$$< x|L >= Ce^{-k|x+X|} \qquad < x|R >= Ce^{-k|x-X|}$$

A properly antisymmetrized wavefunction for two electrons occupying bound states in either of the wells would then have the form

$$|\Psi >= C'(|L_1 R_2 > -|L_2 R_1 >)$$

The normalization condition is

$$1 =< \Psi|\Psi >= 2|C'|^2(1 - | < L|R > |^2)$$

where we have used the fact that the scalar product of two-body quantum states is just the product of the scalar products of the one-body quantum states of each particle, e.g. $< L_1R_2|R_1L_2 >=< L|R >< R|L >= | < L|R > |^2$, $< L_1R_2|L_1R_2 >=< L|L >< R|R >= 1$.

$$< L|R >= C^2 \int_{-\infty}^{+\infty} dx\, e^{-k(|x+X|+|x-X|)} = (1+2kX)e^{-2kX}$$

The Hamiltonian for the system H is the sum of the Hamiltonians for the individual particles h_1 and h_2, each of which consists of the kinetic energy and *both* well potentials. The wavefunction of particle 2 is unaffected by the Hamiltonian of particle 1 (and vice versa) so that in computing the energy $E(X) =< \Psi|H|\Psi >$, for example, $< L_1R_2|H|R_1L_2 >=< L_1|h_1|R_1 >< R_2|L_2 > + < L_1|R_1 >< R_2|h_2|L_2 >= 2 < L|R >< L|h|R >$. Using $< L|R >=< R|L >$, $< L|h|R >=< R|h|L >$, and $< L|h|L >=< R|h|R >$ the system energy simplifies to

$$E(X) =< \Psi|H|\Psi >= 4|C'|^2(< L|h|L > - < L|R >< L|h|R >)$$

The one particle Hamiltonian may be written $h = -\partial_x^2 + U_L(x) + U_R(x)$ with $U_{L,R}$ being the respective well potentials. Since $|L >$ and $|R >$ are eigenstates of the single well problem with eigenvalue $-k^2$, we have $h|L >= (-k^2 + U_R)|L >$, $h|R >= (-k^2 + U_L)|R >$. The required scalar products become

$$\begin{aligned} < L|h|L > &= -k^2 < L|L > + < L|U_R|L >= -k^2 - kbu\, e^{-4kX} \\ < L|h|R > &= -k^2 < L|R > + < L|U_L|R >= -k^2 < L|R > -kbu\, e^{-2kX} \end{aligned}$$

The x integrals over the well potentials are performed assuming that they are delta functions with integral $-bu$.

We are interested in $E(X) - E(\infty)$. At $X = \infty$ there are two independent well systems and the energy is just $-2k^2$. Plugging in the above results for the scalar products gives

$$\begin{aligned} E(X) + 2k^2 &= 4|C'|^2[< L|h|L > - < L|R >< L|h|R > +2k^2/(4|C'|^2)] \\ &= 4|C'|^2(kX)(kbu)e^{-4kX} \end{aligned}$$

In the limit of large X, $|C'|^2 \to 1/2$. Since $E(X)$ is a decreasing function as X increases (for sufficiently large X) the potential is repulsive.

3 Diatomic Linear Chain

If x_j is the displacement of atom j from equilibrium then the equation of motion is

$$M_j \partial_t^2 x_j = k(x_{j+1} + x_{j-1} - 2x_j)$$

where

$$M_j = \begin{cases} M & ; \quad j \text{ even} \\ \alpha M & ; \quad j \text{ odd} \end{cases}$$

Normal modes of the chain will have the form

$$x_j = e^{i[k(ja)-\omega t]} \cdot \begin{cases} A & ; \quad j \text{ even} \\ B & ; \quad j \text{ odd} \end{cases}$$

The coefficients A and B satisfy a matrix equation

$$\begin{pmatrix} -\omega^2 M + 2k & -2k\cos(ka) \\ -2k\cos(ka) & -\omega^2 M\alpha + 2k \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = 0$$

Setting the matrix determinant equal to zero gives the solutions

$$\omega^2 = \frac{k}{M}\left[\left(\frac{1}{\alpha}+1\right) \pm \sqrt{\left(\frac{1}{\alpha}+1\right)^2 - \frac{4}{\alpha}\sin^2(ka)}\right]$$

In the limit $\alpha \to 1$ the dispersion relations for the two branches become

$$\omega = 2\frac{k}{M} \begin{cases} |\cos(\frac{1}{2}ka)| \\ |\sin(\frac{1}{2}ka)| \end{cases}$$

When the masses are unequal, the maximum allowed wavenumber in each branch is $|k| = \pi/(2a)$. When the masses become equal, the maximum wavenumber is doubled, and the cos branch is "shifted" to cover $\pi/(2a) < |k| < \pi/a$. This restores the familiar $|\sin(ka/2)|$ dispersion for the equal mass case.

The dispersion satisfies $\omega^2(1/\alpha) = \alpha\omega(\alpha)$. This is because the transformation $\alpha \to 1/\alpha$ is equivalent to exchanging the masses and rescaling M by α.