

Area C CSEM Preliminary Exam
Wednesday, May 25, 2016

1. Provide short answers and *brief* explanations where needed for the following questions. No analysis is required. If you write more than a sentence or two, you are writing too much.

- (a) What is Cauchy's stress theorem? What principles does it rely on?
- (b) Why is tensor consistency an important constraint on mathematical models of physical systems
- (c) What is material frame indifference, and why is it important?
- (d) What physical principle is the following an expression of?

$$\rho_0 \dot{\eta}_0 + \text{Div} \frac{\mathbf{q}_0}{\theta} - \frac{r_0}{\theta} \geq 0$$

What is the physical meaning of each term?

- (e) What physical phenomenon is expressed in the following equation:

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

and what is a common device that relies on this phenomenon?

- (f) A particle is in quantum state $\psi(\mathbf{x})$. Write an expression for the expected value of the kinetic energy of the particle.
 - (g) You have precise knowledge of two observable quantities, Q and M , in a quantum system with wavefunction ψ . What is the value of $[\tilde{Q}, \tilde{M}]\psi$, where $\tilde{Q}$ and $\tilde{M}$ are operators associated with Q and M ? Why?
 - (h) What is the Pauli principle, and how does it affect the electronic structure of atoms?
 - (i) What are Fermions? Give an example of one.
2. In a linearly elastic solid undergoing small (infinitesimal) deformations the second Piola-Kirchhoff stress tensor S is given by

$$S = \lambda \mathbf{I} \nabla \cdot \mathbf{u} + \mu (\nabla \mathbf{u} + \nabla \mathbf{u}^T)$$

where $\mathbf{u}$ is the small displacement, $\mathbf{I}$ is the identity tensor and λ and μ are constants.

- (a) Assuming no body forces and starting with conservation of momentum, derive an equation for the evolution of $\mathbf{u}$.
- (b) Show that $\mathbf{u} = f(\mathbf{x} \cdot \mathbf{e} - \alpha t)\mathbf{e}$ for any sufficiently smooth f and any unit vector $\mathbf{e}$ is a solution. What is the value of α and what does it represent?
- (c) Show that $\mathbf{u} = f(\mathbf{x} \cdot \mathbf{e} - \beta t)\mathbf{g}$, with $\mathbf{g}$ a unit vector such that $\mathbf{g} \cdot \mathbf{e} = 0$, is a solution. What is the value and interpretation of β .

3. Consider a diatomic molecule consisting of atoms with mass m_1 and m_2 that are separated by a distance R . It is free to rotate around its center of mass. The Hamiltonian for this rotating system is given by:

$$H = \frac{L^2}{2I}$$

where L^2 is the square magnitude of the angular momentum (analogous to the linear momentum) and $I = R^2 \frac{m_1 m_2}{m_1 + m_2}$ is the moment of inertia about the center of mass (analogous to the mass). Recall that the operators $\hat{L}^2$ and $\hat{L}_3$ associated with L^2 and L_3 (the angular momentum in the 3 direction) satisfy the following:

$$\hat{L}^2 Y_{\ell m} = \ell(\ell + 1) \hbar^2 Y_{\ell m}$$

$$\hat{L}_3 Y_{\ell m} = \hbar m Y_{\ell m}$$

where $Y_{\ell m}$ is a spherical harmonic, for this case ℓ is a non-negative integer and m an integer with $|m| \leq \ell$.

- Write the time-independent Schrödinger equation for this system.
- What are the energy levels that the system can access?
- What is the ground state energy?
- If the system transitions from quantum state $\psi = Y_{32}$ to state $\psi = Y_{10}$, what is the frequency of the photon that is emitted.
- If the system is in quantum state $\psi = Y_{21}$, what is the expected value of the energy, of the angular momentum in the x_3 direction, and of the angular momentum in the x_1 direction.

4. Short Answers

- Give an example of a *physical system* which is well-represented by a **micro-canonical** ensemble. State why your system has the appropriate macroscopic variables for the ensemble.
- Repeat (a) for the **grand-canonical** ensemble.
- Within the grand-canonical ensemble, what is the probability of finding N particles in the system?
- Describe in words what the chemical potential of a system is. For an ideal gas in a fixed volume, how does the chemical potential change as more particles are added to the volume? Explain your answer.
- Consider a box of fixed volume containing 100 ideal gas molecules in thermal equilibrium. What is the average energy of the system? What is the standard deviation of the energy fluctuations.
- Show that Boltzmann's entropy is an extensive variable, (i.e. that $S_{1+2} = S_1 + S_2$) for two subsystems, 1 and 2.
- Consider a gas molecule which has two *independent* contributions to its energy; translation with energy levels $E k_i$, and vibration with energy levels $E v_j$. Give an expression for the single particle partition function of the molecule including both translation and vibration.

- (h) The time independent Schrödinger equation has the form

$$-\frac{\hbar^2}{2m} \frac{d^2 u}{dx^2} + V(x) u(x) = E u(x).$$

When we solved for stationary states numerically, we derived the formula

$$u(x+h) = [2 + h^2 f(x)] u(x) - u(x-h)$$

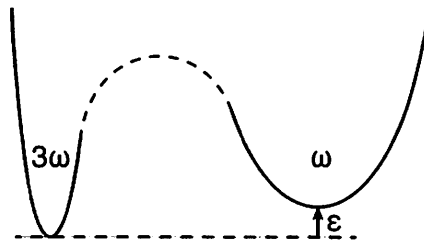
where $f(x) \equiv -\frac{2m}{\hbar^2} (E - V(x))$. Using the method of Taylor expansion, find the leading error term in this numerical algorithm.

- (i) We often described atomic interactions using a pair potential of the Lennard-Jones form, $V_{LJ}(r) = a/r^{12} - b/r^6$. What physical interactions do these two terms most closely describe? Which type of atoms or molecules are best described by this form of potential?
- (j) What is the ergodic hypothesis and why was it important for the concept of ensembles?

5. Quantum to Classical partition functions

- (a) A quantum oscillator has energy levels $E_n = (n + 1/2)\hbar\omega$. Work out the quantum partition function for the oscillator. Clearly state any restrictions on the variables that arise from your calculation and any corresponding physical significance.
- (b) Classically, the harmonic oscillator has an energy $E = kx^2/2 + mv^2/2$. Work out the classical partition function for the oscillator. You may need to use the following relation: $\int e^{-\alpha x^2} = \sqrt{\pi/\alpha}$.
- (c) Take the high-temperature limit of your quantum partition function in (a). At what temperature does the description of the oscillator switch from quantum to classical. Remember that $\omega = \sqrt{k/m}$.
- (d) In order for the classical partition function to agree with the that from quantum mechanics, we had to introduce a factor to our definition of the classical partition function. What is this factor, how is it justified from quantum mechanics, and why could we ignore it for before we talked about chemical equilibrium.

6. Classical equilibrium



The tradeoff between energy and entropy can be investigated by considering a gas molecule which can be in two molecular states. The states are described by harmonic potentials with two different natural frequencies. The smaller of the states has frequency 3ω , and the larger has frequency ω . The minimum potential energy of the larger state is a value ϵ above the minimum potential energy of the smaller state. Consider the system classically.

- (a) If a classical constant-energy trajectory were calculated sketch the probability density of finding the particle as a function of position. Consider a value of the energy which is greater than the barrier between the two states so that the particle can visit both states.
- (b) Repeat (a) for a constant temperature (canonical) trajectory.
- (c) In thermal equilibrium, what is the free energy of the molecule in each of the two states as a function of temperature?
- (d) What is the probability of finding the gas molecule in the larger state (with frequency ω), and how is this probability related to the free energy of this state? Sketch this probability as a function of temperature.

Area C CSEM Preliminary Exam
Wednesday, May 24, 2017

1. Provide short answers and *brief* explanations where needed for the following questions. No analysis is required. If you write more than a sentence or two, you are writing too much.

