# APAM Doctoral Qualifying Examination
# Applied Physics, Applied Mathematics, and Materials Science and Engineering
# Day One Exam

May 3, 2021

- Candidates must complete four (4) questions.
- Questions (**circle** the four submitted)
  1. Classical Mechanics
  2. Electromagnetism
  3. Quantum Mechanics
  4. Linear Alegbra
  5. Partial Differential Equations I
  6. Applied Dynamical Systems
  7. Numerical Methods
  8. Crystallography: Symmetry, Structure, Anisotropy (Crystallography I)
  9. Materials Thermodynamics and Phase Diagrams (Thermodynamics)
  10. Kinetics of Solids (Kinetics)
- Applied Mathematics/Applied Analysis candidates must complete *no fewer than three* (3) of #4, #5, #6, #7; the remaining one (1) question may be chosen either from the fourth of #4-#7 or from one of #1-#3.
- Applied Mathematics/Atmospheric, Earth and Oceanic Physics candidates must complete *any four* (4) of problems #1-#7.
- Applied Physics/Plasma Physics and Applied Physics/Solid State and Optical Physics candidates must complete the three (3) problems #1,#2,#3 and one (1) of #4, #5, #6, and #7.
- Materials Science and Engineering candidates must complete one (1) of problems #4, #5 and all three (3) of problems #8, #9, #10.

- **Rules:** No resources may be used during the exam. The exam is closed book, closed notes, closed computer files, closed internet. Calculators are not allowed. You may not communicate with anyone, in any way, during the exam period.
- Write your student number (*not your name*) and problem number in the top right corner of every page of your exam, in the form $SX - QY$. (Student number = $X$, problem number = $Y$).
- When you have completed your exam, sign the statement below, scan the two instruction pages, followed by your solutions, as a single PDF, and upload the PDF to the courseworks site. Your PDF file must be uploaded **before 3:30 pm ET.**

*I affirm that I have followed the rules specified, that I have not given or received inappropriate help during this exam, and that all work submitted is my own.*

| Signed: | ____________ | ____________ | ____________ | ____________ |
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| | name | **signature** | uni | student # |

## Day 1: Mechanics May 2021

In this problem, you are to determine the linear motion of a three-atom molecule when the atoms are constrained to move in one dimension, along $x$. See the figure below. Please neglect rotations and work in the center-of-mass frame (C.O.M.) and define any constants used in your solution.

Assume the atomic masses are equal and the forces between the atoms are determined solely by the distance separating an outer atom (either $m_1$ or $m_3$) from the middle atom (with mass $m_2$). For example, the force on $m_1$ is determined by the distance, $\Delta x_{12} \equiv (x_2 - x_1)$, and gradient of the potential, $V(\Delta x)$. Note that $m_1 = m_2 = m_3$.

## Part 1

Take the potential energy of interaction between the atoms to be the Lennard-Jones potential, $V(\Delta x) = 4\left[(1/\Delta x)^{12} - (1/\Delta x)^6\right]$. The gradient of this potential vanishes at $\Delta x = 2^{1/6} \approx 1.122$.

- Describe the equilibrium atomic positions (when the forces vanish). Neglect rotation and work in the C.O.M. frame.
- Consider small atomic displacements. Constrain your solution and consider only displacements that leave the center-of-mass location unchanged. Using this constraint, what are the linear equations of motion? How many degrees of freedom are needed?
- Find the normal modes when the relative positions vary in time as $\exp(\gamma t)$. Use this to determine the characteristic frequency of each mode, $\gamma$, and the associated eigenvectors.

## Part 2

Now assume the potential energy of interaction between the atoms is given by $V(\Delta x) = \cos(2\pi\Delta x)$. The gradient of this potential vanishes at several values of $\Delta x$.

For this second part, select two equilibrium atomic positions (again neglecting rotation and translation): one where the atomic positions are $(i)$ stable and the other $(ii)$ unstable.

Like Part 1, constrain the small atomic displacements so that the center-of-mass location remains unchanged. Find the orthogonal modes, and, for each mode, determine the either the frequency of oscillation or the exponential growth rate, and the eigenvectors.

