Answers to Final Exam, Physics 240A

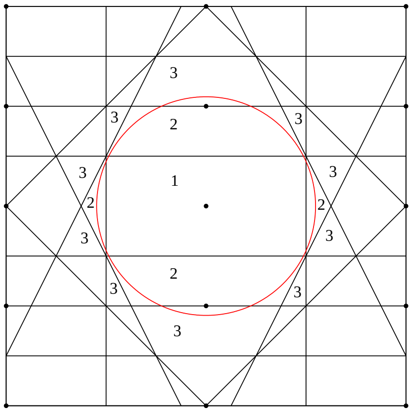
1. The statement is correct. For the Sommerfeld model, electrons are treated as free electrons between collisions. Any interaction with the lattice ions must manifest itself by causing collisions, since it certainly isn't accounted for anywhere else in the model. (This doesn't say whether it's the dominant source of collisions, though.) In the semiclassical model, the periodic potential of the lattice is built into the electron wave functions describing the motion between collisions. The lattice ions are already accounted for before collisions are considered.

2. a) The semiclassical equations of motion are $\hbar\dot{k} = -eE$ and $v(k) = \frac{1}{\hbar}\frac{\partial\varepsilon(k)}{\partial k} = \frac{a}{\hbar}\sin ak + \frac{2a}{\hbar}\sin ak\cos ak = \frac{a}{\hbar}(\sin ak + \sin 2ak)$. From the first equation, k decreases at the same steady rate, regardless of its initial value. The value of v is determined from the second equation and the instantaneous value of k. At $k = \pi/6a$, $v(\pi/6a) = \frac{a}{\hbar}(\sin\pi/6 + \sin\pi/3) = \frac{a}{\hbar}\frac{1+\sqrt{3}}{2}$. As k decreases, both sine functions decrease, so the electron slows down. This is qualitatively correct classically: an electron that initially moves in the direction of an electric field decelerates. At $k = \pi/2a$, $v(\pi/2a) = \frac{a}{\hbar}$. This time as k decreases, $\sin ak$ decreases slowly but $\sin 2ak$ increases quickly. Hence v increases, which is *not* classical: the electric field is accelerating a negative charge in the direction of the field! For $k = \pi/a$, $v(\pi/a) = 0$. As k decreases, v becomes negative. This again is classical behavior, with the electric field accelerating an electron in the direction opposite the field.

b) The band maxima and minima occur when $0 = \frac{\partial\varepsilon}{\partial k}$, or $0 = \sin ak + \sin 2ak = \sin ak + 2\sin ak\cos ak = \sin ak(1 + 2\cos ak)$. It turns out that $k = 0$ and $k = \pi/a$ are minima, while $k = 2\pi/3a$ is a maximum. Finding the effective mass means approximating $\varepsilon(k)$ by a parabola $A(k - k_o)^2$ near an extremum at k_o, and setting $A = \hbar^2/2m^*$ as if the electron is behaving like a free electron except for its altered mass. From Taylor expansions, $A = \frac{1}{2}\frac{\partial^2\varepsilon}{\partial k^2}$. Near $k_o = 0$, $m^* = 2A/\hbar^2 = 3a^2/hbar^2$. Near $k_o = \pi$, $m^* = a^2/\hbar^2$. Near $k_o = 2\pi/3a$, $m^* = -a^2/\hbar^2$, a non-classical result since the mass is negative! In general, the non-classical behavior appears near a band maximum, where the curvature is the opposite from the classical expectation.

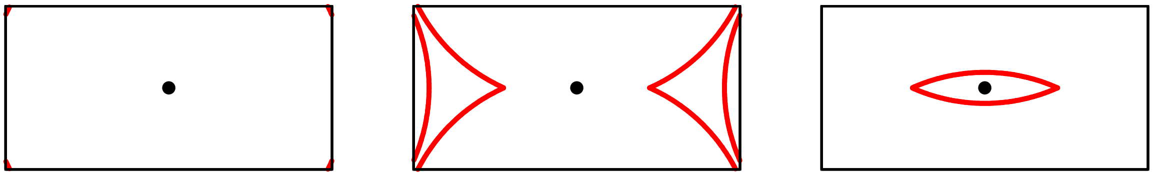
3. a) The rectangular lattice generated by $\mathbf{b_1} = \frac{2\pi}{a}\hat{\mathbf{x}}$ and $\mathbf{b_2} = \frac{\pi}{a}\hat{\mathbf{y}}$. (Note the long side is vertical for the original real lattice but horizontal for the reciprocal lattice.)

b) Note that reaching the nth Brillouin zone from the central lattice point involves crossing exactly $n-1$ of the perpendicular bisectors of lines from the central lattice point to other lattice points. The red circle shows the Fermi surface for part d).



c) Each orbital state takes a k-space area of $(2\pi/L)^2$ for an $L\times L$ sample. With spin, each electron state takes area $2\pi^2/L^2$. The total number of states below the Fermi energy equals the total number of electrons, so $N = (\pi k_F^2)/(2\pi^2/L^2)$, or $n = N/L^2 = k_F^2/2\pi$. The free-electron Fermi surface is a circle of radius k_F, which first touches the (horizontal) edge of the first Brillouin zone for $k_F = \pi/2a$. This gives $n = 7.4\times 10^{14}/\text{cm}^2$.

d) Now $k_F = \sqrt{2\pi n} = 1.5/\text{Å}$. Since $\pi/a = 1.37/\text{Å}$, the Fermi surface (red) extends slightly into the third Brillouin zone. Also, the corners of the first Brillouin zone are at $1.53/\text{Å}$, so they are not included in the Fermi surface. The second-zone part inside the Fermi surface includes the middle of the Brillouin zone and also the portions at the far left and far right. (Figures on top of next page.)