- (a) What is the difference between the Cauchy, first Piola-Kirchhoff and second Piola-Kirchhoff stress tensors. Why do we have these different stress tensors?
- (b) Why is tensor consistency an important constraint on mathematical models of physical systems
- (c) How are intermolecular forces represented in the continuum conservation of momentum equation?
- (d) What physical principle is the following an expression of?

$$\rho_0 \dot{e}_0 = \mathbf{S} : \dot{\mathbf{E}} - \text{Div } \mathbf{q}_0 + r_0$$

What is the physical meaning of each term?

- (e) What physical phenomenon is expressed in the following equation:

$$\nabla \times \mathbf{B} = \mu_0 \mathbf{j} + \mu_0 \epsilon_0 \frac{\partial \mathbf{E}}{\partial t}$$

and what is a common device that relies on this phenomenon?

- (f) A particle with charge q is located at point $\mathbf{x}$ and is traveling with velocity $\mathbf{v}$ in an electric field $\mathbf{E}$ and magnetic field $\mathbf{B}$. What is the force on the particle?
 - (g) A particle is in quantum state $\psi(\mathbf{x})$. Write an expression for the expected value of the momentum of the particle.
 - (h) Atoms of an element at high enough temperature emit radiation at discrete frequencies that are characteristic of the element. Why?
 - (i) An electron is in the spin-up quantum state relative to the x_1 direction. What is the expected value of its spin angular momentum in the x_3 direction and in the x_1 direction?
 - (j) How many electrons can populate the $n = 2$ shell of an atom?
2. Recall that in a continuum, the conservation of momentum implies:

$$\rho_0 \frac{\partial^2 \mathbf{u}}{\partial t^2} = \text{Div } \mathbf{F}\mathbf{S} = \mathbf{f}_0$$

and

$$\rho \left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \text{grad } \mathbf{v} \right) = \text{div } \mathbf{T} + \mathbf{f}$$

in the Lagrangian and Eulerian representation, respectively. Consider the steady constant density incompressible flow of a Newtonian fluid between two parallel planar walls, located at $x_2 = \pm \delta$. A Newtonian fluid obeys the constitutive relation:

$$\mathbf{T} = -p\mathbf{I} + 2\mu\mathbf{D} + \lambda \text{tr } \mathbf{D}$$

where $\mathbf{T}$ is the Cauchy stress tensor, p is the pressure, $\mathbf{D}$ is the strain rate tensor, μ is the shear viscosity and λ is the bulk viscosity.

- (a) What is the statement of conservation of mass simplified for a constant density incompressible flow?
 - (b) Assuming no body forces, what is the statement of conservation of momentum simplified for a constant density incompressible flow of a Newtonian fluid with constant viscosity (including simplifications of the constitutive relation)?
 - (c) What are the boundary conditions at the walls ?
 - (d) The flow is driven by a constant pressure gradient $\text{grad } p = -G\mathbf{e}_1$ in the x_1 direction, and the flow is two-dimensional and fully developed, meaning that the velocity does not change in the flow direction. Simplify the equations to obtain an ODE for the velocity.
 - (e) Solve the ODE (it is simple) to obtain the velocity.
3. Consider a particle of mass m constrained to move in one dimension x , in a potential given by

$$V = \begin{cases} 0 & \text{if } x \in (0, 2) \\ \infty & \text{otherwise} \end{cases}$$

- (a) Write the time-independent Schrödinger equation for the particle, specifying appropriate boundary conditions.
- (b) What is the ground state energy?
- (c) Suppose that the particle is in the quantum state described by the wavefunction

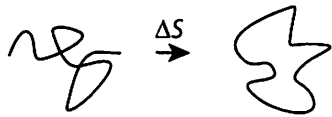
$$\psi(x) = a \sin(2\pi x) + b \sin(3\pi x)$$

How must a and b be related?

- (d) In the same quantum state, what is the expected value of the energy?
- (e) The particle is in the same quantum state, and a measurement of the energy is to be made. What are the possible outcomes of such a measurement, and what are the probabilities of obtaining each.

4. Short problems – the best 4 out of 5 will count toward your grade:

(a) Consider a long DNA molecule on a two-dimensional surface. When it is circularized (i.e., when its two ends meet each other), the resulting entropy change is $\Delta S = a - \delta \log N$, where $N \gg 1$ is the molecule's contour length. What is the numerical value of δ ? Neglect excluded volume interactions (i.e. treat the DNA as a non-self-avoiding random walk in 2D).



(b) Briefly explain why there is no hydrogen or helium in the Earth's atmosphere. Your explanation should be based on a mathematical equation. Hint: hydrogen and helium have the lowest mass of all atoms; if there were some in the atmosphere what would happen to them?

(c) The partition function of a quantum harmonic oscillator with a frequency ω is $q = \frac{1}{2 \sinh(\beta \omega \hbar / 2)}$. Under what condition (what relationship between β and ω) can one take the classical limit in this expression? What is q in the classical limit?

(d). Explain (in no more than 3 sentences) the difference between the canonical and microcanonical ensembles.

(e) Write down the Hamiltonian of the one-dimensional Ising model in the presence of a magnetic field.

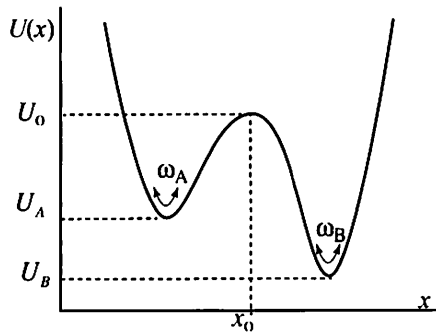
5. Consider a system that consists of $N=2$ indistinguishable, noninteracting particles obeying the Fermi-Dirac statistics. Each particle can be in 3 possible states with the energies $\epsilon_1 < \epsilon_2 < \epsilon_3$.

(a) Assuming the canonical ensemble at temperature T (not grand canonical, N is fixed!), write down the expression for the free energy F of the system.

(b) Using the result from Part (a) find the entropy S of the system.

(c) What will the entropy S become in the limits $T \rightarrow 0$ and $T \rightarrow \infty$?

6. A one-dimensional Brownian particle of mass m is subjected to a double-well potential $U(x)$ shown in the picture below. The temperature of the particle's surroundings is T . The frictional force on the particle is proportional to its velocity and is given by $-\gamma \dot{x}$.



- (a) Write down the Langevin equation describing the motion of the particle and briefly explain the mathematical properties of the noise term
- (b) Write down the Smoluchowski equation for the probability density $w(x,t)$ of finding the particle at x at time t . What is the relationship between the diffusion coefficient and γ ?
- (c) Under what conditions are the Langevin and Smoluchowski descriptions of the same system equivalent?
- (d) We define states A and B as corresponding to the particle being to the left ($x < x_0$) and to the right ($x \geq x_0$) of the barrier, as shown. Assuming that the particle is being observed for a very long time, write down the expression describing the fraction f_A of the total time the particle spends in A. Your answer should be given in terms of the function $U(x)$.
- (e) Using the transition-state theory approximation, estimate the average dwell time within A, $\langle t_A \rangle$, given the parameters shown in the picture.
- (f) Is the exact value of $\langle t_A \rangle$ greater or smaller than the estimate you gave in Part (e)? Briefly explain why.

