Physics 725: Solid State Physics I

Final Exam

Tuesday, December 8, 2015 / 12:00–15:00 / Room 104, Lewis Hall

Student's Name: _____

Instructions

There are 27 questions. You should attempt all of them. Mark your response on the test paper in the space provided. Please use a pen. If in answering a question you sketch a diagram, please provide meaningful labels. Aids of any kind—including class notes, textbooks, cheat sheets, and calculators—are not permitted.

Good luck!

12 points	multiple choice	questions 1–12
12	short answer	13–24
16	mathematical	25–27
40 points		

Useful identities

$$\int_0^\infty \frac{x\,dx}{e^x-1} = \frac{\pi^2}{6} \qquad \int_0^\infty \frac{x\,dx}{e^x+1} = \frac{\pi^2}{12}$$

$$\int_0^\infty \frac{x^3\,dx}{e^x-1} = \frac{\pi^4}{15} \qquad \int_0^\infty \frac{x^3\,dx}{e^x+1} = \frac{7\pi^4}{120}$$

$$\int_0^\infty dx\, e^{-\alpha x^2} = \frac{\sqrt{\pi}}{2\alpha^{1/2}} \qquad \int_0^\infty dx\, x^2 e^{-\alpha x^2} = \frac{\sqrt{\pi}}{4\alpha^{3/2}}$$

$$\cos(A-B) = \cos A\cos B + \sin A\sin B \qquad \cos(x) = 1 - \tfrac{1}{2!}x^2 + \tfrac{1}{4!}x^4 - \cdots$$

$$\sin(A+B) = \sin A\cos B + \cos A\sin B \qquad \sin(x) = x - \tfrac{1}{3!}x^3 + \tfrac{1}{5!}x^5 - \cdots$$

Conversion factors

$$\begin{aligned} 1\,\mathrm{eV} &= k_\mathrm{B}\cdot(11{,}605\,\mathrm{K}) \\ k_\mathrm{B} &= 8.617\times10^{-5}\,\mathrm{eV}\cdot\mathrm{K}^{-1} \\ \hbar &= 6.582\times10^{-16}\,\mathrm{eV}\cdot\mathrm{s} \\ hc &= 1240\,\mathrm{eV}\cdot\mathrm{nm} \end{aligned}$$

Multiple choice questions (12 points)

Answer by circling one of (a), (b), (c), etc. directly on the test paper

1. It takes ~ 1 meV to break a Cooper pair in a superconductor. A bacterium expends ~ 1 MeV to replicate itself. What is the energy scale involved in a typical covalent bond?

   (a) 0.1–1 eV
   (b) 1–10 eV
   (c) 10–100 eV
   (d) 0.1–1 keV
   (e) 1–10 keV

2. An agglomeration of atoms is found at instantaneous positions $\{\boldsymbol{R}_i\}$. The atoms have a hard-core radius $\sigma/2$ and are contained in a region of linear size L. What feature of the pair distribution function

$$g(r) = \left\langle \sum_{i<j} \delta(r - |\boldsymbol{R}_i - \boldsymbol{R}_j|) \right\rangle_{\text{time average}}$$

   signals the onset of crystalline order?

   (a) it vanishes for all $r < \sigma$
   (b) it vanishes at long distances $r \sim L$
   (c) additional weight builds up around $r = \sigma$
   (d) the appearance of distinct peaks at characteristic neighbour distances

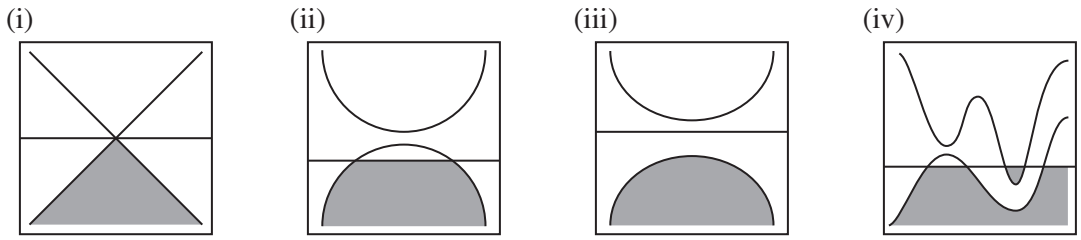
3. Some alloys will form a superlattice structure if they are

