# Physics 725: Solid State Physics I

Practice Midterm Exam

Student's Name: _____

## Instructions

There are 23 questions, some with multiple subparts. 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!

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|---|---|---|
| 15 points | multiple choice | questions 1–13 |
| 15 | short answer | 14–21 |
| 20 | mathematical | 22–23 |
| **50 points** | | |

## Multiple choice questions (15 points)

Answer by circling one of (a), (b), (c), etc. directly on the test paper. Be sure that your selection is clear and unambiguous.

1. All but one of the following is associated with the process of solidification. Which one does not belong in the list?

   (a) "spontaneous" reduction of the translational and rotational symmetry

   (b) truly long-ranged positional order

   (c) latent heat of formation

   (d) continuous phase transition

2. Condensed matter physics largely considers physical processes over what range of energies?

   (a) μeV to eV

   (b) meV to keV

   (c) keV to MeV

   (d) MeV to GeV

3. What is the melting temperature of nickel, an fcc crystal?

   (a) 172,800 K

   (b) 17,280 K

   (c) 1728 K

   (d) 172.8 K

4. Which of the following elements is the least chemically reactive?

   (a) Na

   (b) Mg

   (c) S

   (d) Cl

   (e) Ar

5. For crystals of C ($1s^2 2s^2 2p^2$), Si ([Ne]$3s^2 3p^2$), or Ge ([Ar]$3d^{10} 4s^2 4p^2$) in their diamond configuration, the directionality of the local covalent bonds is which one of the following?

   (a) linear

   (b) trigonal

   (c) tetragonal

(2 points) 6. Assign each of these categories in the periodic table—

(a) semi-metals (b) non metals and halogens (c) noble gases
(d) alkali metals and alkaline earths (e) basic metals

—to the most appropriate group of elements below. Write the corresponding letter in the space provided. Each letter should appear exactly once.

____ C N O P S F Cl Br I

____ B Si As Te

____ Li Na K Rb Cs Be Mg Ca Sr

____ Al Ga In Sn Tl Pb Bi

____ He Ne Ar Kr Xe

7. In its cubic unit cell, $BaTiO_3$ (barium titanate) has barium atoms positioned at the 8 cell corners, a titanium atom in the middle, and oxygen atoms centred at each of the 6 faces. What is the size of the crystal basis?

(a) 3
(b) 4
(c) 5
(d) 8
(e) 15

8. Associate one of the two material descriptions below—

(a) hard and brittle; cleaves rather than deforms; good insulator; transparent
(b) relatively ductile; good electrical and thermal conductors; opaque

—with the following three bonding types. Write the corresponding letter in the space provided. Each letter can be appear more than once or not at all.

____ ionic

____ covalent

____ metallic

9. At small wave vector $\boldsymbol{q}$, the group velocity and phase velocity necessarily coincide for which one of the following categories of phonon mode?

(a) acoustic
(b) optical
(c) longitudinal
(d) transverse

10. The pair distribution function $g(r) \sim \langle \sum_{i<j} \delta(r - |\boldsymbol{R}_i - \boldsymbol{R}_j|) \rangle$ describes the average separation between atoms. For a molten system, it is flat and featureless—aside from a small hard-core exclusion region $0 \le r < \sigma$. When the system is cooled and solidifies, $g(r)$ develops a sequence of strong peaks at positions $r > \sigma$. For each sequence below (showing the first three peak distances), identify the Bravais lattice type as

(a) body-centred cubic, (b) face-centred cubic, or (c) simple cubic.

Write the corresponding letter in the space provided. Each letter should appear exactly once.

____ $\frac{\sqrt{3}}{2}a$, $a$, $\frac{\sqrt{11}}{2}a$, ...

____ $\frac{1}{\sqrt{2}}a$, $a$, $\frac{\sqrt{10}}{2}a$, ...

____ $a$, $\sqrt{2}a$, $\sqrt{3}a$, ...

11. After "integrating out" the valence electron degrees of freedom, the ions in a crystal are described by an effective Hamiltonian

$$H = \sum_i -\frac{\hbar^2}{2M}\left(\frac{\partial}{\partial \boldsymbol{R}_i}\right)^2 + \sum_{i<j} V^{(2)}(\boldsymbol{R}_i, \boldsymbol{R}_j) + \sum_{i<j<k} V^{(3)}(\boldsymbol{R}_i, \boldsymbol{R}_j, \boldsymbol{R}_k) + \cdots$$

that may include two-, three-, and higher-body interactions. Suppose the ions are at positions $\boldsymbol{R}_i$ that deviate only slightly from the minimum-energy, equilibrium positions $\boldsymbol{R}_i^{(0)}$ of a regular solid. Which one of the following statements—written in terms of the differences $\boldsymbol{R}_{ij} = \boldsymbol{R}_i - \boldsymbol{R}_j$ and $\boldsymbol{R}_{ij}^{(0)} = \boldsymbol{R}_i^{(0)} - \boldsymbol{R}_j^{(0)}$—is *not* a sensible interaction term?

