Physics 541: Condensed Matter Physics

Final Exam

Monday, December 17, 2012 / 14:00–17:00 / CCIS 4-285

Student's Name: ________________________

Instructions

There are 24 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!

10 points	multiple choice	questions 1–9
12	short answer	10–20
28	mathematical	21–24
50 points		

Useful identities

$$\int_0^\infty \frac{dx}{e^x - 1} = \infty \qquad \int_{x_0}^\infty \frac{dx}{e^x - 1} = -\log(e^{x_0} - 1) + x_0$$

$$\int_0^\infty \frac{x\,dx}{e^x - 1} = \frac{\pi^2}{6} \qquad \int_0^\infty \frac{x^2\,dx}{e^x - 1} = 2\zeta(3) = 2\left(1 + \frac{1}{2^3} + \frac{1}{3^3} + \frac{1}{4^3} + \cdots\right)$$

$$\int_0^\infty \frac{x^3\,dx}{e^x - 1} = \frac{\pi^4}{15} \qquad \int_0^\infty \frac{x^4\,dx}{e^x - 1} = 24\zeta(5) = 24\left(1 + \frac{1}{2^5} + \frac{1}{3^5} + \frac{1}{4^5} + \cdots\right)$$

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

$$\cos(A - B) = \cos A \cos B + \sin A \sin B$$
$$\sin(A + B) = \sin A \cos B + \cos A \sin B$$

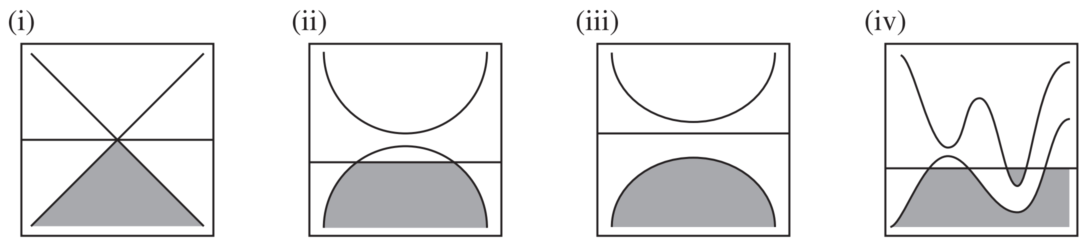
Conversion factors

$$1\,\mathrm{eV} = k_\mathrm{B} \cdot (11{,}605\,\mathrm{K})$$
$$k_\mathrm{B} = 8.617 \times 10^{-5}\,\mathrm{eV} \cdot \mathrm{K}^{-1}$$
$$\hbar = 6.582 \times 10^{-16}\,\mathrm{eV} \cdot \mathrm{s}$$
$$hc = 1240\,\mathrm{eV} \cdot \mathrm{nm}$$

Multiple choice questions (10 points)

Answer by circling one of (a), (b), (c), etc. directly on the test paper—except for question 2, where you'll need to write the letters into the four blanks, and question 3, where you'll circle either true or false. Be sure that each selection is clear and unambiguous.

1. 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 <u>incorrect</u>?

(a) in the case of (iv), there are two contributions of opposite sign to the Hall current
(b) (ii), (iii), and (iv) show a gap in the electronic density of states
(c) (ii) and (iv) are likely to be the best conductors
(d) (i) and (iii) have a vanishing electronic density of states at the Fermi energy.

2. (2 points) Match up these typical condensed matter energy scales

(a) 8 keV, (b) 1.1 eV (c) 0.2 eV (d) 26 meV

with the following descriptions:

____ silicon band gap
____ $k_{\mathrm{B}}T$ for room temperature
____ hydrogen bond
____ x-ray energy for crystal diffraction

3. Indicate whether the following statements about 2 eV photons are true or false.

(t / f) They are in the visible spectrum.
(t / f) They are not quite energetic enough for low energy electron diffraction (LEED)

4. 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 nm
   (b) $\sim$100 nm
   (c) $\sim$1000 nm

5. What physical feature leads to truncation of the Ewald sum in an ionic solid?

   (a) crystal surface
   (b) interstitial or substitutional impurities
   (c) negative index of refraction

6. Which of the carbon orbital hybridizations leads to a trigonal bonding arrangement?

   (a) sp
   (b) sp^2
   (c) sp^3
   (d) all of sp, sp^2, and sp^3
   (e) none of them

7. Which of the following is a typical path through the Brillouin zone in the cubic lattice system?

   (a) A–B–C–A
   (b) I–II–IV–III
   (c) Γ–X–M–Γ–R–X
   (d) Σ–R–W–O–Δ

8. Which Bravais lattice has the largest number of slip planes?

   (a) simple cubic
   (b) face centred cubic
   (c) body centred cubic

9. A cleaved silicon (111) surface can undergo which of the following surface reconstructions?

   (a) 2×1 reconstruction (into orthogonal rows of dimers)
   (b) 3×3 reconstruction
   (c) 5×5 reconstruction
   (d) 7×7 reconstruction

Short answer questions (12 points)

Keep your answers brief and to the point.