1 a) Stress tensors map a normal vector to a force per unit area; they diff in whether the normal, force and area are represented in the reference or current configuration. We have all three because they are more convenient in different situations.

b) So that model predictions are invariant to the coordinate system in which the system is described.

c) Through the stress tensor

d) Conservation of energy

$\rho \dot{e}$ - rate of change of ^{internal} energy, $S : \dot{E}$ - rate of work done by stress

$\text{Div } q_0$ - heat flux τ_0 - volumetric heating

e) Formation of magnetic fields by currents, an electro magnet etc.

f) $E = q(E + v \times B)$

g) $-i\hbar \int \psi^* \nabla \psi dx = \langle p \rangle$

h) The energy states of the electrons in an atom are quantized, and when electrons transition from a higher energy state to a lower they emit a photon at a frequency characteristic of the change in energy, which is thus discrete.

i) $\langle L_3 \rangle = 0$ $\langle L_1 \rangle = \frac{\hbar}{2}$

j) 8

2 a) $\frac{\partial \rho}{\partial t} + \text{div}(\rho \underline{v}) = 0$ for const. density incompressible $\rho = \text{const.}$
then $\boxed{\text{div}(\underline{v}) = 0}$

b) In fluids use Eulerian form of momentum equation

$$\rho \frac{\partial \underline{v}}{\partial t} + \rho \underline{v} \cdot \text{grad} \underline{v} = \text{div} \underline{T} + \underline{f}$$

For constant density incompressible $\text{tr} \underline{D} = 0$ so

$$\underline{T} = -p \underline{I} + 2\mu \underline{D}$$

substituting and dividing through by ρ

$$\frac{\partial \underline{v}}{\partial t} + \underline{v} \cdot \text{grad} \underline{v} = -\frac{1}{\rho} \text{grad} p + 2 \frac{\mu}{\rho} \text{div} \underline{D}$$

$$= -\frac{1}{\rho} \text{grad} p + \frac{\mu}{\rho} \text{div} \text{grad} \underline{v}$$

c) at the wall $\underline{v} = 0$

d) let $x = x_1$, $y = x_2$ $u = v_1$, $v = v_2$

continuity equation

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \Rightarrow v = C, \text{ but } v = 0 \text{ at wall so } v = 0$$

fully developed

x-momentum equation simplification

$$\frac{\partial u}{\partial t} = 0 \quad (\text{steady}) \quad u \frac{\partial u}{\partial x} = 0 \quad (\text{fully developed})$$

$$v \frac{\partial u}{\partial y} = 0 \quad (v = 0) \quad (\text{grad } p)_1 = -G$$

$$(\text{div grad } \underline{v})_1 = \frac{\partial^2 u}{\partial y^2}$$

$$\frac{d^2 u}{dy^2} = -\frac{G}{\mu}$$

$$e) \quad u = -\frac{G}{4\mu} y^2 + C_1 y + C_2$$

$$u(\pm \delta) = 0 \Rightarrow u = -\frac{G}{2\mu} (\delta^2 - y^2)$$

$$3 \quad a) \quad -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} = E \psi \quad \psi(0) = \psi(2) = 0$$

b) Find eigen values + functions -

$$-\frac{d^2 \psi}{dy^2} = \alpha^2 \psi \Rightarrow \psi = A \sin(\alpha x) + B \cos(\alpha x)$$

$$\text{B.C.} \quad \psi(0) = 0 \Rightarrow B = 0 \quad \psi(2) = 0 \Rightarrow \alpha = \frac{n\pi}{2} \quad n = 1, 2, \dots$$

$$\frac{n^2 \pi^2}{4} = \frac{E_n 2m}{\hbar^2} \Rightarrow E_n = \frac{n^2 \hbar^2 \pi^2}{8m} \quad n=1, 2, \dots$$

Ground state is

$$E_1 = \frac{\hbar^2 \pi^2}{8m}$$

c) Normalization:

$$\int_0^L \psi^* \psi dx = 1 \Rightarrow \int_0^L (a^2 \sin^2(2\pi x) + b^2 \sin^2(3\pi x)) dx = 1 \quad (\text{orthogonality})$$

$$\Rightarrow a^2 + b^2 = 1$$

d) $\langle E \rangle = a^2 E_4 + b^2 E_6$ because $\sin(\frac{n\pi x}{L})$ is the eigen function

$$= \frac{(16a^2 + 36b^2) \hbar^2 \pi^2}{8m}$$

e) Possible outcomes: $E = \frac{2\hbar^2 \pi^2}{m}$ or $E = \frac{9\hbar^2 \pi^2}{2m}$
with probabilities a^2 and b^2 respectively.

Area C CSEM Preliminary Exam
Friday, May 25, 2018

1. Provide short answers and *brief* explanations where needed for the following questions. No analysis is required. If you write more than a sentence or two, you are writing too much.

- (a) What is the right Cauchy-Green deformation/stain tensor? What does it express? List two of its properties.
- (b) How is the Green-St. Venant strain tensor related to the Cauchy-Green deformation/stain tensor?
- (c) It is proposed that the following represent models of physical phenomena. For each, state whether or not this is possible and why.

i. $|\mathbf{v}| = \omega^{2/3} S^{1/2}$

ii. $v_i = \sum_{j=1}^3 Q_{ij} f_j$

iii. $\mathbf{v} = \nabla \times \mathbf{g}$

Here $\mathbf{v}$, is a velocity vector with Cartesian components v_i , $\mathbf{f}$ and $\mathbf{g}$ are vectors with components f_j and g_j , and Q_{ij} are components of a second rank tensor. Further, ω and S are angular frequency and slope, respectively.

- (d) What are constitutive relations, and why do we need them?
- (e) What physical principle is the following an expression of?

$$\rho \frac{de}{dt} = \mathbf{T} : \mathbf{D} - \text{div } \dot{\mathbf{q}} + r$$

What is the physical meaning of each term?

- (f) What is Ampère-Maxwell's law, and what does it express? Describe the physical meaning of the different terms in the law.
- (g) A particle with charge q is located at point $\mathbf{x}$ and is traveling with velocity $\mathbf{v}$ in an electric field $\mathbf{E}$ and magnetic field $\mathbf{B}$. What is the force on the particle?
- (h) Let h be Planck's constant and p its momentum. What is the significance of

$$p = \frac{h}{\lambda}$$

Re-express p in terms of energy $E = h\nu$ and speed c , and again explain its significance.

- (i) A particle is in quantum state $\psi(\mathbf{x})$. Write an expression for the expected value of the kinetic energy of the particle.
- (j) Let L_i be the angular momentum in the x_i direction of the motion of a particle, and ψ be the wavefunction of the quantum state. If $L_3\psi = \hbar m\psi$ and $\phi = (L_1 + iL_2)\psi$, what is $L_3\phi$?

2. A cube of incompressible material of dimension a is subjected to a uniaxial load in the x_1 direction, resulting in a deformation that reduces the dimension in the x_1 direction to $\alpha^2 a$, with $0 < \alpha < 1$. The material has an incompressible neo-Hookean strain energy density function:

$$W(\mathbf{E}) = \mu I_{\mathbf{E}},$$

where $\mathbf{E}$ is the strain tensor, $I_{\mathbf{E}}$ is its first invariant and μ is the shear modulus.

- Determine the deformation gradient tensor ($\mathbf{F}$), the right Cauchy-Green deformation tensor ($\mathbf{C}$) and the Green-St. Venant strain tensor ($\mathbf{E}$) in the material.
- How much work was required to deform the material?
- Because the material is incompressible, there is a degeneracy in the stress relation, so that the second Piola-Kirchhoff stress is given by

$$\mathbf{S} = \frac{\partial W}{\partial \mathbf{E}} + p \mathbf{F}^{-1} \mathbf{F}^{-T}$$

where p can be determined from boundary conditions, in this case on the unloaded sides. Determine $\mathbf{S}$.

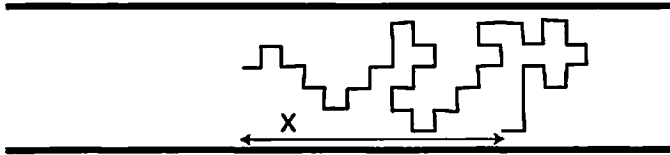
- What is the total load force?
3. Consider a particle of mass m in a rectangular box $\Omega = [0, a] \times [0, b]$, where the potential $V = V(x, y)$ is given by:

$$V(x, y) = \begin{cases} 0 & \text{for } 0 \leq x \leq a, \quad 0 \leq y \leq b \\ \infty & \text{otherwise} \end{cases}$$

- Write the Schrödinger equation (time independent) describing the motion of the particle
- State any boundary conditions that the wavefunction must satisfy in this case
- Derive the general solution of the wavefunction (Hint: separation of variables).
- Derive the expression for the (discrete) energy spectrum.
- For the special case of a square box ($a = b$), determine the energy E for the lowest and the next two higher energy levels.