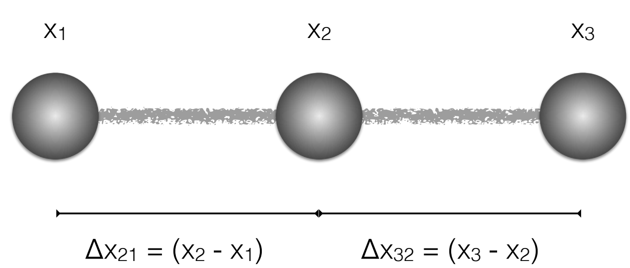



Figure 1: A one-dimensional model of a molecule with three equal mass atoms.

**Day 1: APAM Electromagnetism Qualifying Exam** **May 2021**

1. Consider an electromagnetic field along the z-direction of the form

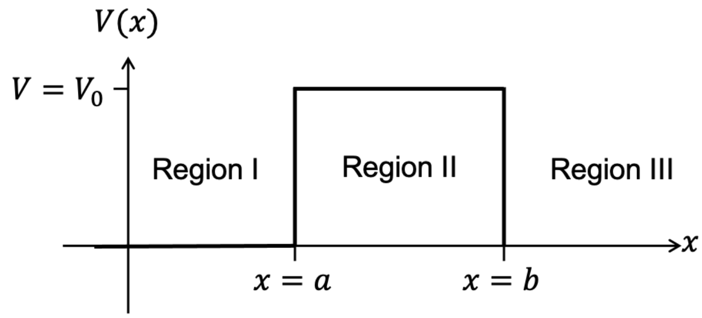
$$\mathbf{E}(z,t) = \hat{\mathbf{x}} E_0 \cos kz \cos \omega t$$

(a) Does this field satisfy the wave equation? Explain.
(a) Find the magnetic field $\mathbf{B}(z,t)$
(c) Find the Poynting vector **S**.
(d) Calculate the intensity at some point $z$. Explain your result.

2. Suppose that we have a rectangular shape wave guide with height $a$ and width $b$ ($a > b$), placed in air.
(a) What is the condition on the wave frequency $\omega$ such that a wave will propagate in the rectangular pipe?
(b) For what range of frequencies will the waveguide support a single TE mode? For what range will only a single TM mode be supported?
(c) If $a = 10$ cm, $b = 5$ cm, how many propagation modes exist for a wave of frequency 1 GHz?

# Day 1: Quantum Mechanics May 2021

Consider a particle of energy $E$ moving in 1D in a region shown.




a) Using the position basis, the wave function for the particle in region I and region II may be written as:

$$\psi_I(x) = Ae^{ikx} + Be^{-ikx}; \text{ and } \psi_{II}(x) = Ce^{ik'x} + De^{-ik'x}$$

Determine $k$ and $k'$.

b) Using the fact that Schrödinger's equation is a linear second order differential equation, provide two relations between the four unknowns $A$, $B$, $C$ and $D$ (i.e. determine the boundary conditions at $x = a$ for solutions in Region I and Region II )

c) Defining two vectors $\Psi_I(x = a)$ and $\Psi_{II}(x = a)$ as:

$$\Psi_I = \begin{bmatrix} Ae^{ika} \\ Be^{-ika} \end{bmatrix}; \text{ and } \Psi_{II} = \begin{bmatrix} Ce^{ik'a} \\ De^{-ik'a} \end{bmatrix}$$

Determine the matrix $M_1$ such that $M_1\Psi_I = \Psi_{II}$.

d) Now consider the particle at $x = a$ within Region II and at $x = b$ in Region II. Determine a matrix $M_2$ such that $M_2\Psi_{II}(x = a) = \Psi_{II}(x = b)$:

e) Determine a matrix $M_3$ such that $M_3\Psi_{II}(x = b) = \Psi_{III}(x = b)$.

f) We can use these matrices ($M_1$,$M_2$ and $M_3$) to determine $\Psi_{III}(x = b)$ given $\Psi_I(x = a)$ by defining a matrix $M_T\Psi_I(x = a) = \Psi_{III}(x = b)$ . Provide an expression for $M_T$.

g) Expressing $M_T$ as:

$$M_T = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix}$$

Consider a particle incident on the potential barrier at $x = a$ in Region I. Determine the probability that it will get transmitted across the barrier to $x = b$ in region III in terms of the elements of the matrix $M_T$.