10. The electronic configuration of copper, written Cu: [Ar] $3d^{10}\,4s^{1}$, is expressed in terms of its 11 valence electrons and an inert inner shell having the same configuration as argon. Write out the electronic configuration of argon. Explain why we call it a *closed shell* configuration.

11. A wavefunction $|\Psi\rangle = \sum_n \Psi_n |n\rangle$ is expanded in a basis $\{|n\rangle\}$ of localized wavefunctions. Explain how this might give rise to a *generalized* eigenvalue equation (matrix times column vector) $H\Psi = ES\Psi$. Be explicit about what S represents.

12. 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 in the crystalline phase. Estimate the binding energy per atom.

13. The wavefunction $\psi(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3)$ for three indistinguishable quantum particles has the property that $\psi(\boldsymbol{r}, \boldsymbol{r}, \boldsymbol{r}') = \psi(\boldsymbol{r}, \boldsymbol{r}', \boldsymbol{r}) = \psi(\boldsymbol{r}', \boldsymbol{r}, \boldsymbol{r}) = 0$. Argue that, in terms of single-particle states $\{\phi_a, \phi_b, \phi_c\}$, the wavefunction necessarily has the form

$$\psi(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3) = \frac{1}{\sqrt{3!}} \Big[\phi_a(\boldsymbol{r}_1)\phi_b(\boldsymbol{r}_2)\phi_c(\boldsymbol{r}_3) - \phi_a(\boldsymbol{r}_1)\phi_c(\boldsymbol{r}_2)\phi_b(\boldsymbol{r}_3) + \cdots \Big]$$

Carefully write out the four terms that have been elided over.

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

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

that is established in thermal equilibrium.

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

16. In Boltzmann theory, the transport lifetime of a particle is given by

$$\frac{1}{\tau_t} = \frac{2\pi}{\hbar} n_{\text{imp}} \int \frac{d^3k'}{(2\pi)^3} |T_{\boldsymbol{k},\boldsymbol{k}'}|^2 \delta(\epsilon_{\boldsymbol{k}} - \epsilon_{\boldsymbol{k}'})(1 - \cos\theta),$$