   (a) annealed
   (b) quenched
   (c) irradiated
   (d) ionized

4. The shape of a Landau level in k-space is

   (a) cylindrical
   (b) spherical
   (c) hyperbolic
   (d) parabolic
   (e) block diagonal

5. The band structures (energy versus wavevector) shown below are all drawn on the same scale. The Fermi energy is indicated with a horizontal line, and the filled states are shaded.



Which of these statements is incorrect?

(a) (i) is a semi-metal with a vanishing density of states at the Fermi level; electronic excitations, however, are not gapped

(b) in the case of (ii) and (iii), the density of states has a gap

(c) in the case of (iv), the lowest-lying excitations traverse an indirect band gap

(d) in the case of (iv), there are contributions of opposite sign to the Hall current

(e) (ii) is a conductor; (iii) is an insulator

6. Suppose that the work function of a metal is $W = 1\,\text{eV}$. What is the critical wavelength of a photon below which it can eject an electron from the metal (i.e., photoemission)?

(a) $\sim 10\,\text{nm}$

(b) $\sim 100\,\text{nm}$

(c) $\sim 1000\,\text{nm}$

7. What physical feature corresponds to truncation of the Ewald sum in an ionic solid?

(a) interstitial or substitutional impurities

(b) negative index of refraction

(c) crystal surface

8. The simple, body-centred, and face-centred cubic lattice structures can be expressed in terms of a *conventional* unit cell that is x, y, and z times larger, respectively, than the *primitive* unit cell. What are the correct values?

(a) $x = y = z = 1$

(b) $x = 1$, $y = 2$ and $z = 4$

(c) $x = 1$, $y = z = 2$

(d) $x = 1$, $y = z = 4$

(e) none of them

9. For electrons in *one* spatial dimension (moving in a linear chain of atoms, say), the electronic density of states $D(\epsilon)$ that is produced by a band edge at $\epsilon = 0$ scales as which of the following?

   (a) $\epsilon^{3/2}$

   (b) $\sqrt{\epsilon}$

   (c) $-\log 1/\epsilon$

   (d) $1/\sqrt{\epsilon}$

   (e) $\epsilon^{-3/2}$

10. Low-energy electron diffraction (LEED) is an experimental technique to measure structure by bombarding the material surface with a collimated beam of low energy electrons. Indicate whether the following statements are true or false.

   (t / f) LEED requires a single-crystal sample with a surface cut along a crystal facet

   (t / f) LEED can image arbitrary arrangements of atoms at the surface, even non-periodic ones.

11. The bare interaction potential between pairs of electrons is given by a transform pair $V(r) \sim 1/r$, $V(q) \sim 1/q^2$ that describes the Coloumb repulsion in real space and Fourier space. In a material environment with mobile charge carriers, however, the potential is screened. The Thomas-Fermi approach is a static approximation (no retardation) that introduces a screening length λ^{-1}. Which of the following forms is <u>not</u> consistent with the Thomas-Fermi theory?

   (a) $V(r) \sim \frac{e^{-\lambda r}}{r}$

   (b) $V(q) \sim \frac{1}{q^2+\lambda^2}$

   (c) $V(q) \sim \frac{e^{-q/\lambda}}{q^2}$

12. We denote the s-wave and p-wave valence orbitals of a carbon atom by $|\mathrm{s}\rangle$ and $|\mathrm{p}_\alpha\rangle$ with $\alpha = \mathrm{x}, \mathrm{y}, \mathrm{z}$. The four linear combinations

