

Physics 240A: Final Exam. 12/12/07

1. Density of States. 15 points.

A two-dimensional material has a “relativistic” dispersion relation $\varepsilon_k = \alpha|\vec{k}|$. [A currently popular example of such a peculiar system is *graphene*, a single layer of graphite.]

(a) Calculate, carefully, the velocity. Make sure your result makes sense physically.

Solution: the velocity is $(1/\hbar)\nabla\varepsilon_k = i(\alpha/\hbar)\hat{k}$. Is this result, a constant velocity directed radially, reasonable? Yes, a simple sketch of ε_k will verify this. **Note:** any time ε_k depends only on $|\vec{k}|$ (i.e. it is isotropic) then the velocity direction is \hat{k} .

(b) Calculate the density of states, showing all work. Strive to get the constants correct, as well as the energy dependence.

Solution:

$$\begin{aligned} N(E) &= \frac{1}{N} \sum_{k,s} \delta(E - \varepsilon_k) = \frac{1}{N} \frac{V}{4\pi^2} 2 \int d^2k \delta(E - \varepsilon_k) = \frac{V_{cell}}{2\pi^2} \int_{S(E)} \frac{dS_k(E)}{|\nabla\varepsilon_k|} \\ &= \frac{V_{cell}}{2\pi^2} \frac{2\pi k(E)}{\alpha} = \frac{V_{cell}}{\pi} \frac{E}{\alpha^2}. \quad \frac{N(E)}{V_{cell}} = \frac{E}{\pi\alpha^2}. \end{aligned}$$

We have used $k(E) = E/\alpha$, a factor of two for spin, and standard factors for 2D. So unlike for a k^2 dispersion where $N(E)$ is constant (for positive energies) in 2D, in this case $N(E) \propto E$.

2. Tight Binding Representation of a Binary Compound in 2D. 15 points.

A binary compound in 2D has a square lattice, with atom A at the origin and atom B in the center of the square.

(a) For a single orbital on each atom (energies $\varepsilon_A, \varepsilon_B$) and near-neighbor hopping of each of the types t_{AA}, t_{BB}, t_{AB} , calculate the expression for all of the independent matrix elements of the tight binding Hamiltonian. You do *not* need to diagonalize.

Solution:

$$H_{AA} = \varepsilon_A + 2t_{AA}[\cos(k_x a) + \cos(k_y a)], \quad (1)$$

$$H_{BB} = \varepsilon_B + 2t_{BB}[\cos(k_x a) + \cos(k_y a)], \quad (2)$$

$$\begin{aligned} H_{AB} &= t_{AB}[1 + e^{i\vec{k}\cdot(-a,0)} + e^{i\vec{k}\cdot(0,-a)} + e^{i\vec{k}\cdot(-a,-a)}] \\ &= t_{AB}[e^{-ik_x a/2}\{e^{ik_x a/2} + e^{-ik_x a/2}\} + e^{-ik_y a} e^{-ik_x a/2}\{e^{ik_x a/2} + e^{-ik_x a/2}\}] \\ &= 2t_{AB}\cos(k_x a/2)e^{-ik_x a/2}[e^{-ik_y a/2}\{e^{-ik_y a/2} + e^{ik_y a/2}\}] \\ &= 4t_{AB}\cos(k_x a/2)\cos(k_y a/2)e^{-i(k_x+k_y)a/2}. \end{aligned}$$

and $H_{BA} = (H_{AB})^*$. This is perhaps the most elegant way to express it.

(b) In the limit where $|\varepsilon_A - \varepsilon_B|$ is large, describe what the bands will look like. The answer can be given in sentences, but use expressions if you want. First describe what should be meant by this limit.

Solution: to be well within this limit, one would estimate something like $|\varepsilon_A - \varepsilon_B| > 8t_{AB}, 8t_{AA}, 8t_{BB}$ (since $8t$ is the bandwidth, and this limit will hold when the bands are separated). The point is that when the separation of the band centers becomes greater than the coupling between them, the A bands and B bands will begin to become nearly independent bands. One limit is simple: if $t_{AB}=0$, then there are separate A and B bands; even if they overlap, they are separate in essence since there is no coupling. These isolated bands will look like the simple 2D near-neighbor TB bands that we have discussed, and which are discussed so much in the context of high temperature superconductors.

