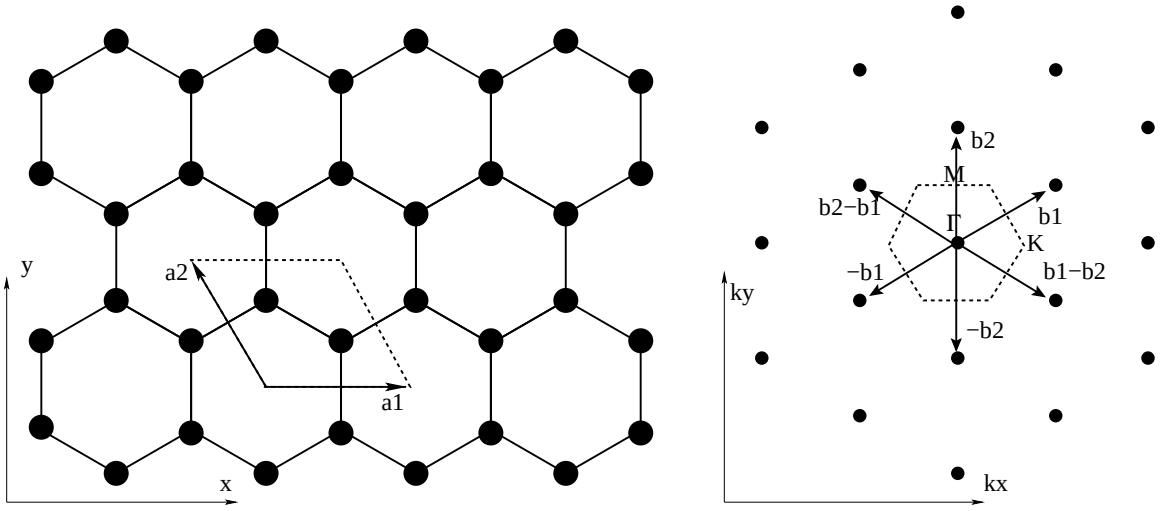
NAME: SOLUTIONS

33-448 Solid State Physics Final Exam #3 Tuesday, May 3, 2016

**1. Band structure of graphene**

The figure below illustrates the real-space structure and diffraction pattern of graphene. The dashed lines outline the unit cell in real space and the first Brillouin zone in reciprocal space. Special reciprocal points are marked $\Gamma$ (center of zone), $K$ (corner of zone) and $M$ (mid-edge of zone). The reciprocal lattice vectors are

$$\mathbf{b}_1 = \frac{2\pi}{a}(\hat{x} + \frac{1}{\sqrt{3}})\hat{y} \qquad \mathbf{b}_2 = \frac{4\pi}{\sqrt{3}a}\hat{y}.$$




*(a)* Sketch and label the vectors $\pm\mathbf{b}_1$, $\pm\mathbf{b}_2$, and $\pm(\mathbf{b}_1 - \mathbf{b}_2)$ on the diffraction pattern.

**Answer:** See figure.

*(b)* Let the electron-lattice interaction potential at $\mathbf{r} = (x, y)$ be

$$U(\mathbf{r}) = U_0 \left[ \cos\left( \frac{2\pi}{a}(x + \frac{1}{\sqrt{3}}y) \right) + \cos\left( \frac{2\pi}{a}(x - \frac{1}{\sqrt{3}}y) \right) + \cos\left( \frac{4\pi}{\sqrt{3}a}y \right) \right].$$

Verify that $U(\mathbf{r})$ obeys the required translational symmetries of the crystal lattice. Hint: this is easiest if you think about reciprocal space, and I will give a simple answer more points than a complicated one.

