

# Comprehensive Examination

Department of Physics and Astronomy

Stony Brook University

Fall 2020

## General Instructions:

Three problems are given. If you take this exam as a placement exam, you must work on all three problems. If you take the exam as a qualifying exam, you must work on two problems (if you work on all three problems, only the two problems with the highest scores will be counted).

Each problem counts for 20 points, and the solution should typically take approximately one hour.

Use one exam book for each problem, and label it carefully with the problem topic and number and your ID number.

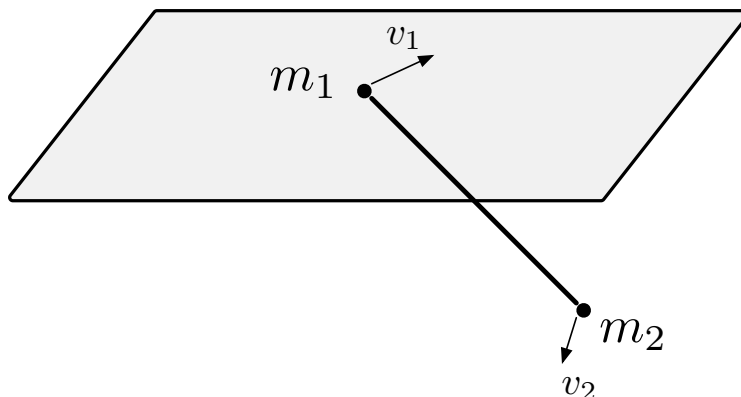
**Write your ID number (not your name!) on each exam booklet.**

You may use, one sheet (front and back side) of handwritten notes and, with the proctor's approval, a foreign-language dictionary. **No other materials may be used.**

# Classical Mechanics 1

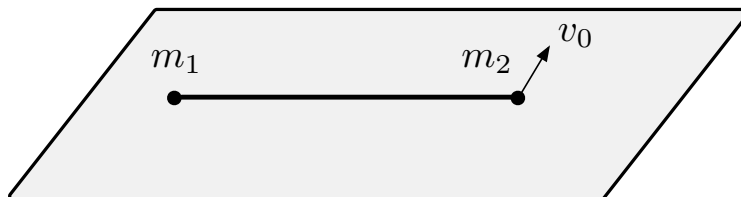
## A sliding conical pendulum

Consider two beads connected by a rod of length  $\ell$ . The first bead has mass  $m_1$  and is constrained to lie in the  $x, y$  plane, but may move freely in this plane. The second bead has mass  $m_2$  and can move freely in all three dimensions, and can pass freely through the  $x, y$  plane. The system sits in the earth's gravitational field  $\mathbf{g} = -g \hat{\mathbf{z}}$ .



- (0 points) Determine the distance from  $m_1$  to the center of mass.
- (6 points) Clearly define some appropriate generalized coordinates for the system, and write down the Lagrangian of the system in terms of these coordinates.
- (5 points) Identify all integrals of the motion.

Now consider the case where the first bead is initially at rest and the second bead initially has velocity  $v_0$  in the  $x, y$  plane, and perpendicular to the rod, before beginning to fall (see below).

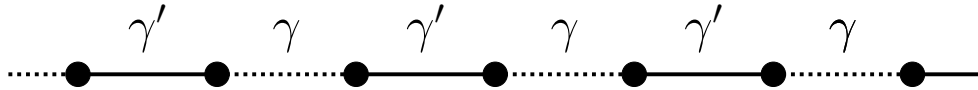


- (1 points) Describe qualitatively the subsequent motion of the system. In what Galilean frame is the motion periodic? Explain.
- (8 points)
  - The pendulum swings down from an initial angle of  $\pi/2$  relative to the vertical to a minimum angle. Determine this minimum angle.
  - Determine the associated period of the motion. You may leave any dimensionless integrals unevaluated. Define what is meant by large and small  $v_0$  and describe the motion qualitatively in these two limits.

# Classical Mechanics 2

## Waves from coupled springs

Consider a one dimensional system of springs, consisting of alternating spring constants  $\gamma$  and  $\gamma'$ , and particles of mass  $m$  as shown below<sup>1</sup>. At rest the springs are unstretched and are separated by a distance  $a$ . Let  $x_i$  and  $u_i$  respectively denote the equilibrium position and small longitudinal displacement of the  $i$ -th oscillator.