4. Short problems – the best 4 out of 5 will count toward your grade:

(a) Consider a two-dimensional self-avoiding lattice random walk of N steps confined to an infinite 2D “tube”. Let $\langle x^2 \rangle = \langle x^2 \rangle(N)$ be the mean square distance traveled in N steps and measured along the tube axis. How does $\langle x^2 \rangle$ scale with N in the limit $N \rightarrow \infty$?



(b) Same question as in (a), but for a non-self-avoiding random walk

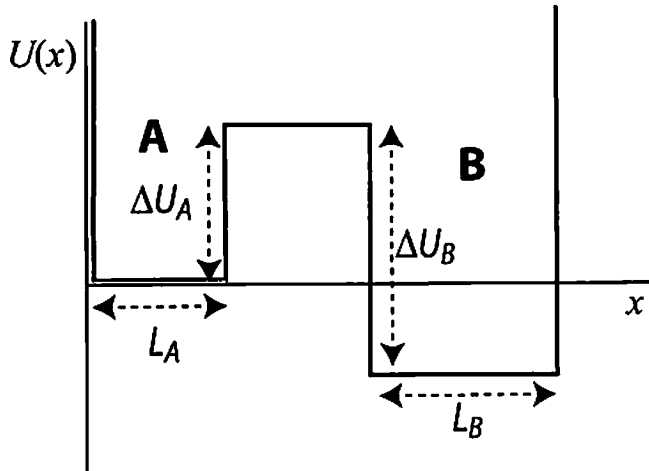
(c) Does the 1D Ising model (with the interaction energy between neighboring spins being equal to J) exhibit a phase transition? If it does, what is the temperature T_c at which the transition happens?

(d) Write down the expression for the partition function of two identical particles obeying Fermi-Dirac statistics at temperature T . Each particle can be in two possible states, with energies ε_1 and ε_2 .

(e) Explain (in no more than 3 sentences) what we mean when we say that the dynamics of some physical quantity, $x(t)$, is ergodic.

5. A one-dimensional particle is subjected to a double-well potential $U(x)$ (shown in the picture below), which consists of two square wells separated by a square barrier. The

temperature of the particle's surroundings is T . Assume $\frac{\Delta U_A}{k_B T}, \frac{\Delta U_B}{k_B T} \gg 1$. The frictional force on the particle is proportional to its velocity and is given by $-\gamma \dot{x}$.

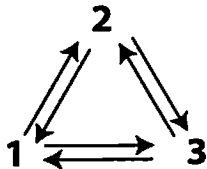


- (a) Assuming overdamped dynamics, write down the Langevin and Smoluchowski equations describing the motion of the particle.
- (b) State the fluctuation-dissipation theorem that relates the random noise term in the Langevin equation to the friction coefficient γ and to the temperature T .
- (c) Estimate the equilibrium probability, w_A , of finding the system within the left potential well. Your answer should be given in terms of the quantities (potential energies and lengths) shown in the picture. (Note that the barrier height is assumed to be much higher than the thermal energy, so the probability to be in the barrier region between A and B can be neglected).

6. A 3-level system obeys stochastic dynamics described by the master equation:

$$\frac{dw_i}{dt} = -\sum_{j \neq i} k_{i \rightarrow j} w_i + \sum_{j \neq i} k_{j \rightarrow i} w_j ,$$

where w_i is the probability of occupying the state i , and $i, j = 1, 2, 3$.



(a) Assuming that all the coefficients $k_{i \rightarrow j}$ are known, what is the average time, $\langle t_2 \rangle$, that the system continuously spends in state 2 before jumping to a different state?

(b) Assuming $k_{1 \rightarrow 2} = k_{2 \rightarrow 3} = k_{3 \rightarrow 1} = 1s^{-1}$ and $k_{2 \rightarrow 1} = k_{3 \rightarrow 2} = k_{1 \rightarrow 3} = 0.01s^{-1}$, is the dynamics of the system time reversible? Recall that we called a stochastic process $i(t)$ (i being the system's discrete state) time reversible if the direct trajectory $i(t)$ and the time-reversed trajectory $i(-t)$ have the same statistical properties.

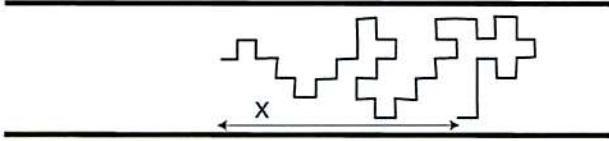
(c) Same question as (b) but for the following set of coefficients, $k_{1 \rightarrow 2} = k_{2 \rightarrow 3} = 1s^{-1}$, $k_{2 \rightarrow 1} = k_{3 \rightarrow 2} = 0.01s^{-1}$, $k_{3 \rightarrow 1} = k_{1 \rightarrow 3} = 0$.

Solutions

4. Short problems – the best 4 out of 5 will count toward your grade:

(a) Consider a two-dimensional self-avoiding lattice random walk of N steps confined to an infinite 2D “tube”. Let $\langle x^2 \rangle = \langle x^2 \rangle(N)$ be the mean square distance traveled in N steps and measured along the tube axis. How does $\langle x^2 \rangle$ scale with N in the limit $N \rightarrow \infty$?

$$\langle x^2 \rangle \propto N^2$$



(b) Same question as in (a), but for a non-self-avoiding random walk

$$\langle x^2 \rangle \propto N \quad \left\{ \begin{array}{l} \text{walks in} \\ x \text{ and } y \\ \text{directions} \\ \text{are decoupled} \end{array} \right.$$

(c) Does the 1D Ising model (with the interaction energy between neighboring spins being equal to J) exhibit a phase transition? If it does, what is the temperature T_c at which the transition happens?

$$\boxed{\text{Yes, } T_c = 0}$$

(d) Write down the expression for the partition function of two identical particles obeying Fermi-Dirac statistics at temperature T . Each particle can be in two possible states, with energies ϵ_1 and ϵ_2 .

$$Q = \frac{1}{2} e^{-\beta(\epsilon_1 + \epsilon_2)}, \quad \beta = (k_B T)^{-1}$$

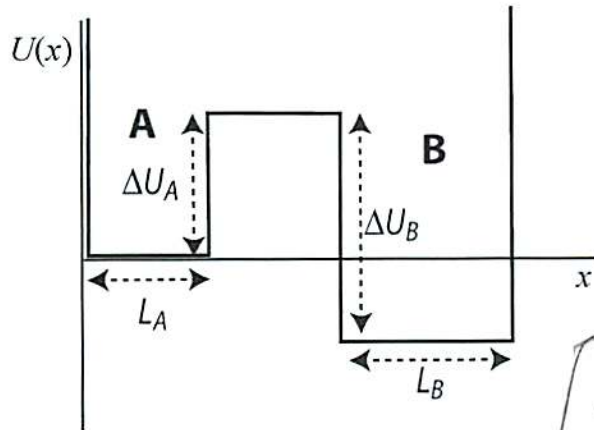
(e) Explain (in no more than 3 sentences) what we mean when we say that the dynamics of some physical quantity, $x(t)$, is ergodic.

Time averages performed over a single long trajectory $x(t)$ are equal to ensemble averages.

5. A one-dimensional particle is subjected to a double-well potential $U(x)$ (shown in the picture below), which consists of two square wells separated by a square barrier. The

temperature of the particle's surroundings is T . Assume $\frac{\Delta U_A}{k_B T}, \frac{\Delta U_B}{k_B T} \gg 1$. The frictional

force on the particle is proportional to its velocity and is given by $-\gamma \dot{x}$.



(a)

$$\gamma \dot{x} = -U'(x) + \eta(t)$$

$$\frac{\partial w}{\partial t} = D \frac{\partial}{\partial x} \left[\beta U'(x) + \frac{\partial}{\partial x} \right] w(x, t)$$

$$D = \frac{k_B T}{\gamma}$$

(a) Assuming overdamped dynamics, write down the Langevin and Smoluchowski equations describing the motion of the particle.