# Doctoral Qualifying Exam
# Linear Algebra question

1. $A$ is a real $3 \times 3$ matrix, and we have that

$$A \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} -2 \\ -2 \\ -2 \end{pmatrix}, \; A \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}, \; A \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}.$$

   (i). (4 points) What are the eigenvalues and associated eigenvectors of $A$? Can we use this set of eigenvectors as a basis for $\mathbb{R}^3$?

   (ii). (4 points) Does the linear system $Ax = b$ have a solution for any $b \in \mathbb{R}^3$? If not, find the subspace of $b$'s such that $Ax = b$ solvable; find the subspace of $b$'s such that $Ax = b$ is not solvable.

   (iii). (4 points) Calculate

$$A^{3000} \begin{pmatrix} 4 \\ -5 \\ 4 \end{pmatrix}.$$

2. (8 points) Let $A \in \mathbb{R}^{n \times m}$, $n \geq m$, $\text{rank}(A) = m$ with singular values $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_m > 0$ and singular value decomposition $A = U\Sigma V^T$. Find the singular value decomposition of the matrices

$$A^T A, \quad (A^T A)^{-1}$$

   in terms of the singular value decomposition of $A$.

3. (5 points) Consider the ODE system

$$\frac{d\mathbf{u}(t)}{dt} = A\mathbf{u}(t), \quad \mathbf{u}(t=0) = \mathbf{u}_0.$$

   with

$$A = \begin{pmatrix} 0 & 1 & -1 & 1 \\ -1 & 0 & -1 & 1 \\ 1 & 1 & 0 & 1 \\ -1 & -1 & -1 & 0 \end{pmatrix}.$$

   Does $\|\mathbf{u}(t)\|_2^2$ change with time? Here $\| \cdot \|_2$ is the usual Euclidean norm.

Day I: # 5. Partial Differential Equations

**1** Let $\Omega = \{\mathbf{x} = (x, y) \in \mathbb{R}^2 : x > 0, y > 0\}$, $\Gamma_1 = \{\mathbf{x} = (x, 0) : x > 0\}$ and $\Gamma_2 = \{\mathbf{x} = (0, y) : y > 0\}$.

a) Find the Green's function (using the method of images) that satisfies: for $\mathbf{x}_0 \in \Omega$,

$$-\nabla^2 G(\mathbf{x}, \mathbf{x}_0) = \delta(\mathbf{x} - \mathbf{x}_0), \text{ in } \Omega, \quad G(\mathbf{x}, \mathbf{x}_0) = 0, \text{ on } \Gamma_1 \text{ and } \Gamma_2.$$

b) Find an integral representation of the solution, using the Green's function found in a), to the following problem in terms of the boundary data:

$$-\nabla^2 u(\mathbf{x}) = 0, \text{ in } \Omega, \; u(x, 0) = g(x), \text{ on } \Gamma_1 \text{ and } u(0, y) = h(y), \text{ on } \Gamma_2,$$

c) Show that, using the integral representation found in b), if $g(x) \geq 0$ and $h(y) \geq 0$ for all $x > 0$ and $y > 0$, then the solution of the problem in b) satisfies $u(\mathbf{x}) \geq 0$ for $\mathbf{x} \in \Omega$.

**2** Consider the eigenvalue problem $\dfrac{d^2\phi}{dx^2} - \dfrac{x}{2}\dfrac{d\phi}{dx} + \lambda\phi = 0$ with boundary conditions $\phi(0) = \phi(2) = 0$ for a nonzero function $\phi(x)$ defined on $[0, 2]$.

a) Find a transformation of variable to reformulate the problem in the Sturm-Liouville form.

b) Use the Rayleigh Quotient to show that $\lambda \geq 0$.

c) In addition, show that the smallest eigenvalue is larger than 0.9.

# Qualifying Exam 2021 - Dynamical Systems Question

1. Consider the following ODE

$$\dot{x} = x(-x - y + 1)\,,$$
$$\dot{y} = y(y - b)\,,$$

where $b \in \mathbb{R}$.

   (a) (5 points) Show that if $x(0), y(0) \geq 0$, then the solutions remain non-negative for all times $t \geq 0$.

   (b) (6 points) Plot the nullclines of the system for different values of $b > 0$ and find the fixed points of the system

   (c) (8 points) Characterize the stability of the different fixed points and describe the bifurcations they undergo. If convenient, plot the relevant bifurcation diagrams.

