

## Condensed Matter Physics I — PHZ5941

### Final Exam

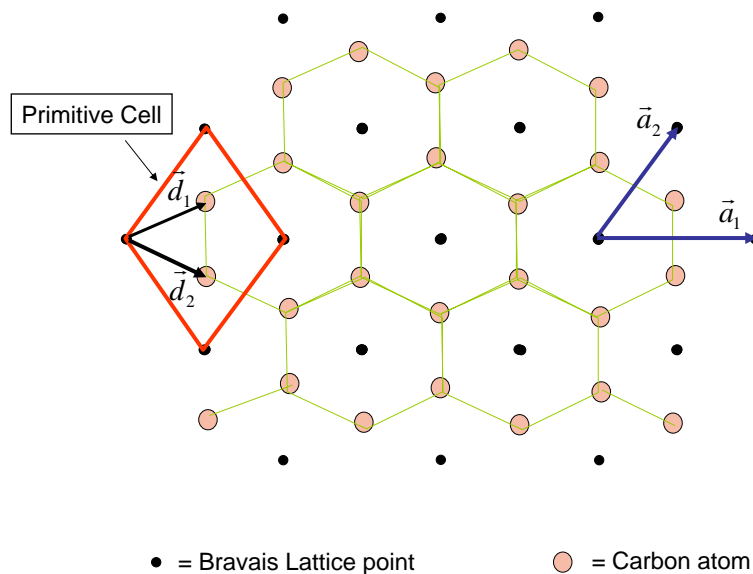
- I** The final is due either in my mail box in the main office in the Keen building or at the Magnet Lab. The due date is Midnight, Thursday, Dec. 13, 2007. There will be no extensions.
- II** In completing the final you may consult any books you wish, and please feel free to ask me any clarifying questions.
- III** *Please do not discuss the final with other members of the class until after the deadline.*
- IV** Good luck!

**1. (60 pts) Electronic Structure of Graphene** — Graphene consists of an atomically thin layer of carbon atoms arranged in a honeycomb lattice. Recently there has been an explosion of work on this fascinating material. For a review see the following Physics Today “Search and Discovery” article:

[http://www.physicstoday.org/vol-59/iss-1/pdf/vol59no1p21\\_23.pdf](http://www.physicstoday.org/vol-59/iss-1/pdf/vol59no1p21_23.pdf)

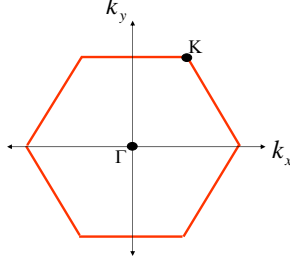
In this problem you will determine the band structure of graphene using the tight-binding approximation.

Recall that the honeycomb lattice is *not* a simple Bravais lattice. Rather, it can be viewed as a triangular Bravais lattice with a two atom basis as shown in the figure below ( $\vec{d}_1$  and  $\vec{d}_2$  are the basis vectors).



The triangular Bravais lattice (represented by black dots in the figure) is generated by the vectors  $\vec{a}_1 = a\hat{x}$  and  $\vec{a}_2 = \frac{a}{2}\hat{x} + \frac{\sqrt{3}a}{2}\hat{y}$  (also shown in the figure).

- (a) Determine the primitive vectors  $\vec{b}_1$  and  $\vec{b}_2$  which generate the reciprocal lattice for this triangular lattice and construct the 1st Brillouin zone. It should look like this:



Determine the value of  $\vec{k}$  at the zone corner, denoted  $\mathbf{K}$  in the figure.

*Tight-Binding Model for Graphene.*— In graphene, each carbon atom forms a double bond with each of its three nearest neighbors. Since carbon has 4 valence electrons, this leaves one electron per carbon atom which is not used to form these double bonds. This extra valence electron occupies a band formed by  $p_z$  orbitals, i.e. the  $2p$  orbitals on each carbon which point out of the page.