(b) State the fluctuation-dissipation theorem that relates the random noise term in the Langevin equation to the friction coefficient γ and to the temperature T .

$$\langle \eta(t) \eta(t') \rangle = 2\gamma k_B T \delta(t - t')$$

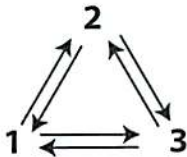
(c) Estimate the equilibrium probability, w_A , of finding the system within the left potential well. Your answer should be given in terms of the quantities (potential energies and lengths) shown in the picture. (Note that the barrier height is assumed to be much higher than the thermal energy, so the probability to be in the barrier region between A and B can be neglected).

$$w_A = \frac{q_A}{q_A + q_B} \approx \frac{L_A e^{\beta \Delta U_A}}{L_A e^{\beta \Delta U_A} + L_B e^{\beta \Delta U_B}}$$

6. A 3-level system obeys stochastic dynamics described by the master equation:

$$\frac{dw_i}{dt} = -\sum_{j \neq i} k_{i \rightarrow j} w_i + \sum_{j \neq i} k_{j \rightarrow i} w_j,$$

where w_i is the probability of occupying the state i , and $i, j = 1, 2, 3$.



(a) Assuming that all the coefficients $k_{i \rightarrow j}$ are known, what is the average time, $\langle t_2 \rangle$, that the system continuously spends in state 2 before jumping to a different state?

$$\langle t_2 \rangle = \frac{1}{k_{2 \rightarrow 1} + k_{2 \rightarrow 3}}$$

(b) Assuming $k_{1 \rightarrow 2} = k_{2 \rightarrow 3} = k_{3 \rightarrow 1} = 1 \text{ s}^{-1}$ and $k_{2 \rightarrow 1} = k_{3 \rightarrow 2} = k_{1 \rightarrow 3} = 0.01 \text{ s}^{-1}$, is the dynamics of the system time reversible? Recall that we called a stochastic process $i(t)$ (i being the system's discrete state) time reversible if the direct trajectory $i(t)$ and the time-reversed trajectory $i(-t)$ have the same statistical properties.

(c) Same question as (b) but for the following set of coefficients, $k_{1 \rightarrow 2} = k_{2 \rightarrow 3} = 1 \text{ s}^{-1}$,

$$k_{2 \rightarrow 1} = k_{3 \rightarrow 2} = 0.01 \text{ s}^{-1}, k_{3 \rightarrow 1} = k_{1 \rightarrow 3} = 0.$$

(b): Time-forward dynamics is mostly clockwise , so time reversed dynamics would be counterclockwise. Not time reversible.

(c) For any scheme like this



with nonzero rate coefficients the dynamics is time-reversible. To see this, note that the steady-state probabilities w_1, w_2, w_3 in this case always satisfy the detailed balance condition:

$$\frac{dw_1}{dt} = -k_{1 \rightarrow 2} w_1 + k_{2 \rightarrow 1} w_2 = 0$$

$$k_{1 \rightarrow 2} w_1 = k_{2 \rightarrow 1} w_2 = 0$$

$$\text{Similarly, } k_{2 \rightarrow 3} w_2 = k_{3 \rightarrow 2} w_3$$

1. (30 points) Provide short answers and *brief* explanations where needed for the following questions. No analysis is required. If you write more than a couple of sentences, you are writing too much.

- (a) (2 pts) What is Cauchy's stress theorem? What principles does it rely on?
- (b) (4 pts) What is the difference between the Cauchy, first Piola-Kirchhoff and second Piola-Kirchhoff stress tensors. Why do we have these different stress tensors?
- (c) (4 pts) It is proposed that the following represent models of physical phenomena. For each, state whether or not this is possible and why.

i. $c_{ij} = b_{ik} a_{kj} b_{ll}^{-1}$

ii. $\mathbf{v} = \nabla \times \mathbf{g}$

Here $\mathbf{v}$, is a velocity vector with Cartesian components v_i , $\mathbf{g}$ is a vector with components g_j , and a_{ij} , b_{ij} , c_{ij} are components of second rank tensors.

- (d) (2 pts) What is material frame indifference, and why is it important?
- (e) (4 pts) The Clausius-Duhem inequality (in the Lagrangian frame) is:

$$\rho_0 \dot{\eta}_0 + \text{Div} \frac{\mathbf{q}_0}{\theta} - \frac{r_0}{\theta} \geq 0$$

What physical principle is it an expression of? What is the physical meaning of each term?

- (f) (4 pts) What physical principle is the following an expression of?

$$\rho \frac{de}{dt} = T : D - \text{div} \dot{q} + r$$

What is the physical meaning of each term?

- (g) (4 pts) In the year 1900 three laws were in existence to describe the average energy per oscillator at temperature T and frequency ν of a black body:

- Wien's law (with constants a, b):

$$\hat{\epsilon} = a \nu \exp \left\{ -b \frac{\nu}{T} \right\} \quad (1)$$

- Rayleigh-Jeans' law:

$$\hat{\epsilon} = \frac{1}{2} k_B T \quad (2)$$

- Planck's law:

$$\hat{\epsilon} = \frac{h \nu}{\exp \left(\frac{h \nu}{k_B T} \right) - 1} \quad (3)$$

with h Planck's constant, k_B Boltzmann constant.

How do they differ? What are their range of validity?

- (h) (2 pts) What is the photoelectric effect? How is it related to Planck's law?
- (i) (2 pts) What is the wave-particle duality? Write expressions in both angular frequency and wavenumber domain.

- (j) (2 pts) Let L_i be the angular momentum in the x_i direction of the motion of a particle, and ψ be the wavefunction of the quantum state. If $L_3\psi = \hbar m\psi$ and $\phi = (L_1 + iL_2)\psi$, what is $L_3\phi$?
2. (40 pts) The incompressible Navier-Stokes equations for a fluid in a uniform gravitational field with acceleration vector $\mathbf{g}$ can be written in several different forms, two of them are:

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \text{grad}) \mathbf{v} = -\frac{1}{\rho} \text{grad } p + \nu \Delta \mathbf{v} + \mathbf{g} \quad (4)$$

$$\frac{\partial \mathbf{v}}{\partial t} - \mathbf{v} \times \boldsymbol{\omega} = -\frac{1}{\rho} \text{grad } p - \frac{1}{2} \text{grad } |\mathbf{v}|^2 + \nu \Delta \mathbf{v} + \mathbf{g} \quad (5)$$

where $\boldsymbol{\omega} = \text{curl } \mathbf{v}$ is the vorticity, ν is the kinematic viscosity and Δ is the Laplacian operator.

- (a) (20 pts) Show that these two forms of incompressible Navier-Stokes are in fact equivalent (**Hint:** You might find this easiest in index notation).
- (b) (20 pts) One way to write Bernoulli's equation (the most famous equation in fluid mechanics) is:

$$\mathbf{e} \cdot \text{grad} \left(p + \frac{1}{2} \rho |\mathbf{v}|^2 - \rho \mathbf{x} \cdot \mathbf{g} \right) = 0$$

where $\mathbf{e}$ is some unit vector. However, this is not true in general. There are several different sets of conditions under which Bernoulli's equation is true. Determine two such sets from the Navier-Stokes equations. You may use the equivalent forms of the Navier-Stokes equations listed above.

3. (30 pts) Consider a particle of mass m constrained to move in one dimension x , in a potential given by $V = m\omega^2 x^2/2$.

- (a) (5 pts) Write Schrödinger's equation for the particle.
- (b) (5 pts) The ground-state wave function is given by

$$\psi(x) = ae^{-x^2/2\alpha^2}$$

where $\alpha^2 = \hbar/m\omega$. What is the ground state energy?

