PHYS4450 Solid State Physics

SAMPLE QUESTIONS FOR DISCUSSION in Week 12 EXERCISE CLASS (10 April 2013)
You may want to think about them before attending exercise class.

SQ23 is an extension of SQ18 on the tight-binding model with two atoms per unit cell to the particular case of graphene. SQ24 serves to illustrate that for a Bloch state $\psi_k(\mathbf{r})$, the quantity $\hbar\mathbf{k}$ looks like a momentum, but actually $\psi_k(\mathbf{r})$ is not an eigenstate of the momentum operator.

SQ23 **Graphene p_z bands.** Carbon atoms in graphene make use of sp^2 hybridization to form the strong honeycomb framework. Each carbon atom still has an electron in the $2p_z$ atomic orbital not engaged in the σ-bonds. These p_z orbitals form bands. As discussed, graphene has a basis of two carbon atoms in a unit cell. TA will apply the formalism in SQ18 to obtain the bands formed by linear combining these p_z orbitals. Since we have two atoms in a unit cell and each atom contributes one p_z orbital, the result is that two bands are formed. These two bands just touch each other. Filling in the electrons give graphene the property of being a gapless semiconductor. The band structure near the touching bands can be described by the Dirac equation for massless fermions.

SQ24 **Bloch state is NOT an eigenstate of the momentum operator.** For an electron in a Bloch state with wavefunction $\psi_k(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_{\mathbf{k}}(\mathbf{r})$, the quantity $\hbar\mathbf{k}$ acts like momentum, e.g., it appears in the semiclassical equation of motion in the presence of an applied force. However, it is not the physical momentum of an electron. A reason comes from the semiclassical equation of motion that relates the rate of change of $\hbar\mathbf{k}$ ONLY to the external applied force (but NOT the TOTAL force that should include the internal forces due to the periodic array of ions). TA: Another way to illustrate the point is to work out $\hat{\mathbf{p}}\psi_k(\mathbf{r})$ directly and show that the Block state is NOT an eigenstate of the momentum operator $\hat{\mathbf{p}}$. [Note: There is one trivial case when ψ is indeed an eigenstate of $\hat{\mathbf{p}}$ though, as you will see from the answer.] The concept in this SQ is also closely related to the idea of defining an effective mass.

SQ-TA **Contact your TA for help.** To give you a chance to talk to the TA on your preparation of the presentation, I will ask the TWO TAs to be present in this week's exercise class. Although the time will not be sufficient for you to ask all your questions and for them to answer the questions, I hope that it will serve as a catalyst for you to make an appointment with the TA to discuss your progress.