$$
\begin{aligned}
|1\rangle &= \frac{1}{2}|\mathrm{s}\rangle + \sqrt{\frac{2}{3}}|\mathrm{p_x}\rangle - \frac{1}{2\sqrt{3}}|\mathrm{p_z}\rangle \\
|2\rangle &= \frac{1}{2}|\mathrm{s}\rangle - \frac{1}{\sqrt{6}}|\mathrm{p_x}\rangle + \frac{1}{\sqrt{2}}|\mathrm{p_y}\rangle - \frac{1}{2\sqrt{3}}|\mathrm{p_z}\rangle \\
|3\rangle &= \frac{1}{2}|\mathrm{s}\rangle - \frac{1}{\sqrt{6}}|\mathrm{p_x}\rangle - \frac{1}{\sqrt{2}}|\mathrm{p_y}\rangle - \frac{1}{2\sqrt{3}}|\mathrm{p_z}\rangle \\
|4\rangle &= \frac{1}{2}|\mathrm{s}\rangle + \frac{\sqrt{3}}{2}|\mathrm{p_z}\rangle
\end{aligned}
$$

   represent sp^n hybridization with what geometry?

   (a) $n = 1$, linear

   (b) $n = 2$, trigonal

   (c) $n = 3$, tetrahedral

Short answer questions (12 points)

Keep your answers brief and to the point.

13. At what angle do the (110) and (111) planes of a simple cubic crystal intersect?

14. Explain what a *contact potential* is.

15. The pair potential for a collection of N atoms has the Lennard-Jones form

$$V(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right].$$

Estimate their equilibrium separation at low temperature. Estimate the binding energy per atom, assuming a crystalline phase with lattice coordination z (the number of nearest neighbours).

16. How do the heat capacity of an ideal quantum gas and an ideal classical gas differ? In what temperature regime do they coincide?

17. As you showed in Assignment 3, the electronic chemical potential shifts away from its zero-temperature value (ϵ_F) according to $\mu \approx \epsilon_F - [\pi^2 k_B^2 D'(\epsilon_F)/6D(\epsilon_F)]T^2$. Explain why the temperature variation might be much weaker than $O(T^2)$ in a two-dimensional electron gas.

18. Explain what we mean by *thermionic emission*. Justify the temperature dependence of the current

$$j = -\frac{em}{2\pi^2\hbar^3}(k_B T)^2 e^{-W/k_B T}$$

that is established in thermal equilibrium.

19. Explain why you can have neither van Hove singularities nor Fermi surface nesting in the case of electrons whose dispersion $\varepsilon_{\boldsymbol{k}} = \hbar^2 k^2 / 2m^*$ is perfectly free-electron-like.

20. What does it mean that the gap in one semiconductor is *direct* and in another *indirect*? Why does the distinction matter?

21. Describe the competing effects that govern surface roughening.

22. What is the distinction between *lattice relaxation* and *surface reconstruction* in a finite crystal?

23. We can write the work function of a metal as $W = -E_F + e\int \boldsymbol{E} \cdot d\boldsymbol{r}$. Explain what these terms mean and where they come from. In particular, how does the field $\boldsymbol{E}$ arise?

24. At the junction between n-type and p-type regions of a doped semiconductor, there is a *depletion layer*. What is that? And what governs its width?