(a) long-range dipolar $V^{(2)} \sim \{3[(\boldsymbol{R}_{ij} - \boldsymbol{R}_{ij}^{(0)}) \cdot \hat{\boldsymbol{R}}_{ij}^{(0)}]^2 - (\boldsymbol{R}_{ij} - \boldsymbol{R}_{ij}^{(0)})^2\}/(8\pi\epsilon_0 |\boldsymbol{R}_{ij}^{(0)}|^3)$

(b) bond stretching $V^{(2)} \sim (|\boldsymbol{R}_{ij}| - |\boldsymbol{R}_{ij}^{(0)}|)^2$

(c) bond bending $V^{(3)} \sim (\boldsymbol{R}_{ij} \cdot \boldsymbol{R}_{ik} - \boldsymbol{R}_{ij}^{(0)} \cdot \boldsymbol{R}_{ik}^{(0)})^2$

(d) bond scissoring $V^{(3)} \sim [(\boldsymbol{R}_{ij} \times \boldsymbol{R}_{ik}) \cdot \boldsymbol{R}_{ij} - (\boldsymbol{R}_{ij}^{(0)} \times \boldsymbol{R}_{ik}^{(0)}) \cdot \boldsymbol{R}_{ij}^{(0)}]^2$

(e) plaquette distortion $V^{(4)} \sim [(\boldsymbol{R}_{ij} \times \boldsymbol{R}_{il}) \cdot (\boldsymbol{R}_{kj} \times \boldsymbol{R}_{kl}) - (\boldsymbol{R}_{ij}^{(0)} \times \boldsymbol{R}_{il}^{(0)}) \cdot (\boldsymbol{R}_{kj}^{(0)} \times \boldsymbol{R}_{kl}^{(0)})]^2$

12. Which of the following crystal forms is incompatible with a strongly ionic solid?

(a) face-centred cubic

(b) body-centred cubic

(c) simple cubic

(2 points) 13. Indicate whether these are true or false statements.

(t / f) pure crystals are thermodynamically unstable to contamination by impurities

(t / f) near special stoichiometric ratios, alloys of two elements can form superlattices

(t / f) binary mixtures will always alloy rather than phase separate

(t / f) the dynamics of phase separation are diffusive

## Short answer questions (15 points)

Try to provide answers in concise prose. At most a few sentences are required for each question.

14. In what (mathematical) sense are the Bravais lattice vectors and reciprocal lattice vectors of a crystal *dual* to each other?

(2 points) 15. Provide a sketch of Bragg scattering from a crystal plane. Use it to motivate and explain the Bragg scattering condition.

(2 points) 16. The layered alloy CuAu can form when a high-temperature liquid mixture of roughly 50% copper and 50% gold is cooled. What experimental signature marks the formation of the new intermetallic crystalline compound? What are the different outcomes when the system is quenched versus annealed?

(3 points) 17. The coherence energy per unit cell of an ionic solid is approximated by

$$E_{\text{coh}} = -\alpha \frac{e^2}{4\pi\epsilon d} + \frac{C}{d^{12}}.$$

Explain the meaning of each term on the right hand side. Determine the equilibrium separation.

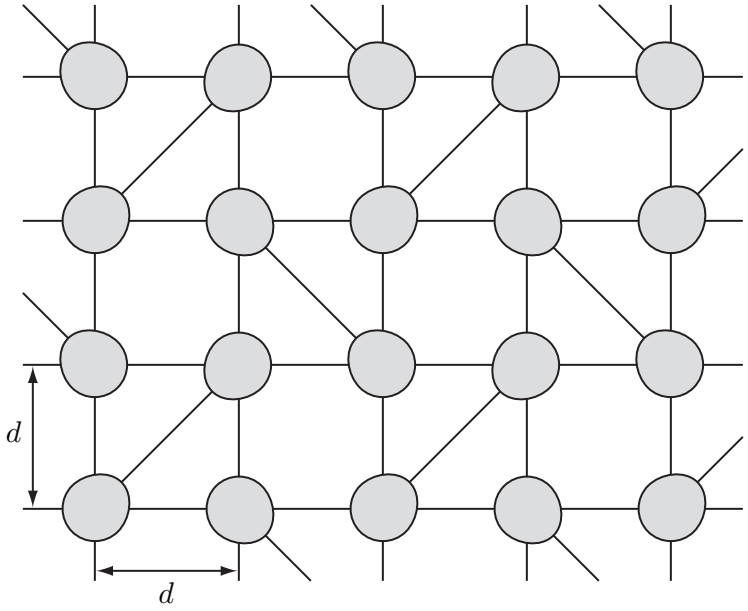
(2 points) 18. Explain why a liquid can be supercooled below its solidification temperature, whereas $^4$He always becomes superfluid at exactly $T_c = 2.17$ K.