- (a) (7 points) Write down the Lagrangian for the system of springs and determine the equations of motion. Show that the normal modes of the system take the form

$$u_i = A \xi_1 e^{-i\omega t + kx_i}, \quad (1a)$$

$$u_{i+1} = A \xi_2 e^{-i\omega t + kx_{i+1}}, \quad (1b)$$

where  $i$  runs over the even sites. Explicitly write down the system of equations (in matrix form) that must be solved to determine the eigen-frequencies and associated vectors  $\vec{\xi} = (\xi_1, \xi_2)$ , but *do not* try to solve this system explicitly yet.

- (b) (6 points) Determine the eigen-frequencies  $\omega_{\pm}^2(k)$ . Expand your eigen-frequencies at small  $k$  to quadratic order, and sketch the behavior of  $\omega_+(k)$  and  $\omega_-(k)$  at small  $k$ .
- (c) For long wavelengths  $ka \ll 1$  the fluctuations of the oscillators can be treated as a continuous system with a field  $u(t, x)$  proportional to the displacements. Consider a continuous action of the form

$$S[u(t, x)] = \int dt dx \left( \partial_t u(t, x)^2 - c_1 (\partial_x u(t, x))^2 - c_2 (u(t, x))^2 \right), \quad (2)$$

where  $c_1$  and  $c_2$  are constants.

- (i) (4 points) Determine the equation of motion for  $u(t, x)$  from this action, and compute the dispersion relation  $\omega^2(k)$  from the resulting equation.
- (ii) (3 points) How should the “low-energy” constants  $c_1$  and  $c_2$  be chosen to correctly model the fluctuations of part (c) for the positive mode  $\omega_+(k)$ , and how should they be chosen to correctly model the negative mode  $\omega_-(k)$ .

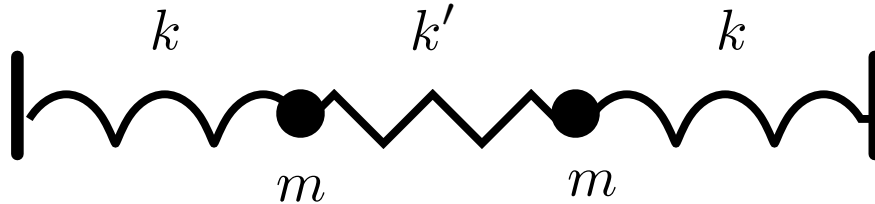
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<sup>1</sup>To avoid confusion with the wavenumber  $k$  in Eq. (1), we are using  $\gamma$  and  $\gamma'$  for the spring constants instead of  $k$  and  $k'$ .

# Classical Mechanics 3

## Oscillations with similar frequencies

Consider two particles of mass  $m$  coupled to the walls via springs with spring constant  $k = m\omega_0^2$ . The two particles are weakly coupled by a third spring with spring constant  $k' = m\omega'^2$  as shown below. The particles can move only in the  $x$ -direction, and the springs are unstretched when the system is at rest. Assume that  $\omega' \ll \omega_0$ .



- (a) (3 points) If at time  $t = 0$  the left particle is displaced by an initial position  $x_0$  and the right particle is at rest, determine the subsequent oscillations of the system.
- (b) (4 points) Plot qualitatively  $x_1(t)$  and  $x_2(t)$ . Show all relevant features, minding the strong inequality  $k' \ll k$ .

Now consider the case when the particles also experience dissipation. The drag force on the particles is

$$F_{\text{drag}} = -m\eta \frac{dx}{dt}, \quad (1)$$

and the drag coefficient is small  $\eta \ll \omega' \ll \omega_0$ . Starting at  $t=0$ , external forces are applied to the particles. The forces on the first and second particles are  $F(t)$  and  $-F(t)$  respectively. The particles are at rest for  $t < 0$ .

- (c) (6 points) Determine the positions of the particles for  $t > 0$  as an explicit integral over  $F(t)$ .
- (d) (3 points) Determine the energy of the system for  $t > 0$  as a double integral over  $F(t)$ .
- (e) (4 points) If  $F(t)$  is a time-dependent random force satisfying<sup>2</sup>

$$\begin{aligned} \langle F(t) \rangle &= 0, \\ \langle F(t)F(t') \rangle &= 2Tm\eta\delta(t - t'). \end{aligned}$$

Determine how the energy of the system evolves in time.

Here  $T$  is a constant parameter that can be interpreted as the temperature of an external bath provided the force  $F(t)$ .