**Answer:** Note that the arguments of the cosines are, respectively, $\mathbf{b}_1 \cdot \mathbf{r}$, $(\mathbf{b}_1 - \mathbf{b}_2) \cdot \mathbf{r}$, and $\mathbf{b}_2 \cdot \mathbf{r}$. Thus

$$U(\mathbf{r}) = \frac{U_0}{2} \sum_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}}$$

where the sum on $\mathbf{G}$ runs over the set of smallest nonzero reciprocal lattice vectors. By the definigion of reciprocal lattice vector, $\exp(i\mathbf{G} \cdot \mathbf{T}) = 1$ for all lattice translations $\mathbf{T}$. Hence, $U(\mathbf{r} + \mathbf{T}) = U(\mathbf{r})$.

*(c)* Based on your knowledge of the origin of band gaps, estimate the band gap $E_g$ at the special point $M$ predicted by the nearly free electron model. Be sure to fully define any symbols or quantities you introduce. You may wish to recall the "central equation",

$$(\lambda_{\mathbf{k}} - E)C(\mathbf{k}) + \sum_{\mathbf{G}} U_{\mathbf{G}} C(\mathbf{k} - \mathbf{G}) = 0,$$

but do **not** attempt to solve it.

**Answer:** Recall that a term in the Fourier series of a potential $U_{\mathbf{G}} \exp(i\mathbf{G} \cdot \mathbf{r})$ creates a gap at $\mathbf{k} = \mathbf{G}/2$ of magnitude $E_g = 2U_{\mathbf{G}}$. Hence the gap $E_g = U_0$.

*(d)* Is there a band gap at the special point $K$? Briefly explain why or why not.

**Answer:** There is no gap at $K$ because $K \neq \mathbf{G}/2$ for any reciprocal lattice vector $\mathbf{G}$.

**2. Bloch oscillations**

Consider an electron moving in a one-dimensional periodic potential $V(x+a) = V(x)$. The electron accelerates in the presence of an applied force $F$, but as long as $F$ is finite the energy must change continuously. Hence the electron energy is confined to a single band. Let the dispersion relation be $E(k) = -A\cos(bk)$ within this band.

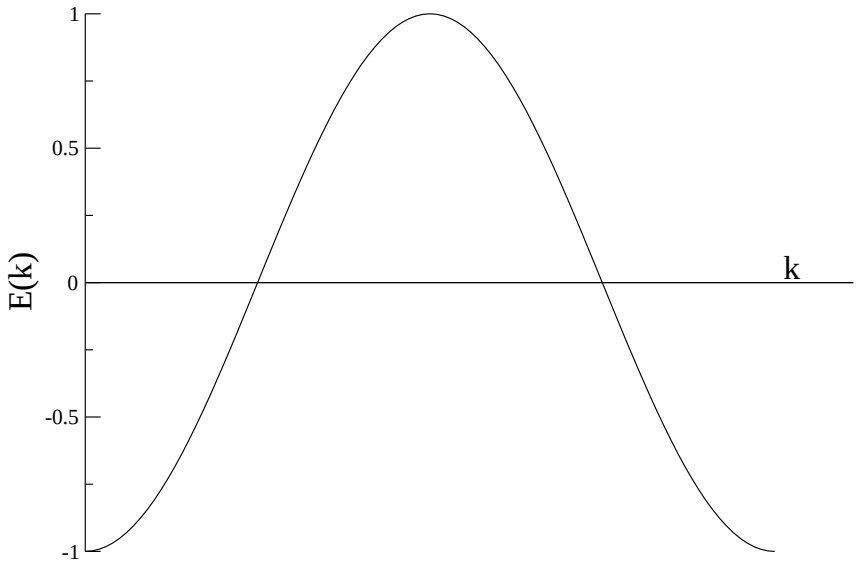
*(a)* What is the value of $b$? What is the *group* velocity of the electron with wavenumber $k$?

> **Answer:** The first reciprocal lattice vector is $G = 2\pi/a$. Requiring $E(k+G) = E(k)$ demands that $bG = 2\pi$ so that $b = a$. Group velocity is
> $v_g = (1/\hbar)dE/dk = (aA/\hbar)\sin(ak)$.