- (c) (10 pts) In some quantum state, the wavefunction is given by:

$$\psi(x) \propto \begin{cases} (\beta - |x|)/\beta^2 & -\beta \leq x \leq \beta \\ 0 & \text{otherwise} \end{cases}$$

What are $\langle x \rangle$ and $\langle E \rangle$, the expected values of the position and energy of the particle.

- (d) (10 pts) For the same quantum state as in (c), what is the probability that the particle will be observed with $x \geq \beta/2$?

4. (50 pts)

(a) (10 pts) A one-dimensional quantum particle on-a-ring is described by the Hamiltonian $\hat{H} = \frac{\hat{p}^2}{2I}$, $\hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial \varphi}$, where φ is the angular coordinate of the particle.

What are the stationary states $\psi_n(\varphi)$ (i.e. the solutions of the time-independent Schrödinger equation)?

(b) (10 pts) For a classical monoatomic gas consisting of atoms of mass m , at temperature T , write down the expression $P(v)$ describing the distribution of the absolute velocity of its

atoms, $v = \sqrt{v_x^2 + v_y^2 + v_z^2}$.

(c) (10 pts) For a one-dimensional classical harmonic oscillator with the Hamiltonian

$H = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}$ at temperature T , write down the distributions $P(x)$ and $P(v)$ of its

coordinate and velocity. What is the expectation value $\langle E \rangle$ of the oscillator's *total* energy?

(d) (10 pts) Write down the Langevin equation describing the motion of a one-dimensional free Brownian particle with coordinate x at temperature T . The friction force on the particle is proportional to its velocity, with a proportionality coefficient γ . State the fluctuation-dissipation theorem in this case. How is the friction coefficient γ related to the diffusion coefficient of the particle?

(e) (10 pts) For a non-self-avoiding random walk on a lattice, the probability of returning to the site from which the walk has originated scales with the number of steps N ($N \gg 1$) as $p(N) \propto N^{-\alpha}$. What are the values of α in one, two and three dimensions?

5. (25 pts)

Consider the one-dimensional Ising model with nearest neighbor interactions at zero magnetic field. The number of spins in the model is N ($N \gg 1$), and the interaction energy between neighboring spins is J ($J > 0$).

- (a) (10 pts) At temperature T , estimate the probability that exactly n spins are up and, correspondingly, $N - n$ spins are down. Assume that $n \ll N$.
- (b) (5 pts) Make a qualitative sketch of the expectation value of a spin $\langle s \rangle$ as a function of temperature T (Note: do not use the mean-field approximation to answer this question).
- (c) (5 pts) Assuming the mean field approximation for the 1D Ising model, how does the temperature T_c at which the order-disorder transition takes place depend on the parameters of the model?
- (d) (5 pts) Is the mean-field theory a good approximation for the Ising model in 1D? In particular how does the mean-field value of T_c differ from its exact value?

6. (25 pts)

Consider an ideal gas of $N \gg 1$ indistinguishable, noninteracting particles obeying the Bose-Einstein statistics.

(a) (20 pts) Assuming that each particle can be in just two possible states with the energies ϵ_1 and ϵ_2 ($\epsilon_2 > \epsilon_1$), what is the expectation number of the number of particles n_2 found in the second state at temperature T ?

(b) (5 pts) Answer the question of Part A assuming that the particles are distinguishable.

Area C CSEM Preliminary Exam

Monday, August 3, 2020

You may use your class materials (notes, textbook, old exams, cheat sheet, etc.) on this exam.

1. Provide short answers and *brief* explanations where needed for the following questions. No analysis is required. If you write more than a sentence or two, you are writing too much.

- (a) What is Cauchy's stress theorem? What principles does it rely on?
- (b) Why is tensor consistency an important constraint on mathematical models of physical systems
- (c) What is material frame indifference, and why is it important?
- (d) What physical phenomena give rise to the Cauchy stress term in the momentum equation, and why do we need a constitutive relation for this term?
- (e) What physical principle is the following an expression of?

$$\rho_0 \dot{\eta}_0 + \text{Div} \frac{\mathbf{q}_0}{\theta} - \frac{r_0}{\theta} \geq 0$$

What is the physical meaning of each term?

- (f) What physical phenomenon is expressed in the following equation:

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

and what is a common device that relies on this phenomenon?

- (g) A particle with charge q is located at point $\mathbf{x}$ and is traveling with velocity $\mathbf{v}$ in an electric field $\mathbf{E}$ and magnetic field $\mathbf{B}$. What is the force on the particle?
- (h) In quantum mechanics what observable is represented by the operator $-i\hbar\nabla$
- (i) A particle is in quantum state $\psi(\mathbf{x})$. Write an expression for the expected value of the position of the particle.
- (j) In a quantum system with wavefunction ψ , you have precise knowledge of an observable Q . What does this tell you about ψ ?

Solve only two of the following three problems

2. A cube of incompressible material of dimension a is subjected to a shear load on the faces normal to the x_1 direction, resulting in a deformation that displaces these faces relative to each other in the direction normal to one of the other faces (call it the x_2 direction) by an amount αa . The material has an incompressible neo-Hookean strain energy density function:

$$W(\mathbf{E}) = \mu I_{\mathbf{E}},$$

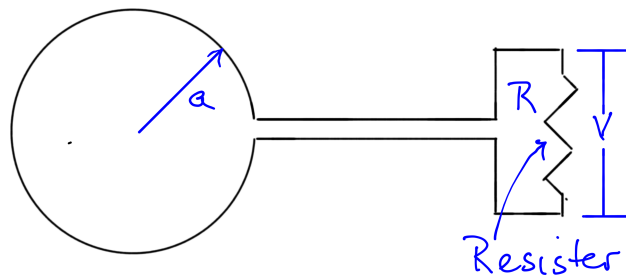
where $\mathbf{E}$ is the strain tensor, $I_{\mathbf{E}}$ is its first invariant and μ is the shear modulus.

- (a) Determine the deformation gradient tensor ($\mathbf{F}$), the right Cauchy-Green deformation tensor ($\mathbf{C}$) and the Green-St. Venant strain tensor ($\mathbf{E}$) in the material.
- (b) How much work was required to deform the material?
- (c) Because the material is incompressible, there is a degeneracy in the stress relation, so that the second Piola-Kirchhoff stress is given by

$$\mathbf{S} = \frac{\partial W}{\partial \mathbf{E}} + p\mathbf{F}^{-1}\mathbf{F}^{-T}$$

where p can be determined from boundary conditions, in this case on the unloaded sides. Determine $\mathbf{S}$.

- (d) What is the total load force.



3. You are interested in measuring the time varying magnetic field $\mathbf{B}(\mathbf{x}, t)$ at a point $\mathbf{x}$. It is proposed that a planar circular loop of wire of radius a be used as a probe. We will use Farady's law to analyze how that might work.
 - (a) Let $\mathbf{n}$ be a unit normal to the plane of the wire loop and assume that a is small enough that variations in $\mathbf{B}$ over the interior of the loop are negligible. If the center of the loop is placed at the point $\mathbf{x}$, what is the energy per unit charge gained/lost when the charge moves around the loop once? Does it matter how fast the charge is moving?
 - (b) A real wire has resistance R , so that energy is dissipated at the rate $I^2 R$ when a current I flows through it. If the wire loop has resistance R_l , what is the current flowing through the wire so that the energy imparted to the charges balances the dissipation?
 - (c) If an electrical resistor with resistance $R \gg R_l$ is placed in the wire loop circuit as shown in the figure, then the effective resistance of the loop is R (Note: the wires going from the loop to the resistor are so close together that the net effect of the magnetic field on them is negligible). The voltage difference between the two sides of a resistor is $V = IR$. What is V for the resistor in the figure, if the loop is placed as in (a)?
 - (d) If one measures V , what can one infer about the magnetic field?
4. Consider a particle of mass m constrained to move only along the x axis in a potential given by:

$$V(x) = \begin{cases} 0 & 0 \leq x \leq a \\ \infty & \text{otherwise} \end{cases}$$

- (a) Write the Schrödinger equation (time independent) describing the motion of the particle, stating any boundary conditions the wavefunction must satisfy

- (b) Determine the energy levels and associated wave functions.
- (c) Let $\tilde{Q}$ be the operator

$$\tilde{Q}\psi = \frac{d^2\psi}{dx^2} \quad 0 \leq x \leq a.$$

Is the associated quantity Q an observable? Why or why not? If so what is the physical observable?