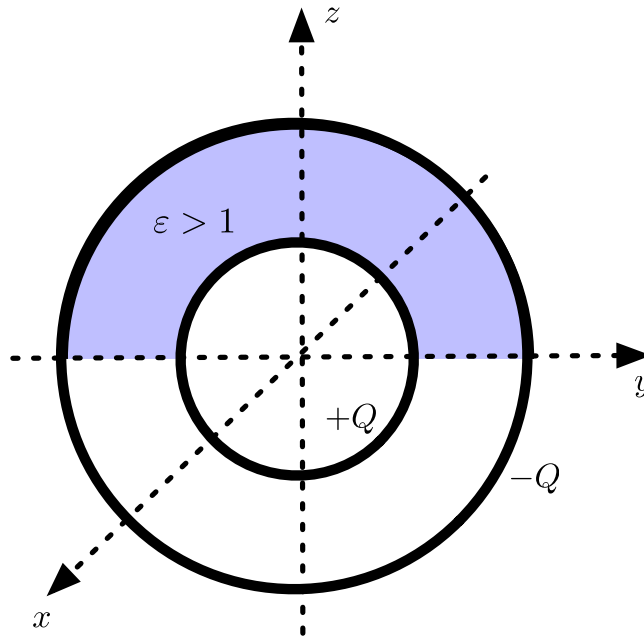
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<sup>2</sup>Imagine discretizing the system into steps of size  $\Delta t$ , the force in each  $\Delta t$  is  $F(t) = \pm 2Tm\eta/\sqrt{\Delta t}$  where each sign occurs with 50% probability.

# Electromagnetism 1

## Half-spherical capacitor

Two concentric conducting spheres of inner and outer radius  $a$  and  $b$  respectively, carry charges  $\pm Q$ . The empty space between the spheres is half-filled by a shell of dielectric with dielectric constant  $\epsilon$  as illustrated in the figure.



- (a) (8 points) Find the electric field everywhere between the spheres.

*Hint:* Assume that the electric field is directed radially and show that the equations of motion and all electrostatic boundary conditions are satisfied with this ansatz.

- (b) (6 points) Calculate the charge per area on the inner sphere, and the polarization charge per area induced on the surface of the dielectric at  $r = a$ .
- (c) (6 points) Calculate the magnitude and direction of the net electrostatic force on the inner sphere.

# Electromagnetism 2

## Radiation from non-relativistic motion

- (a) (8 points) Consider a relativistic charged particle of charge  $q$  and trajectory  $\mathbf{r}_0(t)$ . Recall that the Lienard-Wiechert potentials are<sup>3</sup>

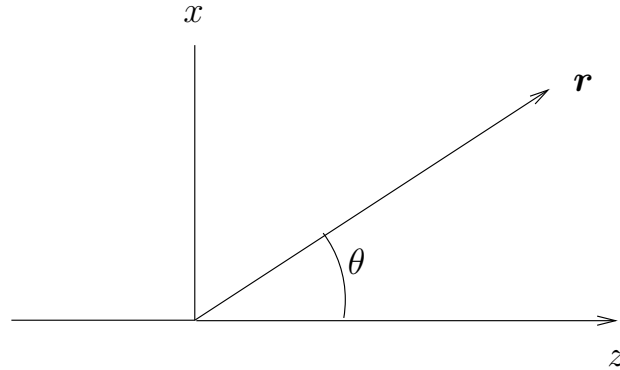
$$\varphi(t, \mathbf{r}) = \frac{q}{4\pi\epsilon_0} \left[ \frac{1}{R(1 - \mathbf{n} \cdot \mathbf{v}_0/c)} \right]_{\text{ret}}, \quad (1a)$$

$$\mathbf{A}(t, \mathbf{r}) = \frac{q}{4\pi\epsilon_0 c} \left[ \frac{\mathbf{v}_0/c}{R(1 - \mathbf{n} \cdot \mathbf{v}_0/c)} \right]_{\text{ret}}, \quad (1b)$$

where  $\mathbf{v}_0 = \dot{\mathbf{r}}_0$ ,  $\mathbf{R} \equiv \mathbf{r} - \mathbf{r}_0$ , and  $\mathbf{n} = \mathbf{R}/R$ .  $[\ ]_{\text{ret}}$  indicates that  $\mathbf{r}_0$  and  $\mathbf{v}_0$  are to be evaluated at the *retarded* time  $T \equiv t - |\mathbf{r} - \mathbf{r}_0(T)|/c$ .