*(b)* A constant applied electric field $\vec{\mathcal{E}} = -\mathcal{E}\hat{x}$ accelerates the electron. What is $dk/dt$? Neglect any scattering by impurities, defects or phonons, *i.e.* take the mean free time $\tau \to \infty$.

> **Answer:** According to semiclassical dynamics, $\hbar dk/dt$ equals the force on the electron, which is $(-e)(-\mathcal{E})$. Thus $dk/dt = e\mathcal{E}/\hbar$. If we wish we may restrict $k$ to the first Brillouin zone through "Umklapp" by taking the value of $k$ modulo $G$, but this is not necessary.

*(c)* Assume the electron is initially localized around the origin $x \approx 0$ in a wave packet with $k \approx 0$. Qualitatively describe the motion of the electron in response to the applied field, and comment on how the motion differs from that of a free particle. Use the figure below to assist your explanation.




**Answer:** Since $k$ increases linearly in time, the group velocity $v_g$ must oscillate sinusoidally. Thus the particle initially moves to the right, until $k = \pi/a$ at which point its velocity reverses, and the particle returns to the origin $x = 0$ once $k = 2\pi/a$. Thus the motion is oscillatory (and will thus emit radiation), while a free electron in contrast will simply accelerate.

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**3. Quantum well density of states**

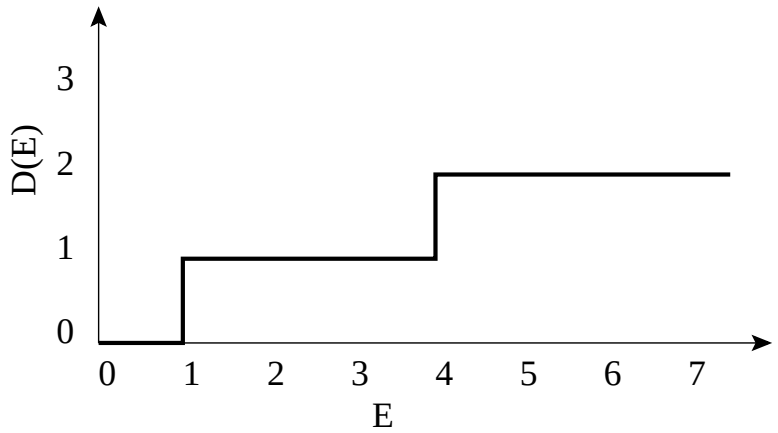
*(a)* For free electron motion in two dimensions, the electronic density of states $D(E) \sim E^p$. State the value of $p$ and briefly justify your answer.

**Answer:** For a massive particle $E \sim k^2$. Consider the reciprocal space surface $k(E)$ of constant energy $E$. Its area=$\pi k(E)^2 \sim E$ contains a number of states $\mathcal{N}(E) \sim E$. The density of states $D(E) = d\mathcal{N}(E)/dE$ is independent of $E$, hence $p = 0$.

*(b)* A quantum well formed in a semiconductor heterostructure can be modeled with a potential

$$V(x,y,z) = \begin{cases} 0 & (|z| < a/2) \\ +\infty & (a/2 < |z|). \end{cases}$$

On the axes below, sketch the density of states $D(E)$ for this quantum well and comment on any notable features. On this figure, the units of energy are $[(\hbar^2/2m)(\pi/a)^2]$ and the units of $D(E)$ are arbitrary. You may wish to recall the solution of the "particle in a box" problem, $E_n = (\hbar^2/2m)(n\pi/a)^2$ with $n \geq 1$ a positive integer.




**Answer:** No state has energy less than $E_1$. For $E_1 < E < E_2$, we have $D(E)$ constant (the motion is free in the $xy$ plane and $n = 1$ along $z$. For $E_2 < E < E_3$ we have both $n = 1$ and $n = 2$ $z$-states, each of which has a constant constribution to $D(E)$.