Physics 361 **Problem set 2** **due October 18, 2002**

P2.1 scattering from a honeycomb lattice The nearest neighbor distance of the honeycomb lattice of Fig. 4.17 is denoted b. a)draw the reciprocal lattice out to the 4th smallest reciprocal lattice vector. b) Indicate the relative intensities of waves diffracted for each of the indicated reciprocal lattice points.

P2.2 exchange repulsion This problem aims to reveal how the overlap of atomic wave-functions leads to repulsion between atoms. For this purpose we model the atom as a one-dimensional square well representing the ion core of the outer electron. This outer electron is a Shroedinger particle experiencing this potential. The well depth is u; the width is b, the bound-state energy is $-\epsilon$. We take units such that the mass is $\frac{1}{2}$ and $\hbar = 1$. Thus the wave-function outside the well has the form $C\exp(-\epsilon^{1/2}|x|)$. Here x is the position. The well is very narrow and deep, so that virtually all of the wavefunction lies outside the well.

a) Find the relationship between ϵ, u and b in this limit.
b) Find the normalization constant C.

Consider a pair of these atoms at positions X and $-X$. We take X to be much larger than $\epsilon^{-1/2}$ so that their wave-functions overlap very little. The wavefunction $\psi(1,2)$ of the system depends on both electron co-ordinates, 1 and 2. This ψ is virtually the same as though X were infinite. Our object is to calculate the energy of the system $E(X) - E(\infty)$, to see the magnitude of the attraction or repulsion at large separation. We ignore the electrons' mutual interaction and their spin. Thus the hamiltonian is the sum of single-electron hamiltonians $h_1 + h_2$. In our units h_1 has the form $h_1 = -\frac{d^2}{dx_1^2} + U_L(x_1) + U_R(x_1)$, where U_L is the square well at $-X$ and U_R is the square well at $+X$. The state of an electron in the L well is denoted $|L\rangle$ and that in the right-hand well as $|R\rangle$ †. That is, $\langle x|L\rangle = C\exp(-\epsilon^{1/2}|x-X|)$, and $\langle x|R\rangle = C\exp(-\epsilon^{1/2}|x+X|)$. We can denote a two-particle state with particle 1 in the left well and particle 2 in the right well by $|L\rangle_1 |R\rangle_2$. The system contains an electron in each well. Its wavefunction must be antisymmetric underchange of the two electron co-ordinates 1 and 2:

$$|\psi\rangle = C'(|L\rangle_1 |R\rangle_2 - |R\rangle_1 |L\rangle_2)$$

The normalization constant C' is set by the condition $\langle\psi|\psi\rangle = 1$. The energy of the system $E(X)$ for large X is $\langle\psi|\, h_1 + h_2\,|\psi\rangle$. Writing out these inner products and separating out the objects that depend on co-ordinate 1 from those that depend on co-ordinate 2, the normalization condition can be written

$$1 = C'^2\,(\ \langle L|_1 L\rangle_1 \langle R|_2 R\rangle_2 \pm \langle R|_1 R\rangle_1 \langle L|_2 L\rangle_2 \pm \langle L|_1 R\rangle_1 \langle R|_2 L\rangle_2 \pm \langle R|_1 L\rangle_1 \langle L|_2 R\rangle_2\ ) \qquad *$$

Here I've deliberately left the signs of some terms unspecified. Likewise, $\langle\psi|\, h_1\,|\psi\rangle$ has the form

$$\langle\psi|\, h_1\,|\psi\rangle = C'^2\,(\ \langle L|_1 h_1|L\rangle_1 \langle R|_2 R\rangle_2 \pm \langle R|_1 h_1|R\rangle_1 \langle L|_2 L\rangle_2 \pm \langle L|_1 h_1|R\rangle_1 \langle R|_2 L\rangle_2 \pm \langle R|_1 h_1|L\rangle_1 \langle L|_2 R\rangle_2\ )\ **$$

Now that all the $\langle ...|\,...\,|...\rangle$ expressions refer to the same co-ordinate, we no longer need the $_1$ and $_2$ subscripts. Thus, *eg.* $\langle L|_2 R\rangle_2$ is simply $\langle L|R\rangle$. Note also that $\langle L|\, h_1\,|L\rangle \equiv -\epsilon'$ is not simply $-\epsilon$, because h_1 includes both wells, while ϵ was the energy in a single well.

c) Simplify the expressions * and **, and figure out the correct signs, to obtain an expression for $E(X)$ as a function of ϵ, ϵ', $\langle L|R\rangle$ and $\langle L|\, h_1\,|R\rangle$. The answer in c) shows that the overlap of the atomic wave-functions affects the energy of the system. There are several effects—some attractive, some repulsive. We now determine which of these effects dominate at large separation X.
d) Using parts a) and b) find $\langle L|R\rangle$ as a function of X, for $X\epsilon^{1/2} \gg 1$.
e) Calculate $\langle L|\, h_1\,|R\rangle$ and find the dominant term for large X.
f) Express $E(X)$ in the form $E(X) = -2\epsilon + f(X)$, giving the asymptotic form of f for large X. Is the interaction attractive or repulsive?

† I'm using the Dirac notation where $\langle\phi|\, h\,|\psi\rangle$ is a shorthand for $\int_{-\infty}^{\infty} dx\ \phi(x)\ h\ \psi(x)$.

P2.3 Diatomic Linear chain A line of atoms in one dimension are connected by identical springs as in Chapter 22. However, the masses alternate between two values: M and αM.

a) Adapt the derivation in the chapter to find the vibrational frequency as a function of wavenumber k.

b) Discuss the form of the "dispersion relation" in a) when the masses become equal.

c) What is the relation between $\omega^2(\alpha)$ and $\omega^2(1/\alpha)$? Why is it independent of k?