- (i) Find approximate expressions for these potentials in the far field limit (large  $\mathbf{r}$ ), and for non-relativistic particles to first order in  $\mathbf{v}_0/c$ .
  - (ii) Derive an expression for the corresponding electric field  $\mathbf{E}(t, \mathbf{r})$  (in the far field and non-relativistic limits) directly from the definition of field strength tensor  $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$  and the potentials of (i).
- (b) (8 points) Consider a plane wave of light propagating in the  $z$  direction which is polarized in the  $x$  direction,  $\mathbf{E}(t, \mathbf{r}) = E_0 \cos(\omega t - kz) \hat{\mathbf{x}}$  (see below). The incoming light is incident upon an electron of charge  $q$  and mass  $m$  situated at the origin. The motion of the electron is non-relativistic.

Determine the radiated electric field in the far field at an angle  $\theta$  relative to the  $z$  axis, and in the  $xz$  plane (see below). For these conditions, give explicit expressions for the Cartesian components of the (real) electric field as a function of  $r$ ,  $\theta$ , and time  $t$ .




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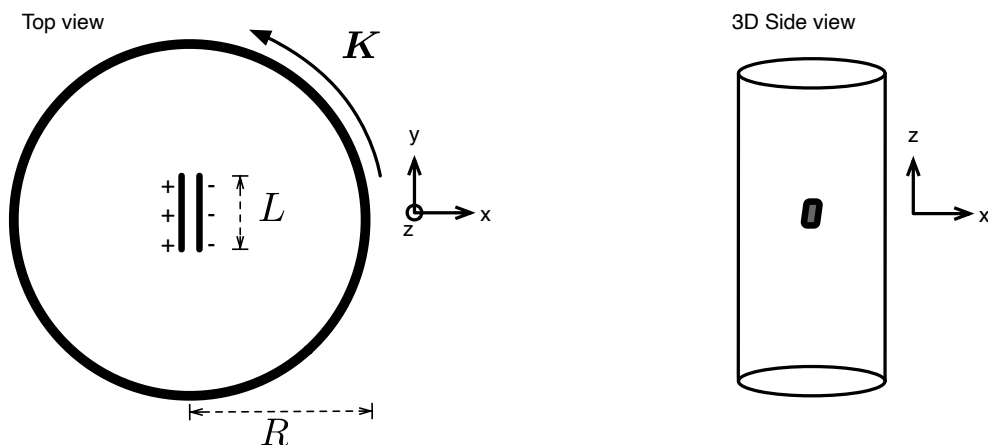
<sup>3</sup>We have given the potentials in the SI system of units. In Gaussian units we substitute  $q/(4\pi\epsilon_0) \rightarrow q$  and  $q/(4\pi\epsilon_0 c) \rightarrow q$  in the equations  $\varphi$  and  $\mathbf{A}$  respectively. In the Heaviside Lorentz units we substitute  $q/(4\pi\epsilon_0) \rightarrow q/4\pi$  and  $q/(4\pi\epsilon_0 c) \rightarrow q/4\pi$ .

- (c) (4 points) Determine the power per unit solid angle scattered at the angle  $\theta$  of part (b) for light polarized in the  $xz$  plane,  $dP_{xz}(\theta)/d\Omega$ , and out of the  $xz$  plane,  $dP_y(\theta)/d\Omega$ . Give a qualitative explanation for the differences in the scattered intensities for the two cases.

# Electromagnetism 3

## A capacitor in a magnetic field

Consider two square non-conducting uniformly charged parallel plates of mass  $M$ , charge  $\pm Q$ , area  $A = L^2$ , and fixed separation  $d$ , with  $d \ll L$ . The center of plate assembly is placed precisely at the center of a long conducting tube of radius  $R$ , with  $R \gg L$ . The normal vector to the plates points along the  $x$ -axis, with the positively charged plate on the left at  $x = -d/2$  when viewed from above (see below). Initially, the tube carries surface current  $\mathbf{K} = K_0 \hat{\phi}$  as shown below.



- (a) (2 points) Compute the magnitude and direction of the momentum  $\mathbf{P}_{\text{field}}$  stored in the initial configuration of electromagnetic fields, *neglecting* the fringing electric fields of the plates.

In part (d), you will show that the total momentum in the fields, *including* the fringing fields, is exactly half of this partial result.