2. For each of the following statements, determine whether it is true or false. Prove or cite relevant result if true, and provide a counter example if false.

   (a) (2 points) A two-dimensional autonomous system of ODEs with no fixed points has a periodic solution.

   (b) (2 points) A three-dimensional autonomous system of ODEs cannot have periodic solutions which are not constant in time (fixed points).

   *(hint - what about a* 2021*-dimensional autonomous system of ODEs?)*

   (c) (2 points) Let $\dot{\underline{x}} = f(\underline{x})$ be an autonomous ODE in two dimensions with $f : \mathbb{R}^2 \to \mathbb{R}^2$ smooth. Suppose that solutions are confined to $S = \{(x, y) \in \mathbb{R}^2 \;\mid\; |x|, |y| \leq 1\}$, i.e., if $x(t_0) \in S$ for some $t_0 \in \mathbb{R}$, then $x(t) \in S$ for all times. Then there exists either a fixed point or a periodic trajectory inside $S$.

# Day 1: Numerical Methods 2021

Consider 3 points $U_n, U_{n+1}, U_{n+2}$, evenly spaced in time which are discrete samples of some continuous function $U(t)$ sampled at times $t_n, t_{n+1}, t_{n+2}$ where $t_n = n\Delta t$.

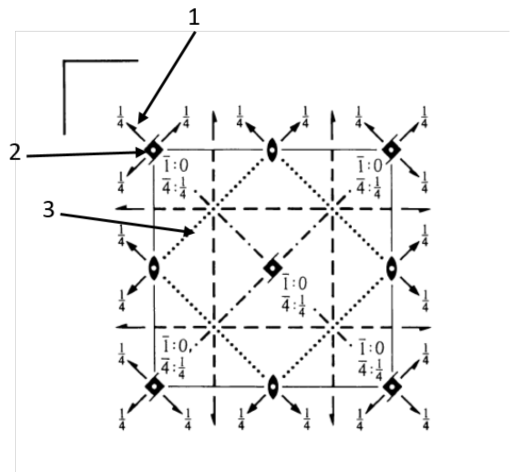
Do the following.

1. (*5 pts* ) Find the polynomial $P(t)$ that exactly interpolates the three points $U_n, U_{n+1}, U_{n+2}$.
2. (*5 pts*) Find an expression for the second order finite difference approximation of $P'(t)$ evaluated at $t = t_{n+2}$.
3. (*5 pts*) Consider the general ODE
$$\frac{du}{dt} = f(t, u) \tag{1}$$
Use your results from question 2 to construct a linear multi-step scheme that uses function values $U_n, U_{n+1}, U_{n+2}$ and one function evaluation at $f(t_{n+2}, U_{n+2})$. (hint: this is the second-order backward differentiation scheme BDF-2)
4. (*10 pts*) Consider the specific RHS $f(t, u) = \lambda u$
   (a) Derive the stability polynomial for the BDF-2 scheme
   (b) Show that this scheme is stable for all timesteps $\Delta t > 0$ for $\lambda \in \mathbb{R} < 0$ and calculate the stability criterion in the limit $\Delta t \to \infty$ (i.e. show that BDF-2 is L-stable)

CRYSTALLOGRAPHY: STRUCTURE, SYMMETRY, ANISOTROPY

a. (4) Compare and contrast close packed and topologically close packed structures. Give an example of each and specify either the structure type or the Strukturbericht designation of your example structures.
b. (3) What is the factor group of a group? In the context of space groups, what was the factor group used to accomplish?

The following questions pertain to the space group with its diagram shown below.




c. (3) The origin of the diagram is placed at center$(2/m)$ at $4_2/m1n$. Explain what this statement means and what each of the symbols is referring to.
d. (6) Using the ITA designation, specify the symmetry operators labelled 1-3 marked on the diagram. Also specify the operator type in words.
e. (3) Generate the coordinates of the symmetry equivalent point to the general point $(x, y, z)$ by the action of operator (3). Use the 3D matrix approach in deriving your answer.
f. (3) Would a single crystal of a material with this space group be piezoelectric? Why or why not? Be certain to include the rank of the tensor in making your argument.
g. (3) What is the plane group symmetry of the [001] projection of this space group? Explain how you arrived at your answer.