To construct a tight-binding description of this system consider Bloch states of the form

$$\Psi_{\vec{k}}(\vec{r}) = \sum_{\vec{R}} \left( A\phi(\vec{r} - \vec{R} - \vec{d}_1) + B\phi(\vec{r} - \vec{R} - \vec{d}_2) \right) e^{i\vec{k} \cdot \vec{R}}.$$

Here  $\phi(\vec{r} - \vec{R} - \vec{d}_s)$  is the atomic  $p_z$  orbital associated with the carbon atom at the point  $\vec{R} + \vec{d}_s$  for  $s = 1, 2$ . In what follows we will assume that the atomic states  $\phi$  are normalized. The coefficients  $A$  and  $B$  are to be determined.

(b) Let  $H$  be the full crystal Hamiltonian for an electron in graphene. By taking the inner product of both sides of the Schrödinger equation

$$H\Psi_{\vec{k}}(\vec{r}) = \mathcal{E}\Psi_{\vec{k}}(\vec{r}),$$

with the states  $\phi(\vec{r} - \vec{d}_1)$  and  $\phi(\vec{r} - \vec{d}_2)$  obtain the following system of equations,

$$\begin{aligned} -\sum_{\vec{R}} (A\gamma_{11}(\vec{R}) + B\gamma_{12}(\vec{R}))e^{i\vec{k} \cdot \vec{R}} &= \mathcal{E} \sum_{\vec{R}} (A\beta_{11}(\vec{R}) + B\beta_{12}(\vec{R}))e^{i\vec{k} \cdot \vec{R}}, \\ -\sum_{\vec{R}} (A\gamma_{21}(\vec{R}) + B\gamma_{22}(\vec{R}))e^{i\vec{k} \cdot \vec{R}} &= \mathcal{E} \sum_{\vec{R}} (A\beta_{21}(\vec{R}) + B\beta_{22}(\vec{R}))e^{i\vec{k} \cdot \vec{R}}. \end{aligned} \quad (1)$$

where

$$\begin{aligned} \gamma_{ss'}(\vec{R}) &= -\int d^3\vec{r} \phi^*(\vec{r} - \vec{d}_s) H \phi(\vec{r} - \vec{R} - \vec{d}_{s'}), \\ \beta_{ss'}(\vec{R}) &= \int d^3\vec{r} \phi^*(\vec{r} - \vec{d}_s) \phi(\vec{r} - \vec{R} - \vec{d}_{s'}). \end{aligned}$$

*Approximations.*— Because the overlap of  $p_z$  orbitals on neighboring lattice sites is small we can make the following approximation for the  $\beta$  integrals,

$$\beta_{ss'}(\vec{R}) \simeq \delta_{ss'} \delta_{\vec{R},0}.$$

For the  $\gamma$  integrals, following arguments similar to those described in Chap. 10 of A&M, for  $\vec{R} = 0$  and  $s = s'$ , we may take

$$\gamma_{11}(0) = \gamma_{22}(0) \simeq -E_p,$$

where  $E_p$  is the energy of an atomic  $p_z$  orbital. For the other  $\gamma_{ss'}(\vec{R})$ 's we need only keep those matrix elements of  $H$  between  $p_z$  orbitals on nearest neighbor carbon atoms. Furthermore, by symmetry we know that all these matrix elements will have the same value (which I'll denote  $t$ ).

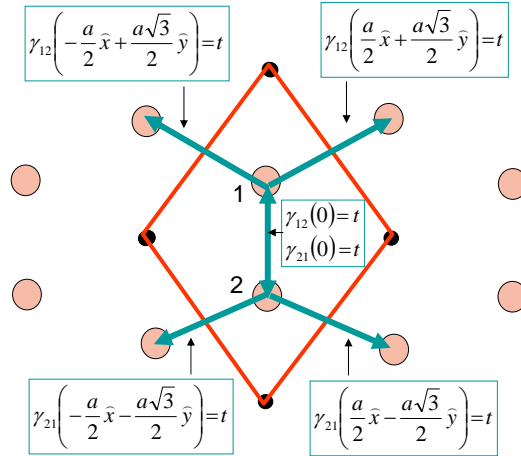
Thus we have

$$\gamma_{12}(0) = \gamma_{12} \left( \frac{a}{2} \hat{x} + \frac{a\sqrt{3}}{2} \hat{y} \right) = \gamma_{12} \left( -\frac{a}{2} \hat{x} + \frac{a\sqrt{3}}{2} \hat{y} \right) = t,$$

and

$$\gamma_{21}(0) = \gamma_{21} \left( \frac{a}{2} \hat{x} - \frac{a\sqrt{3}}{2} \hat{y} \right) = \gamma_{21} \left( -\frac{a}{2} \hat{x} - \frac{a\sqrt{3}}{2} \hat{y} \right) = t,$$

(see figure).