- (d) What is the expected value of the kinetic energy of the particle if its wavefunction is given by $a\psi_n + b\psi_m$, where $a^2 + b^2 = 1$ and ψ_i is the wavefunction associated with i th energy level?

You are required to solve one and only one of the following two problems

5. We consider the Kepler problem for two bodies of masses m_1 and m_2 and positions $\mathbf{r}_1$ and $\mathbf{r}_2$, respectively. The masses interact via the gravitational attraction, with a gravitational constant $G = 6.67 \cdot 10^{-11} \text{ m}^3\text{kg}^{-1}\text{s}^{-2}$.

- (a) Write the potential energy of this system of masses in terms of m_1 , m_2 , $\mathbf{r}_1$, $\mathbf{r}_2$, and G . [1]
- (b) Write the Lagrangian for this problem. [1]
- (c) Let us call $\mathbf{R}$ the position of the center of mass of this system, and $\mathbf{r}$ the position of m_2 relative to m_1 . Perform a coordinate transformation in order to write the Lagrangian from (b) in the center-of-mass reference frame. The expression for the center-of-mass coordinates is known from the lecture notes. [3]
- (d) Check that each term in the Lagrangian obtained in (c) has the correct dimensions of an energy. [1]
- (e) The total angular momentum of this system is $\mathbf{L} = \mathbf{r} \times \mu \dot{\mathbf{r}}$, where $\mu = m_1 m_2 / (m_1 + m_2)$ denotes the reduced mass. Using the Euler-Lagrange equation, show that $\mathbf{L}$ is a constant of motion. [3]
- (f) Show that the trajectory $\mathbf{r} = \mathbf{r}(t)$ lies in a plane passing through the origin of the reference frame and perpendicular to $\mathbf{L}$. [2]
- (g) We orient the Cartesian axes of the center-of-mass reference frame so that the z axis points along the direction of the total angular momentum $\mathbf{L}$. Determine the Lagrangian of the system in the two-dimensional polar coordinates r and θ , having defined: [3]

$$x = r \cos(\theta), \quad y = r \sin(\theta).$$

- (h) Determine the canonical momenta p and p_θ conjugated to the coordinates r and θ , respectively. [4]

- (i) Using the results of (h) and the Legendre transform, show that the Hamiltonian of this system can be written as: [3]

$$H = \frac{p^2}{2\mu} + \frac{p_\theta^2}{2\mu r^2} - \frac{k}{r}.$$

- (j) Using Hamilton's equations, prove that the canonical momentum p_θ is a constant of motion. [1]
- (k) Sketch the effective potential energy $p_\theta^2/2\mu r^2 - Gm_1m_2/r$, and explain the physical meaning of each term. [2]
- (l) Discuss qualitatively the nature of the trajectory $[r(t), \theta(t)]$ for the case when the total kinetic and potential energy of the system corresponds exactly to the bottom of the potential well sketched in (k). Determine the radius of this trajectory. [3]
- (m) Using the radius determined in (l), calculate the average Moon's distance from Earth. The masses of Earth and Moon are $m_E = 5.97 \cdot 10^{24}$ kg and $m_M = 7.34 \cdot 10^{22}$ kg, respectively. [3]
6. A possible realization of a quantum computer consists of a semiconductor with an ordered array of impurities, where each impurity atom carries an electron spin that serves as a quantum bit of information. The spins are oriented parallel ($\uparrow$) or antiparallel ($\downarrow$) to the z direction of a Cartesian reference frame, and interact with an external magnetic field whose component along the z direction is B . We model each of these spins using a two-level quantum system with energies $E_\uparrow = -e\hbar B/m$ and $E_\downarrow = e\hbar B/m$. Here e and m denote the charge and mass of an electron, respectively, and $\hbar$ is the reduced Planck constant. There is no interaction between spins.
- (a) Write the canonical partition function Z of this system as a function of the temperature T . [2]
- (b) Using the definition of canonical partition function, show that the thermodynamic average of the energy of each spin at equilibrium is:

$$\langle E \rangle = -\frac{\partial}{\partial \beta} \log Z, \quad \beta = \frac{1}{k_B T},$$

where T is the absolute temperature and k_B is Boltzmann's constant. [3]

- (c) Starting from the definition of Gibbs' entropy, express the entropy associated with each spin in terms of the partition function Z and the temperature T . [4]
- (d) Combine the results of (a) and (b) to obtain the Helmholtz free energy of each spin at equilibrium. [3]
- (e) It can be shown that the thermodynamic average of the magnetization per spin can be obtained from the Helmholtz free energy via:

$$\langle M \rangle = -\frac{\partial F}{\partial B}.$$

Using this relation, express the average magnetization of the system in terms of e , $\hbar$, m , B , and $k_B T$. [5]

- (f) Sketch the dependence of the average magnetization obtained in (c) on the magnetic field B , at fixed temperature. Indicate the scales in your plot. [3]
- (g) Describe the spin configuration of the system in the limit $|B| \gg mk_{\text{B}}T/e\hbar$. [1]
- (h) Sketch the dependence of the average magnetization obtained in (c) on the temperature T , at fixed magnetic field $B > 0$. Indicate the scales in your plot. [3]
- (i) Describe the spin configuration of the system in the limit $T \gg e\hbar|B|/mk_{\text{B}}$. [1]
- (j) The Curie-Weiss model discussed in the lecture notes exhibits a paramagnetic-ferromagnetic phase transition at a critical temperature. Provide a tentative explanation for why, unlike the Curie-Weiss model, the system studied here does not exhibit a phase transition. [3]
- (k) Calculate the magnetic field B required to achieve 99% of the maximum possible magnetization at room temperature (300 K). [2]

CSEM Area C Preliminary Exam
The University of Texas at Austin
Monday, May 24, 2021

The exam consists of three parts, Part A (short questions), Part B (long questions about topics covered during the first semester), and Part C (long questions about topics covered during the second semester).

You are required to answer all the short questions in Part A; one question in Part B; and one question in Part C. The total numbers of points is 10 (Part A) + 30 (Part B) + 30 (Part C).

You can use your lecture notes. The deadline for submission is 3PM CST.

Part A: Answer all of the following ten short questions

1. (10pts total) Provide short answers and *brief* explanations where needed. No analysis is required.

- (a) (1 pt) What is the Cauchy hypothesis in continuum mechanics, and why do we need it?
- (b) (1 pt) What are the physical principles expressed in the following relations and what is the physical meaning of each term?

$$\dot{\rho} = -\rho I : D$$

- (c) (1 pt) Let F be the deformation gradient tensor. What is the kinematical interpretation of the following relationship:

$$\frac{d}{dt}(\det F) = (\det F) \operatorname{tr}(F^{-1} \dot{F})$$

- (d) (1 pt) What is material frame indifference, and why is it important?
- (e) (1 pt) What is the difference between the Cauchy, first Piola-Kirchhoff and second Piola-Kirchhoff stress tensors. Why do we have these different stress tensors?
- (f) (1 pt) State the canonical quantization conditions for the position and momentum of a particle.
- (g) (1 pt) Sketch the bonding and antibonding wavefunctions of an electron in the H_2^+ molecular cation.
- (h) (1 pt) State the symmetry of fermionic and of bosonic wavefunctions under particle exchange.
- (i) (1 pt) Explain why we can think of light as a collection of discrete energy quanta called photons.
- (j) (1 pt) Explain how the notion of temperature arises in the context of statistical mechanics.

Part B: Answer one and only one of the following two questions (q. 2 or q. 3)

2. Consider a body undergoing arbitrary rigid motions

$$\varphi(\boldsymbol{\xi}, t) = \boldsymbol{\Lambda}(t) \boldsymbol{\xi} + \mathbf{c}(t)$$

where φ are points in the reference configuration, $\boldsymbol{\Lambda}(t)$ is a time-varying rotation, and $\mathbf{c}(t)$ is a time-varying vector.