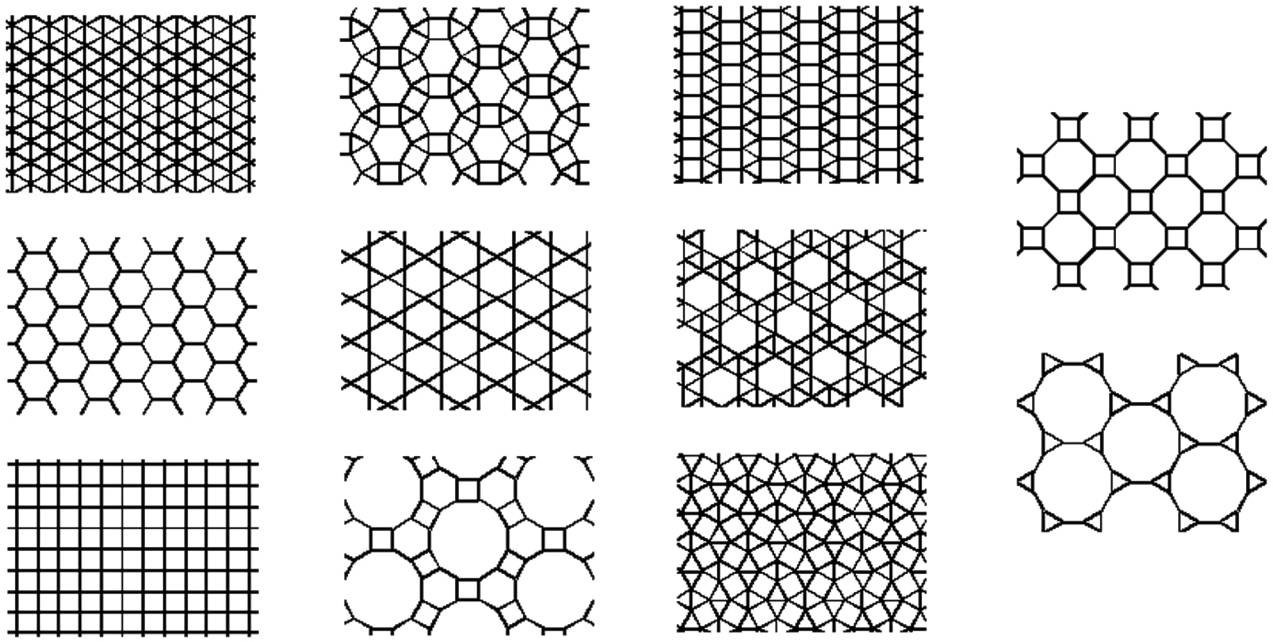
Mathematical problems (16 points)

25. (2 points) A gas of independent electrons moving in a periodic background potential has density

$$n = 2 \sum_{\alpha} \int \frac{d^3k}{(2\pi)^3} f(\varepsilon_{\boldsymbol{k},\alpha} - \mu),$$

where the dispersion $\varepsilon_{\boldsymbol{k},\alpha}$ is a function of a wave vector $\boldsymbol{k}$ in the Brillouin Zone and a band index α. Show that, at low temperatures, the electronic compressibility $\partial n/\partial \mu$ is proportional to the density of states at the Fermi level.

26. (2 points) Consider the 11 Archimedean lattices (two-dimensional) shown below.



Each of these can be expressed as a Bravais lattice plus a basis. Indicate how many basis elements are required in each case.

27. Consider a triangular lattice in two dimensions (see the top-left diagram in question 26), rotated such that one of the lattice vectors coincides with the x axis.

    (a) (1 point) Write down an appropriate set of lattice vectors.

    (b) (2 points) Construct the corresponding reciprocal lattice vectors and the (Wigner-Seitz) Brillouin Zone.

(c) (3 points) Assume that there is a single electronic orbital on each site having overlap s and hopping integral $-t$ with its nearest neighbours only. Show that the tight-binding band structure is of the form

$$\varepsilon_{\boldsymbol{k}} = \frac{-2t\gamma_{\boldsymbol{k}}}{1 + 2s\gamma_{\boldsymbol{k}}}$$

and report an expression for $\gamma_{\boldsymbol{k}}$ in terms of cosines only. (If you don't know how to proceed, solve the problem for $s = 0$.)

(d) (2 points) Expand $\gamma_{\boldsymbol{k}}$ around the bottom of the band ($\boldsymbol{k} = 0$) in powers of k_x and k_y. Keep terms at order zero, two, and four.

(e) (2 points) Compute the effective mass at very low band filling. It will be a function of both s and t.

(f) (2 points) Explain why it is legitimate to write the density of states as

$$D(\epsilon) = \int_{-\frac{2\pi}{a}}^{\frac{2\pi}{a}} dk_x \int_{-\frac{2\pi}{\sqrt{3}a}}^{\frac{2\pi}{\sqrt{3}a}} dk_y \, \delta(\varepsilon_{\boldsymbol{k}} - \epsilon).$$

(*Hint:* I'm looking for a geometrical argument in k-space that explains the limits of integration.)

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