Finally, we can assume to a good approximation that all other  $\gamma$ 's are zero.

- (c) Show that using the approximations outlined above the system of equations given in Eq. (1) take the following form,

$$\begin{aligned} E_p A - t \left( 1 + 2e^{i\sqrt{3}k_y a/2} \cos \frac{k_x a}{2} \right) B &= \mathcal{E} A \\ -t \left( 1 + 2e^{i\sqrt{3}k_y a/2} \cos \frac{k_x a}{2} \right) A + E_p B &= \mathcal{E} B \end{aligned} \quad (2)$$

- (d) Solve the eigenvalue problem given by Eq. (2) for the energy  $\mathcal{E}$  and show that the resulting energy bands are

$$\mathcal{E}_{\pm}(\vec{k}) = E_p \pm t \sqrt{1 + 4 \cos^2 \frac{k_x a}{2} + 4 \cos \frac{k_x a}{2} \cos \frac{k_y a \sqrt{3}}{2}}.$$

Note that there are two bands (a consequence of having two atoms per unit cell). In graphene the  $\mathcal{E}_-$  band is the (full) valence band, and the  $\mathcal{E}_+$  band is the (empty) conduction band. ( $\mathcal{E}_-(\vec{k})$  and  $\mathcal{E}_+(\vec{k})$  are the two bands shown in Fig. 1b in the Physics Today article referenced above.)

- (e) Taylor expand  $\mathcal{E}_{\pm}(\vec{k})$  about the point  $\vec{K}$  at the zone corner (found in part (a)) and show that the resulting dispersion near this point is

$$\mathcal{E}_{\pm}(\vec{k}) \simeq E_p \pm \hbar v_0 \sqrt{(k_x - K_x)^2 + (k_y - K_y)^2} = E_p \pm \hbar v_0 |\vec{k} - \vec{K}|.$$

Determine the velocity  $v_0$  in terms of  $t$  and  $a$ . Note that unlike the case of semiconductors, for which the electron and hole dispersions are quadratic in the momentum, here they are *linear*. This linear dispersion, (shown in Fig. 1c of the Physics Today article), is analogous to that of a *relativistic* electron (with  $v_0$  playing the role of the speed of light). This unusual dispersion is responsible for many of the fascinating properties of graphene.

**2. (40 pts) Debye Specific Heat for One-Dimensional Phonons.**— Consider a one-dimensional monatomic crystal with a single phonon mode  $\omega(k)$ . The lattice specific heat for this solid is given by the following expression

$$c_v = \frac{\partial}{\partial T} \int \frac{dk}{2\pi} \frac{\hbar \omega(k)}{e^{\beta \hbar \omega(k)} - 1},$$

where the integration is over the first Brillouin zone.

In the Debye approximation the phonon dispersion is assumed to be linear for all  $k$ , with  $\omega(k) = c|k|$ , where  $c$  is the speed of sound. Note that in one dimension the Debye wave vector,  $q_D$ , will simply be equal to  $\pi/a$ .

- (a) Obtain an expression for  $c_V$  for this one-dimensional crystal analogous to the three-dimensional expression given in Eq. 23.26 in A&M. As in that expression, your result should be expressed in terms of  $k_B$ ,  $T$ ,  $\Theta_D$  (the Debye temperature), and the number density of lattice ions,  $n$ . It will also involve a definite integral similar to, but not exactly the same as, the integral over  $x$  in Eq. 23.26 in A&M.

- (b) Obtain an approximate expression for  $c_V$  valid in the limit  $T \ll \theta_D$ .
- (c) Obtain an approximate expression for  $c_V$  valid in the limit  $T \gg \theta_D$ . Comment on the significance of your result.