- (b) (6 points) At  $t = 0$  the current is slowly switched off over a time  $T$ ,  $K(t) = K_0 (1 - t/T)$ . Starting with the Lorentz force law,

$$\mathbf{F} = q(\mathbf{E} + \frac{\mathbf{v}}{c} \times \mathbf{B}), \quad (21)$$

determine the magnitude and direction of the force on each plate. Compute the total impulse  $\Delta \mathbf{P}$  (both magnitude and direction) delivered to the plates over time  $T$ . Is this the same as part (a)? Explain.

- (c) (6 points) If the parallel plates are replaced by an assembly consisting of two irregularly shaped non-conducting objects of charges  $\pm Q$  and characteristic size  $L \ll R$  and arbitrary orientation, show that the net force on the assembly is determined by its electric dipole moment and the changing magnetic field,  $\dot{\mathbf{B}}$ . Check that your general result is consistent with (b).



- (d) (6 points) Recompute the total momentum stored in the initial fields of part (a), this time *including* the fringing electric fields. Show that the result is exactly half of (a) and related to the electric dipole moment of the the plates.

*Hint:* Prove the vector identity  $\int_V d^3\mathbf{r} \, E_i = - \oint_S da_i \, \phi$  where  $\phi$  is the scalar potential, and use the result to rewrite the total momentum stored in the field as a surface integral over the cylinder (where the dipole approximation for the electric field is valid). Some elementary integrals are given below.

**Elementary integrals:**

$$\int_{-\infty}^{\infty} \frac{dx}{(1+x^2)^{n/2}} = \begin{cases} \pi & n = 2 \\ 2 & n = 3 \\ \frac{\pi}{2} & n = 4 \\ \frac{4}{3} & n = 5 \end{cases} \quad (22)$$

# Quantum Mechanics 1

## 1D hydrogen atom

An image force attracts an electron to a flat surface. The dynamics of the electron at a distance  $x$  from the surface is governed then by the Hamiltonian

$$H = \frac{p^2}{2m} + V(x), \quad V(x) = \begin{cases} +\infty, & x < 0, \\ -k/x, & x > 0, \end{cases}$$

where  $k > 0$  is a constant.

- (a) (2 pts) Write down the WKB quantization condition appropriate for the potential  $V(x)$ .
- (b) (4 pts) Find explicitly the energies  $E_n$  of the stationary states of the electron bound to the surface in the WKB approximation.

In the rest of the problem you need to find the energies  $E_n$  exactly by solving the Schrödinger equation using the method of the series expansion of the solution.

- (c) (4 pts) Write down the Schrödinger equation and find the main part,  $a(x)$ , of the asymptotic behavior of the wavefunctions  $\psi(x)$  of the bound states at  $x \rightarrow \infty$ :  $\psi(x) \simeq a(x)$ . Derive the form of the Schrödinger equation this equation takes in terms of  $f(x)$  that is defined as the remaining part of  $\psi(x)$ :  $\psi(x) = f(x)a(x)$ .
- (d) (4 pts) Representing  $f(x)$  as a power series, obtain the recurrence relation the coefficients of this series from the Schrödinger equation.
- (e) (4 pts) Use the recurrence relation derived in (d) to find the energies  $E_n$  of the stationary states. Very briefly compare the exact energies  $E_n$  to their values in the WKB approximation.
- (f) (2 pts) Find the wavefunction of the ground state of this “1D hydrogen atom”.

# Quantum Mechanics 2

## Spin angular momentum and an antiferromagnetic spin chain

Consider the spin operators in units of  $\hbar$ ,  $\hat{S}^\alpha$  with  $\alpha=x, y, z$ , which satisfy the usual commutation relations  $[\hat{S}^\alpha, \hat{S}^\beta] = i \sum_\gamma \varepsilon_{\alpha\beta\gamma} \hat{S}^\gamma$ . The spin raising and lowering operators are  $\hat{S}^\pm = \hat{S}^x \pm i\hat{S}^y$ . The spin magnitude  $S$  can take any half-integer or integer value, and is given by the standard relation  $S(S+1) = \sum_\alpha (\hat{S}^\alpha)^2$ .