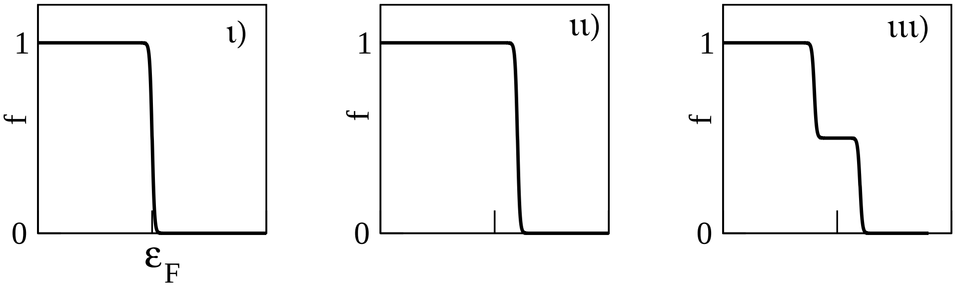
e) Gaps open up at crossings, which in this case means boundaries between Brillouin zones. The Fermi surface also rounds out and becomes perpendicular to the zone edges. At each edge, the energy of states moves down slightly in the lower zone (so the Fermi surface moves outward) and up slightly in the higher zone (so the Fermi surface moves inward). That means the first zone region gets larger (or perhaps fills the entire zone), the second-zone pieces mapped back into the first zone move inward at the edges and outward in the middle (the part that comes from the boundary with the third zone), and the third-zone piece gets smaller.

f) The strongest coupling is to states that have the same energy AND differ in k by exactly a reciprocal lattice vector. There are three: $\mathbf{k} = (\frac{3\pi}{2a}, -\frac{\pi}{2a})$, $\mathbf{k} = (-\frac{\pi}{2a}, \frac{3\pi}{2a})$, and $\mathbf{k} = (-\frac{\pi}{2a}, -\frac{3\pi}{2a})$. The relevant q's are, respectively, $(0, \frac{\pi}{a})$, $(\frac{2\pi}{a}, -\frac{\pi}{a})$, and $(\frac{2\pi}{a}, \frac{2\pi}{a})$. (Using the negatives of these q's is equivalent, since $U_q = U^*_{-q}$.)

g) You need to diagonalize a 4×4 matrix, and some of the matrix elements are given by links among the three k-vectors that couple to the original k. So the coefficients for $q = (\frac{2\pi}{a}, -\frac{2\pi}{a})$, $q = (\frac{2\pi}{a}, \frac{\pi}{a})$, and $q = (0, \frac{3\pi}{a})$ are needed.

4. a) The Fermi surface.

b)



A magnetic field shifts the relative energies of up spins and down spins, so that their occupation numbers are not equal and a nonzero $\mathbf{M}$ develops.

c) Minima occur at complete filling. (This is a minimum of $\mathbf{M}$ as well as a minimum of χ.) There is no flexibility for an electron to flip its spin by moving to a state with higher orbital energy, unless it moves to the next Landau level at a considerable price in orbital energy. So very few electrons can change spin in response to a changing magnetic field. Similarly, maxima occur at half-filling because there is the most freedom for electrons to change spin at low energy cost.

d) Look at oscillations in H and from them calculate $\Delta(\frac{1}{H})$. For the more rapid oscillation, corresponding to the larger cross-sectional area, about 8 periods from 3.85 T to 3.90 T means 8 periods from 2.564×10^{-5} to 2.597×10^{-5} gauss, so $\Delta(\frac{1}{H}) = 4.2 \times 10^{-8}$ gauss. Then use $A = 2\pi e/\hbar c\Delta(\frac{1}{H}) = 2.3 \times 10^{15}/\text{cm}^2$. Since this ellipse has one axis a factor of five longer than the other, $\pi ab = 5\pi a^2 = 2.3 \times 10^{15}$ gives 1.2×10^7/cm and 6.0×10^7/cm for the half-axes of the ellipsoid. (The axes are twice these lengths, of course.)

e) If $k_B T$ is comparable to the energy spacing between levels, $\hbar\omega_c = \hbar eH/m^*c$, the oscillations will be smeared out; so clearly the temperature is much lower. In the absence of information on m^* (you would need to know something about how quickly the energy changes upon moving perpendicular to the Fermi surface) you might as well approximate it by m. This gives $T << \hbar eH/mck_B = 5$ K.