Appendix B

Thursday, March 03, 2011

2x2 matrix and the perturbation theory

I've been speaking about the perturbation theory in class, as it is a useful technique to understand the nearly free electron model. The fact is though it is really not essential to know the perturbation theory in order to understand what is going on. So, here is the version of the nearly free electron model, without using the perturbation theory language.

For this version, we simply consider a 2x2 matrix only, with a general statement that the same qualitative behavior holds even when you have higher dimensional matrices (readers could/should "play with" matrix diagonalization on a computer to verify this). Let us call our model a "2 band" model, since the dimensionality of our matrix determines the number of bands that we are considering.

The matrix in question is presented in prob. 3 of Homework 7. Except here, we are not necessarily restricting $E_1 \approx E_2$; they can be much different.

The matrix is of the form $H = \begin{pmatrix} E_1(k) & U^* \\ U & E_2(k) \end{pmatrix}$, where U is some constant, and $E_1(k) \neq E_2(k)$ in general. We will assume that $E_1(k) \leq E_2(k)$.

Within the two band model, H is the total Hamiltonian, and all we need to do is to diagonalize it to obtain band energies.

The diagonalization is easy enough. It is a bit like doing the phonon problem with two atoms per basis, except the matrix is a bit simpler since the off-diagonal matrix element is just a constant: $\epsilon_{\pm}(k) = \frac{E_1(k)+E_2(k)}{2} \pm \frac{\sqrt{(E_1(k)-E_2(k))^2+4|U|^2}}{2}$, where $+$ corresponds to the upper band, and $-$ corresponds to the lower band.

From this solution, the two different regimes appear. (Note that $E_2 - E_1 \geq 0$, by our choice/convention.)

Regime 1: $E_2(k) - E_1(k) \ll 2|U|$ (Bragg diffraction on or near BZ boundary).

$$\epsilon_{\pm}(k) \approx \frac{E_1(k) + E_2(k)}{2} \pm |U|$$

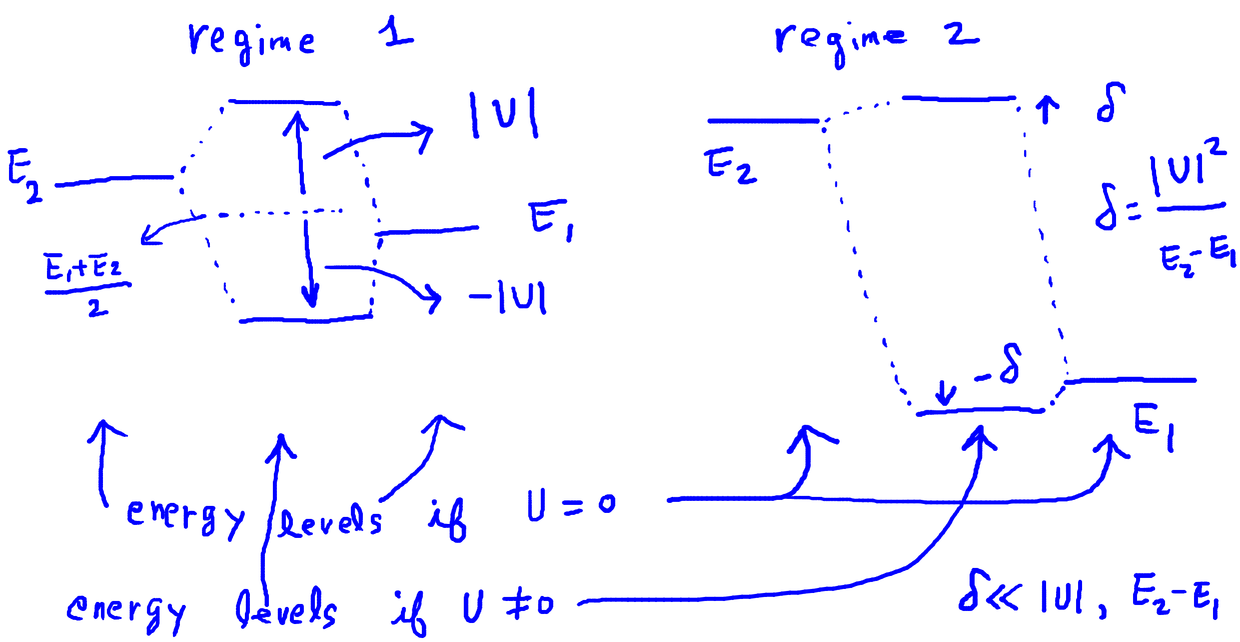
Regime 2: $E_2(k) - E_1(k) \gg 2|U|$ (Bragg scattering far away from BZ boundary).

$$\epsilon_-(k) \approx E_1(k) + \frac{|U|^2}{E_1(k) - E_2(k)}$$

$$\epsilon_+(k) \approx E_2(k) + \frac{|U|^2}{E_2(k) - E_1(k)}$$

It is important to see that in general, what we have is a level repulsion. That is the nature of the 2x2 matrix problem at hand. In regime 1, that repulsion is much more substantial (first order in U) than in regime 2.

The following type of "hybridization" diagram, commonly seen in chemistry literature, can be helpful to visualize these important behaviors.



These behaviors are, of course, identical with what you would expect from the degenerate (regime 1), and the non-degenerate (regime 2) time-independent perturbation theory.

A solid understanding of all the stuff above using a 2x2 matrix should be enough for grasping the essential physics of the nearly free electron band theory, as far as this course is concerned. Indeed, such understanding should be essential for doing problems of Homework.

If one generalizes this to 3x3 and 4x4 matrices, etc., and if the 3rd energy level (E_3) and the 4th energy level (E_4), and so on., are far away, then the above results will remain good approximations. If E_3 and E_4 and so on happen to be close to E_2, then what we say above would need to be modified. Again the sensible thing to do would be to identify two (or a few) levels that are nearly degenerate, and then diagonalize the Hamiltonian submatrix, since that would give the largest effect. In all of this, note that the lowest energy level is always pushed down by the off-diagonal matrix element.