MATERIALS THERMODYNAMICS AND PHASE DIAGRAMS

a. (6) Two identical bodies have heat capacities (at constant volume) of $C(T) = a/T$. The initial temperatures are $T_{10}$ and $T_{20}$, with $T_{20} = 3T_{10}$. The two bodies are to be brought to thermal equilibrium with each other (maintaining both volumes constant) while delivering as much work as possible to a reversible work source. What is the final equilibrium temperature, and what is the maximum work delivered to the reversible work source? Briefly explain what you are doing at each step of your answer.

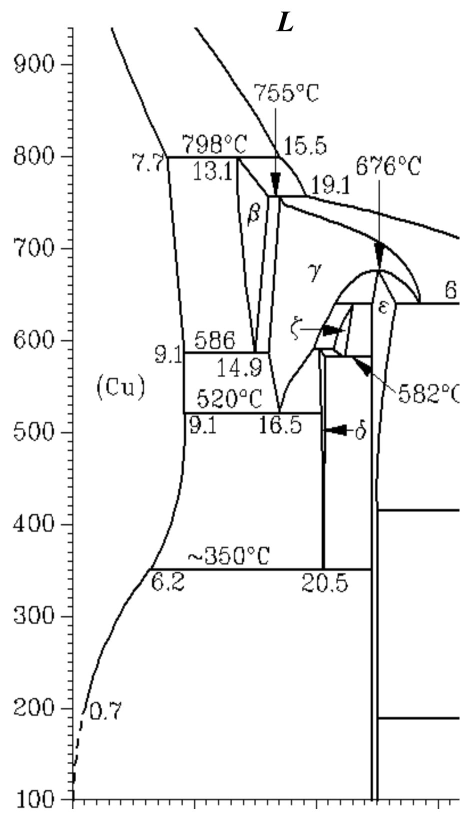
b. (3) For the fundamental relation in the entropic representation give an example of an extensive thermodynamic parameter. What is the conjugate thermodynamic parameter to your chosen extensive parameter? How do these parameters differ, and how are they related?

c. (6) With the aid of schematic diagram(s), explain in your own words what a Gibbs-Wulff plot is, how it is constructed, and how it relates to the equilibrium shape of crystals.

The remainder of this question pertains to the section of the Cu-Sn phase diagram shown below. The vertical axis is in °C and the horizontal axis in at%, in divisions of one percent.

d. (5) Write the reactions for temperatures of 798 °C, 676 °C, and 582 °C in the direction of heating. Identify the reactions as eutectic, peritectic, etc. You do **not** need to give the phase compositions

e. (5) Draw the microstructure at 400 °C of a Cu-10at%Sn alloy that has been slowly cooled from 1000 °C to 400 °C. Clearly label and identify all the phases in your diagram and briefly explain how you arrived at your answer.



## KINETICS OF TRANSFORMATIONS

**Doctoral Qualifying Exam**
**MAY 2021**

In answering the following questions, clearly define and identify the physical quantities and variables. Do explain the critical steps that are involved in your derivation. You do not need, and **are not permitted to use a calculator or any other devices** during this exam.

Consider the phenomenon of spinodal decomposition.

(a) (i) First, explain what the phenomenon is all about, and (ii) then graphically and qualitatively describe, using appropriately drawn phase diagram and the solution free energy vs. composition curve (i.e, $G_{SOL}$ vs. $x_B$), the region in the phase diagram within which slight compositional fluctuations occurring in an initially homogeneous solution would be thermodynamically favored to grow. Also (iii) identify the sub-region within the two phase region wherein slight compositional fluctuations will decay and, subsequently, the separation process must proceed via nucleation and growth (i.e., where large compositional fluctuations are needed).

(b) Now, quantitatively support and substantiate the argument you make above by (i) first deriving the relationship that shows that the free energy change (i.e., $G_{SOL}$) as a result of the development of compositional fluctuations depends on the curvature of $G_{SOL}$ vs. $x_B$, and further that (ii) by showing that the phenomenon of uphill diffusion (which makes the growth of the fluctuations possible) can be related to the curvature.

(c) Identify and elaborate on the physical factors that can oppose the development of these compositional fluctuations. How does the value of fluctuation wave number, $\beta$, affect the situation (i.e., a very small $\beta$ vs. a very big $\beta$)? Explain and describe, to the extent you can, the wavenumber expected to be manifested, at least in the early phase of spinodal decomposition.