19. What sets the upper limit for the phonon occupation number in a crystal?

(2 points) 20. The optical phonon modes in silicon $\hbar\omega_{\boldsymbol{q}} \approx \hbar\omega_0 \approx 60$ meV are weakly dispersing. What does this imply for thermal occupation of these modes well below room temperature? How is this different for the acoustic modes?

(2 points) 21. We say that a purely hard sphere system (classical and noninteracting except for the excluded volume constraint) is *entropic*. What does that mean? Suppose that we drive a system of hard spheres in a container from gas phase to solid by turning up the pressure. What is (qualitatively) the thermodynamic mechanism at work?

## Mathematical problems (20 points)



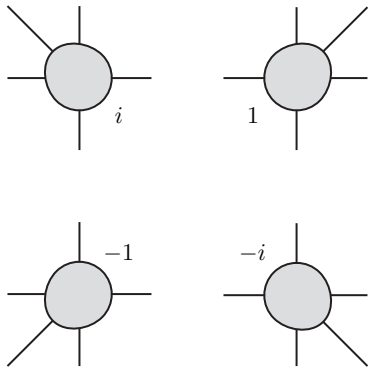

(12 points) 22. The figure above is a schematic representation of a two-dimensional crystal. Express all your answers with respect to the length scale set by the underlying square grid of size $d$.

(a) Find lattice vectors and a basis for the crystal.

(b) Compute the area of the unit cell.

(c) Determine the corresponding reciprocal lattice vectors.

(d) Sketch the Brillouin zone that results from the Wigner-Seitz construction.




(e) Using the reciprocal lattice vectors $\boldsymbol{g}_1$ and $\boldsymbol{g}_2$ that you computed in part (c), parameterize arbitrary points in the reciprocal lattice with the linear combination

$$\boldsymbol{G} = \boldsymbol{G}(n_1, n_2) = n_1\boldsymbol{g}_1 + n_2\boldsymbol{g}_2$$

for integers $n_1$ and $n_2$. Assume atomic form factors $f_{\boldsymbol{\tau}}$ as depicted above and determine the geometric structure factor as a function of $n_1$ and $n_2$. For which reciprocal lattice vectors do the x-ray scattering peaks vanish exactly?

(8 points) 23. The vector $\boldsymbol{u}(\boldsymbol{R}+\boldsymbol{\tau}, t)$ describes the time-varying displacement of an atom residing in the crystal at position $\boldsymbol{R}+\boldsymbol{\tau}$. Here, $\boldsymbol{R}$ denotes a point in the Bravais lattice and $\boldsymbol{\tau}$ an element in the basis. In a simple model of *bond-directed forces*, the displacement obeys a harmonic equation of motion

$$m_{\boldsymbol{\tau}} \frac{\partial^2}{\partial t^2} \boldsymbol{u}(\boldsymbol{R}+\boldsymbol{\tau}, t) = \sum_{\boldsymbol{\eta}} K(\boldsymbol{\eta}) \{\hat{\boldsymbol{\eta}} \cdot [\boldsymbol{u}(\boldsymbol{R}+\boldsymbol{\tau}+\boldsymbol{\eta}, t) - \boldsymbol{u}(\boldsymbol{R}+\boldsymbol{\tau}, t)]\} \hat{\boldsymbol{\eta}}.$$

Here, $\hat{\boldsymbol{\eta}}$ is a unit vector pointing in the direction of $\boldsymbol{\eta}$. This, in turn, is a vector that connects the atom at $\boldsymbol{R}+\boldsymbol{\tau}$ to another at $\boldsymbol{R}+\boldsymbol{\tau}+\boldsymbol{\eta} = \boldsymbol{R}'+\boldsymbol{\tau}'$ for some $\boldsymbol{R}'$ and $\boldsymbol{\tau}'$. We'll use a model in which the spring constant has value $K_1$ between all nearest-neighbour atoms and value $K_2$ between next-nearest-neighbour atoms that are connected by a bond in the diagram on page 8.

(a) What is the rank of the dynamical matrix? In other words, how many propagating harmonic modes are there?

(b) Solve for all the phonon modes in the limit $K_2 = 0$. Determined their dispersion and label them longitudinal (L) or transverse (T), acoustic (A) or optical (O), as appropriate.

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