- (a) (4 pts) Use the commutation relations between the  $\hat{S}^\pm$  and  $\hat{S}^z$  operators to show that under the rotation  $U_z(\theta) = e^{-i\theta\hat{S}^z}$  the operator  $\hat{S}^\pm$  transforms as  $U_z(\theta)\hat{S}^\pm U_z(\theta)^\dagger = e^{\mp i\theta}\hat{S}^\pm$ . Use this result and the permutation  $x \rightarrow z \rightarrow y$  to show that  $e^{-i\pi\hat{S}^y}\hat{S}^z e^{i\pi\hat{S}^y} = -\hat{S}^z$ .

Now consider a chain of such spins on  $N$  sites (with  $N$  even) interacting with a nearest-neighbor antiferromagnetic Heisenberg interaction. The sites are labeled from  $j = -N/2$  to  $j = N/2 - 1$  and arranged in a circle, so that the  $(N/2)$ -th site is the same as  $(-N/2)$ -th site. The Hamiltonian of the chain is then:

$$H = \sum_{j=-N/2}^{N/2-1} (\hat{S}_j^x \hat{S}_{j+1}^x + \hat{S}_j^y \hat{S}_{j+1}^y + \hat{S}_j^z \hat{S}_{j+1}^z) = \sum_{j=-N/2}^{N/2-1} \left[ \frac{1}{2} (\hat{S}_j^+ \hat{S}_{j+1}^- + \hat{S}_j^- \hat{S}_{j+1}^+) + \hat{S}_j^z \hat{S}_{j+1}^z \right]. \quad (1)$$

The chain is invariant under: (i) spatial translations, (ii) spatial reflections, and (iii) rotations of the spin operators, as illustrated below. The reflection can be about any site, but we will only consider the reflection about the origin,  $j = 0$ .

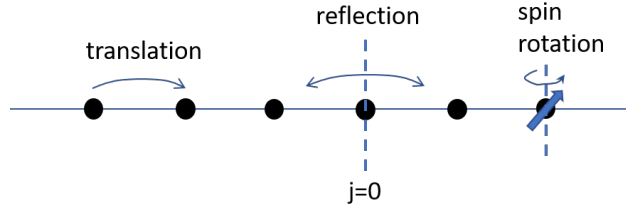


Figure 1: A linear chain of spins with  $N = 6$  sites.

- (b) (2 points) Prove that the Hamiltonian is invariant under a global rotation of spins via the rotation operator,  $U_z(\theta) = e^{-i\theta \sum_j \hat{S}_j^z}$ , i.e. show that  $U_z(\theta) H U_z(\theta)^\dagger = H$ .

The Hamiltonian is also obviously invariant under the translations and reflections.

- (c) (4 points) The ground state of the chain  $|\psi_0\rangle$  has energy  $e_0$  per site, i.e.

$$H|\psi_0\rangle = N e_0 |\psi_0\rangle.$$

Assume that this ground state respects the symmetries of the Hamiltonian, including the rotation symmetry, which makes the  $x, y, z$  axes of the coordinate system equivalent. Use this assumption to determine the expectation values  $\langle \psi_0 | \hat{S}_j^+ \hat{S}_{j+1}^- | \psi_0 \rangle$  and  $\langle \psi_0 | \hat{S}_j^- \hat{S}_{j+1}^+ | \psi_0 \rangle$  in terms of  $e_0$ .

- (d) (5 points) Now consider a non-uniform rotation  $U_{\text{NU}}$  which acts on the middle  $(2n+1)$  sites of the chain  $j \in [-n, n]$  with  $n < N/2$ , and rotates each spin in this range by a site-dependent angle  $\theta_j$  that increases linearly with  $j$  from zero to  $2\pi$ :

$$U_{\text{NU}}^\dagger \equiv \exp \left( i \sum_{j=-n}^n \theta_j \hat{S}_j^z \right), \quad \text{where} \quad \theta_j \equiv \pi(j+n)/n. \quad (2)$$

The operator  $U_{\text{NU}}$  changes the ground state into another state  $|\psi_1\rangle \equiv U_{\text{NU}}^\dagger |\psi_0\rangle$ , creating an excitation of length  $2n+1$ .

- (i) Determine how  $U_{\text{NU}}^\dagger$  transforms under the combination of the reflection with respect to the origin, and a uniform spin rotation by  $\pi$  around  $y$  axis.

*Hint:* The combined action of these transformations on a single site operator  $\hat{S}_j^z$  is such that  $\hat{S}_j^z \rightarrow -\hat{S}_{-j}^z$ .

- (ii) Use the result of (i) to show that  $\langle \psi_1 | \psi_0 \rangle = 0$ , when the spin magnitude  $S$  on each site is a half-integer.