3. Lattice Questions. 10 points.

(a) Describe a rhombohedral Bravais lattice.

Solution: Mathematically, it is specified by $a = b = c$, $\alpha = \beta = \gamma \neq 90^\circ$. Physically, and not very precisely, one might say it has equal length direct lattice vectors symmetrically placed around a single three-fold axis, with angles such that it is not *fcc*.

(b) How many Bravais lattices are there in 3D? Give the names of seven of them.

Solution: 14 Bravais lattices. *sc*, *bcc*, *fcc*; *tetragonal*, *bct*; *orthorhombic*, *b(ase)co*, *b(od)co*, *fcc*; *monoclinic*, *bcm*; *triclinic*; *hex*, *rhombohedral*.

(c) Given direct lattice vectors $\vec{R}_1, \vec{R}_2, \vec{R}_3$, give the expression(s) for the reciprocal lattice vectors.

Solution:

$$\vec{G}_i = 2\pi \frac{\vec{R}_j \times \vec{R}_k}{\vec{R}_i \cdot \vec{R}_j \times \vec{R}_k}.$$

with i, j, k being cyclic integers 1, 2, 3.

4. Structure Factor. 10 points.

(a) Write the **general** expression for the structure factor of a crystal. Define/specify all quantities that enter the expression carefully.

Solution: the structure factor is

$$S_G = \sum_j f_j(G) e^{i\vec{G} \cdot \vec{\tau}_j},$$

where the sum runs over all atoms in the unit cell, at positions $\vec{\tau}_j$. The ‘form factor’ $f_j(G)$ is atom-dependent, being the Fourier transform of the charge density of the atom.

(b) For a square lattice (lattice constant a) in 2D with atom K (potassium) at the origin and atom Cl at $(1,1)a/2$, write the structure factor for an arbitrary reciprocal lattice vector \vec{G} in as simple and informative form as possible.

Solution: Let a general RLV be denoted $\vec{G} = h\vec{G}_1 + k\vec{G}_2$ in terms of the primitive RLVs, h, k are integers. Then

$$S_G = f_K(G) + f_{Cl}(G) e^{i\pi(h+k)} = f_K(G) + (-)^{h+k} f_{Cl}(G).$$

(c) In (b), K and Cl just labeled different atoms. But K ($Z=21$) and Cl ($Z=19$) are similar in size and number of electrons; in fact, K^+ and Cl^- are isoelectronic. For KCl in this square lattice, what more can be said about the structure factor?

Solution: The structure factors are nearly equal, so let $f_K = \bar{f} + \delta$; $f_{Cl} = \bar{f} - \delta$ define the average and the difference. Then

$$\begin{aligned} S_G &= \bar{f}[1 + (-)^{h+k}] + \delta[1 - (-)^{h+k}]. \\ &= 2\bar{f}, \quad h+k = \text{even} \\ &= 2\delta, \quad h+k = \text{odd}. \end{aligned}$$

I.e. the structure factor is large (diffraction spot is bright) for the even $h+k$ points in the plane, and small for odd $h+k$. In the limit that the atoms become identical, the lattice is a square lattice rotated by 45° with half the area per cell, the reciprocal lattice becomes twice as large (in area) because some of the RLVs have “disappeared” ($\delta \rightarrow 0$). It is the odd $h+k$ spots that have vanished.

5. Heat Capacity of an Electron Gas. 15 points.

(a) What would be the specific heat of an electron gas of density n if electrons were classical particles?

Solution: The internal energy is $\frac{3}{2}Nk_B T$ for N particles, so the specific heat (heat capacity per unit volume here) is $\frac{3}{2}bk_B$.

(b) Give the expression for the electronic specific heat C_V for a metal at temperature T , assuming T is much smaller than the Fermi temperature.

Solution: the essential aspects are that C_V is proportional to T (not independent of it), and also proportional to $N(E_F)$. More specifically,

$$C_V = \frac{\pi^2}{3}k_B^2 T N(E_F) = \frac{\pi^2}{3}k_B \times [k_B T N(E_F)].$$

Here $N(E_F)$ is the DOS per unit volume, and it is important to know that the last factor in brackets is very small.

(c) Explain this classical \leftrightarrow quantum difference in a few sentences.