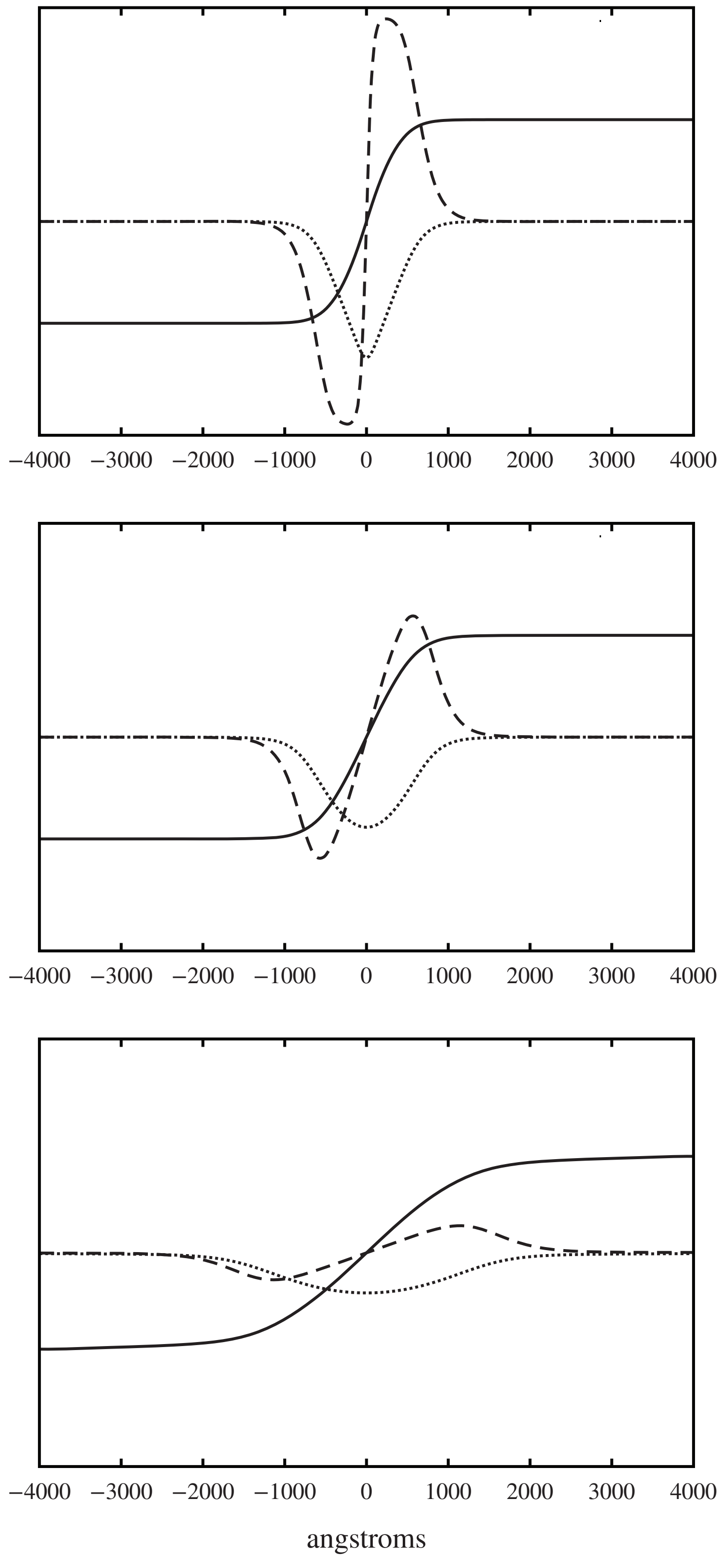
where $kk' \cos\theta = \boldsymbol{k} \cdot \boldsymbol{k}' = kk'(\hat{\boldsymbol{k}} \cdot \hat{\boldsymbol{k}}')$. What happens if the scattering matrix element $T_{\boldsymbol{k},\boldsymbol{k}'}$ is nonzero only when $\hat{\boldsymbol{k}} \approx \hat{\boldsymbol{k}}'$, and what is the consequence for electrical conduction? Conversely, what's the story if $T_{\boldsymbol{k},\boldsymbol{k}'}$ is nonzero only when $\hat{\boldsymbol{k}} \approx -\hat{\boldsymbol{k}}'$?

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

18. Describe how a DC electric field might produce Bloch oscillations in a metal. Why don't we ever observe Bloch oscillations in real materials?

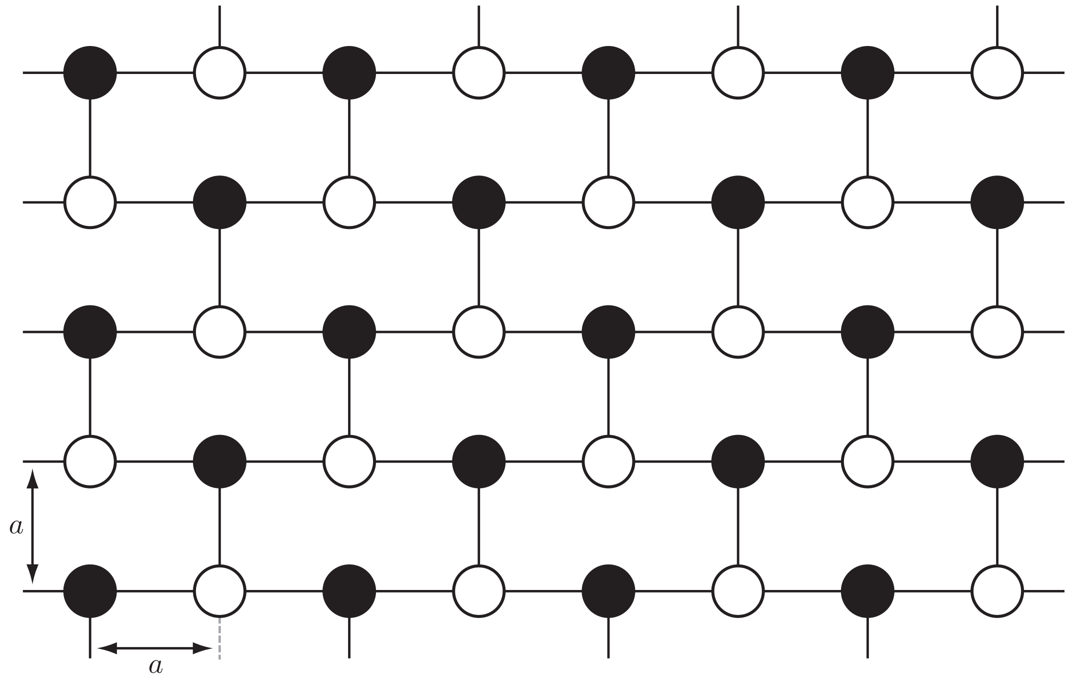
19. In the context of band structure calculations, what problem is the orthogonalized plane wave (OPW) approach meant to solve.