- (a) (6 pts) Show that the following relationship holds between the 1st Piola-Kirchhoff tensor $\mathbf{P}$ and the 2nd Piola-Kirchhoff tensor $\boldsymbol{\Sigma}$:

$$\mathbf{P} : \dot{\mathbf{F}} = \frac{1}{2} \boldsymbol{\Sigma} : \dot{\mathbf{C}}$$

with deformation gradient $\mathbf{F}$ and right Cauchy strain tensor $\mathbf{C}$.

- (b) (6 pts) Show that $\mathbf{P} : \dot{\mathbf{F}}$ vanishes for arbitrary rigid motions.
(c) (6 pts) Let the internal energy density e and heat flux $\mathbf{q}$ fields be given by constitutive relations of the form:

$$\begin{aligned} e &= \alpha \theta \\ \mathbf{q} &= -\kappa \nabla \theta \end{aligned}$$

where α and κ are scalar constants, and θ is absolute temperature. Show that the conservation equation for energy reduces to

$$\rho_0 \alpha \frac{\partial \theta}{\partial t} = \kappa \Delta \theta + r_0$$

with ρ_0 and r_0 density and heat supply in the reference configuration, and differential operators ∇ and Δ taken with respect to reference configuration space, $\boldsymbol{\xi}$.

- (d) (6 pts) Suppose the constitutive relation for e is replaced by a constitutive relation for the Helmholtz free energy ψ and entropy η of the form

$$\begin{aligned} \psi &= \hat{\psi}(\theta) \\ \eta &= -\frac{d\hat{\psi}(\theta)}{d\theta} \end{aligned}$$

for a given function $\hat{\psi}$. Then, re-derive the conservation equation of energy in terms of $\hat{\psi}(\theta)$ and θ .

- (e) (6 pts) Assuming a constitutive relation as in part (d), determine for which parameter range of κ the Clausius-Duhem inequality is satisfied for arbitrary rigid body motions and temperature fields. What is the implication (i.e., physical meaning) for those parameters, for which the inequality is *not* satisfied?

3. (30 points) In a linearly elastic solid undergoing small (infinitesimal) deformations the second Piola-Kirchhoff stress tensor Σ is given by

$$\Sigma = \lambda \nabla \cdot \mathbf{u} \mathbf{I} + \mu (\nabla \mathbf{u} + \nabla \mathbf{u}^T)$$

where $\mathbf{u}$ is the small displacement, $\mathbf{I}$ is the identity tensor and λ and μ are constants.

- (a) (6 pts) Assuming no body forces and starting with conservation of momentum, derive an equation for the evolution of $\mathbf{u}$.
- (b) (6 pts) Show that these equations admit two classes of wave solution, one in which the displacements are in the direction of wave propagation, and one in which the displacements are orthogonal to the direction of propagation.
- (c) (6 pts) Determine the velocities of these waves.
- (d) (6 pts) Determine the spin tensor W for this problem.
- (e) (6 pts) What are the implications of these solutions on the shaking you would feel during an earthquake?

Part C: Answer one and only one of the following two questions (q. 4 or q. 5)

4. (30 points) We consider the time-independent Schrödinger equation for an electron in the hydrogen atom:

$$-\frac{\hbar^2}{2m}\nabla^2\psi - \frac{e^2}{4\pi\epsilon_0 r}\psi = E\psi, \quad (1)$$

where m and e are the electron mass and charge, respectively, $\hbar$ is the Planck constant and ϵ_0 is the dielectric permittivity of vacuum. The proton is located at the origin of the reference frame. r indicates the distance between the electron and the proton.

- (a) (6pts) Let r , θ , and ϕ indicate the electron position in spherical coordinates. Consider the function defined by $\psi(r, \theta, \phi) = r^{-1}u(r)Y_{lm}(\theta, \phi)$, where Y_{lm} denotes a spherical harmonic. Show that, after replacing this expression in Eq. (1), one obtains the following equation for $u(r)$:

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}u - \frac{e^2}{4\pi\epsilon_0 r}u = Eu \quad (2)$$

Indicate the intermediate steps in your derivation.

- (b) (4pts) Determine the normalization condition that the function u must fulfil for the wavefunction ψ to be correctly normalized.
- (d) (4pts) Consider the function

$$u(r) = A r \exp(-\lambda r)$$

where A and λ are real-valued positive constants. Express A in terms of λ by requiring that the wavefunction ψ given in (a) be normalized.

- (e) (6pts) After setting $l = 0$ in Eq. (2), show that the expectation value of the electron energy on the normalized wavefunction determined in (a), as a function of the parameter λ , is given by:

$$\langle E \rangle_\lambda = \frac{\hbar^2}{2m}\lambda^2 - \frac{e^2}{4\pi\epsilon_0}\lambda$$

- (f) (4pts) Determine the minimum of the expectation value $\langle E \rangle_\lambda$ with respect to the parameter λ , and express your result in terms of the Hartree energy.
- (g) (3pts) Provide a physical interpretation for the energy minimum $\langle E \rangle_\lambda$ determined in (f) and for the corresponding parameter λ .
- (h) (3pts) Antihydrogen is the antimatter counterpart of hydrogen. It consists of an anti-electron, a particle with the same mass of an electron but positive charge $+e$, and an antiproton, a particle with the same mass of a proton but negative charge $-e$. This atom of antimatter can be produced in particle accelerators. Find the energy of the ground state of the antielectron in the antihydrogen atom.

5. (30 points) We describe the vibrations of a silicon crystal as a set of N independent quantum harmonic oscillators, all with the same oscillation frequency ω . We want to investigate the statistical properties of this system within the canonical ensemble.

- (a) (4pts) Let us assume that the first oscillator is in the n_1 -th quantum state, with n_1 being a non-negative integer, the second oscillator is in the quantum state n_2 , and so on. Write the total energy of this system as a function of $n_1, n_2, \dots, n_N$ and ω .
- (b) (6pts) Derive the canonical partition function Z for this system, and express your result as a function of ω , temperature T , and number of oscillators N .
- (c) (5pts) The canonical average of the number of phonons in each oscillator at the absolute temperature T can be evaluated as:

$$\langle n \rangle = -\frac{1}{2} - \frac{k_B T}{N\hbar} \frac{\partial \log Z}{\partial \omega},$$

where $\hbar$ and k_B are the Planck and Boltzmann constants, respectively. Using this expression together with the results of (a) and (b), show that the average number of phonons $\langle n \rangle$ in each oscillator coincides with the Bose-Einstein distribution:

$$n(\omega, T) = \left[\exp \left(\frac{\hbar \omega}{k_B T} \right) - 1 \right]^{-1}.$$

- (d) (5pts) Let us call $\mathbf{u}$ the vector corresponding to the displacement of a given atom in the above crystal from its equilibrium site. Write an expression for the mean-square displacement $\langle |\mathbf{u}|^2 \rangle$ at the temperature T , as a function of the frequency ω and the mass M of a silicon atom (Hint: This question does not require derivations, and the use of the lecture notes is allowed).
- (e) (4pts) The mass of a silicon atom is $M = 4.66 \cdot 10^{-26}$ kg, and the oscillation frequency is $\omega = 14$ THz. Calculate the average root mean-square displacement, $\sqrt{\langle |\mathbf{u}|^2 \rangle}$, of a silicon atom at room temperature ($T = 300$ K). Compare your result with the equilibrium distance between nearest-neighbor atoms in the silicon crystal, $0.235 \cdot 10^{-9}$ m.
- (f) (6pts) In order to determine the melting point of a crystal, we can assume that the solid/liquid phase transition occurs when the root-mean-square displacement of the atoms in the solid reaches 50% of the interatomic distance at equilibrium. Using the interatomic distance given in (e), determine the melting temperature of the silicon crystal, and compare your estimate with the measured melting point 1683 K.