Solution: in the classical gas the electrons are completely independent of each other. In the quantum Fermi gas, the electrons are identical and only one can occupy any given state. At $T=0$ they occupy all states up to the Fermi energy (the Fermi sphere). At $T > 0$ the only electrons that can be thermally excited (and have energy $\sim k_B T$) are those within $\sim k_B T$ of E_F . The rest of the electrons, almost all of them in fact, are frozen out by the Fermi exclusion principle.

6. Homogeneous Electron Gas in 2D. 10 points.

For a homogeneous electron gas in two dimensions with density n , derive the expression for the Fermi energy $E_F(n)$.

Solution:

$$N = 2 \sum_k \Theta(\varepsilon_k - E_F) = 2 \frac{A}{(2\pi)^2} \int_0^{k_F} 1 d^2k = \frac{A}{2\pi^2} \pi k_F^2.$$

Then $n = N/A = k_F^2/2\pi$, so $E_F(n) = \hbar^2 k_F^2/(2m) = (\hbar^2/2m)2\pi n = (\pi\hbar^2/m)n$.

7. Electronic Structure Methods. 10 points.

(a) Describe, mostly using words, the main *similarities* and *differences* (several of each) between the Hartree-Fock method and the Density Functional Theory approach.

Similarities:

both are many-body theories for the energy (they treat interacting electrons, not non-interacting ones);

they both construct and minimize an energy functional;

they both lead to “single particle” eigenfunctions and dispersion relation.]]

Differences:

HF is based on a many-electron wavefunction; DFT hardly mentions the wavefunction and focuses on the density (both for the ground state, of course);

HF has a perfectly known but approximate energy functional based on an approximate wavefunction, while DFT has an imperfectly known functional that in principle generates the exact energy and density.

(b) Each of these two methods is applied to the (interacting) homogeneous electron gas. Describe the wavefunctions, dispersion relation $\varepsilon_{k,n}$, and contributions to the total energy E_{tot} , for each method. [Some of (b) may overlap with (a), that's OK.]

Wavefunctions: HF provides an (approximate) g.s. many-particle wavefunction based on variationally optimized single-particle orbitals. DFT expands the density in terms of single-particle orbitals. In each method, these orbitals are the solution of a set of coupled single-particle-like ‘Schrödinger equations’, they simply have different effective potentials. HF has an explicit (and non-local, hence complicated) exchange potential; DFT has an exchange potential and correlation potential that must be approximated somehow.

Dispersion relations: for each, $\varepsilon_{k,n}$ result from the ‘Schrödinger equations’, and although they differ considerably in specific details, on the large scale they have a lot of similarities. These provide the ‘band structure’ in each method.

Total Energy: in each case these are obtained from the functional, with a lot of similarities: kinetic energy part, interaction with external potential, Hartree interaction amongst electrons. HF has in addition an ‘exact’ exchange energy; DFT has an approximate exchange energy and a correlation energy. Each method allows the calculation of properties that can be obtained from the electronic ground state: equation of state and structural transitions under pressure; phonon dispersion curves; ...

8. Bloch's Theorem. 15 points.

(a) State Bloch's theorem, using the appropriate mathematical expressions.

Solution: each single-particle wavefunction (or 'orbital') is given by the form

$$\psi_{k,n}(r) \propto e^{i\vec{k}\cdot\vec{r}} u_{k,n}(r),$$

where \vec{k} is a 'quantum number' associated with the translational symmetry of the state. The function $u_{k,n}$ is periodic from unit cell to unit cell, hence it only needs to be determined in a single cell.

(b) Describe, using one approach (there are a few), the steps that are involved in proving Bloch's theorem. You're not being asked to give a proof. A full proof will get full credit, but a correct statement of the necessary steps will also get full credit.

Example: a state ψ_k must 'contain the same physical information' in each unit cell, based on symmetry grounds. Thus $\psi_k(r + R)$ in another cell must be just some constant C times its value in the cell at the origin $\psi_k(r)$. Applying this rule to cell 1, then cell 2, then 3,... leads to the constant in cell j satisfying $C_j = (C_1)^j$. To keep the wavefunction regular at very large R requires $|C| = 1$. Then applying periodic boundary conditions in our big, macroscopic supercell of N cells leads to $C_j = e^{i\vec{k}\cdot\vec{R}}$. This requirement in term leads to the Bloch form of wavefunction.

Alternatively: you can try to explain how this form results from the symmetry of the differential equation (Floquet's theorem).