20. (2 points) The figure on the next page shows three linear p-n junctions with the donor density $N_{\mathrm{D}}(x)$ and acceptor density $N_{\mathrm{A}}(x)$ switching from their uniform bulk values over length scales $\ell = 10\,\text{Å}$, $100\,\text{Å}$, and $1000\,\text{Å}$. Please properly label the potential ϕ, the electric field E, and the total charge density $\rho_{\mathrm{tot}} = p - n + N_{\mathrm{D}} - N_{\mathrm{A}}$. (In other words, indicate which of the three curves—solid, dashed, dotted—corresponds to what.) Explain what effect increasing ℓ has on the operation of the device.


−4000 −3000 −2000 −1000 0 1000 2000 3000 4000
−4000 −3000 −2000 −1000 0 1000 2000 3000 4000
−4000 −3000 −2000 −1000 0 1000 2000 3000 4000
angstroms

Mathematical problems (28 points)

All questions in this section refer to the two-dimensional crystal shown below. Two species of atom (with masses m_A and m_B) are laid out in a "brick wall" pattern.



21. (a) (2 points) Find a set of lattice vectors and basis vectors that describe the crystal.

    (b) (2 points) Compute the corresponding reciprocal lattice vectors.

(c) (2 points) Determine the Brillouin zone using the Wigner-Seitz construction.

(d) (2 points) Provide the correct limits of integration for the summation

$$\sum_{\boldsymbol{k}} \to V \int_{?}^{?} dk_x \int_{?}^{?} dk_y$$

over all wavevectors in the Brillouin zone.

22. (4 points) Compute the crystal's structure factor in terms of form factors f_A and f_B. How does it relate to the scattering intensity of incident x-rays? What is the condition for *extinction*?

23. (a) (6 points) Determine the band structure in the tight-binding picture. Assume that there is exactly one (s-wave) electronic orbital per lattice site and that there is no substantial overlap between the orbitals on different sites. Only the hopping integrals $-t$ and $-t'$ between nearest- and next-nearest-neighbour sites contribute.

(b) (4 points) Compute the 2×2 effective mass tensor for an electron at the bottom of the conduction band in the two distinct limits $t = 1, t' = 0$ and $t = 0, t' = 1$.

24. (6 points) This question deals with the model of "bond-directed" pair potentials, in which each atom i that has been displaced (by $\boldsymbol{u}_i$) from its equilibrium position ($\boldsymbol{R}_i^{(0)}$) feels a Hooke's law restoring force directed along the lines to its immediate neighbours. Specifically,

$$\text{restoring force on atom } i = \sum_j K_{ij}[\hat{\boldsymbol{\eta}}_{ij} \cdot (\boldsymbol{u}_j - \boldsymbol{u}_i)\, \hat{\boldsymbol{\eta}}_{ij}].$$

Here, we've defined the unit vectors $\hat{\boldsymbol{\eta}}_{ij} = (\boldsymbol{R}_i^{(0)} - \boldsymbol{R}_j^{(0)})/|\boldsymbol{R}_i^{(0)} - \boldsymbol{R}_j^{(0)}|$ and the spring constant

$$K_{i,j} = \begin{cases} K & \text{between neighbouring sites } i \text{ and } j, \\ 0 & \text{otherwise.} \end{cases}$$

Construct the rank-4 dynamical matrix, and do your best to solve for the phonon modes (dispersion relations and polarizations). You may want to simplify things by treating the special case of $m_A = m_B$ and/or considering only small wavectors $q \ll \pi/a$.

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