- (e) (5 points) Calculate the energy difference between the states  $|\psi_1\rangle$  and  $|\psi_0\rangle$ :

$$\delta E \equiv \langle \psi_1 | H | \psi_1 \rangle - \langle \psi_0 | H | \psi_0 \rangle. \quad (3)$$

Show that the energy difference is of order  $\mathcal{O}(1/n)$  and approaches zero for large  $n$ .

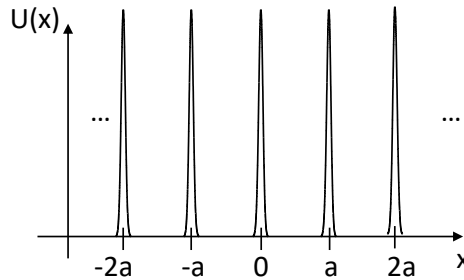
*Hint:* Use the results of parts (a) and (c) applied to the chain.

This problem shows that  $|\psi_1\rangle$  is orthogonal to  $|\psi_0\rangle$  and has the approximately the same energy for large wavelengths,  $n \rightarrow \infty$ . The problem provides one particular example of the so-called Lieb-Schultz-Mattis (LSM) theorem which states that a 1D spin system with translation and spin rotation symmetry, and half-integer spin per unit cell, does not admit a gapped symmetric non-degenerate ground state.

# Quantum Mechanics 3

## Particle in a periodic potential

Consider a particle of mass  $m$  in a periodic potential made of delta functions  $U(x) = \alpha \sum_{n=-\infty}^{\infty} \delta(x - na)$  representing an idealized one-dimensional crystal. This problem will consider the energy spectrum of the particle in the potential, both for the case of discrete translational invariance, and for the case of an additional localized defect.



In the “potential-free” regions  $na < x < (n+1)a$ , the wavefunction  $\psi$  of the particle can be written as a superposition of plane waves,  $A_n e^{ik(x-na)} + B_n e^{-ik(x-na)}$ , where  $k = k(E) = \sqrt{2mE}/\hbar$  is the wavenumber and  $E$  is the particle’s energy.

- (a) (3 points) Provide arguments to show that  $\psi(x)$  must fulfill the condition  $\psi(x+a) = \mu\psi(x)$ . What are the possible values of  $\mu$ ? Relate  $\mu$  to the so-called quasimomentum  $q$ , where  $q \in [-\pi/a, \pi/a]$ . (Note: this is known as Bloch’s theorem.)
- (b) (6 points) From the Schrödinger equation, find the matching conditions for  $\psi$  and its spatial derivative at the points  $x = na$ . Using these conditions, show that the relationship between  $E$  and  $\mu$  can be written as

$$\mu^2 - 2\mu f(E) + 1 = 0$$

and find  $f(E)$  in terms of the wavenumber  $k = k(E)$ .

- (c) (3 points) From the constraint on  $\mu$ , find the range of allowed values of  $f(E)$ .
- (d) (5 points) The function  $f(E)$  encodes the spectrum of the particle in the potential. Use Bloch’s theorem and the result from the previous part to derive an equation that relates  $f(E)$  to the quasimomentum  $q$ . Solve the obtained relation by iteration in the limit of a large potential,  $\alpha \rightarrow \infty$  (introducing the dimensionless parameter  $\lambda \equiv \alpha ma/\hbar^2$ ) to get the terms up to and including the order  $1/\alpha$ . Provide a very brief interpretation of the zero-order and the first order terms in  $1/\alpha$ .
- (e) (3 points) Based on the above, sketch the function  $E = E(q)$ , indicating bands and band gaps, and briefly discuss the qualitative behavior of this function for arbitrary potential strength.

# Statistical Mechanics 1

## Vibrations of a string

Consider a uniform violin string of length  $L$  with constant tension  $\sigma$  and total mass  $M = \rho L$ . Both ends of the string ( $x = 0$  and  $x = L$ ) are fixed. This string may have small vibrations in the perpendicular directions  $|y|, |z| \ll L$

$$y_n(x, t) = A_n \sin\left(\frac{\pi n}{L} x\right) \cos(\omega_n t + \phi_n), \quad n = 1, 2, \dots,$$

with kinetic and potential energies

$$U_n = \sigma \Delta L = \sigma \int_0^L dx \left( \sqrt{1 + (y')^2} - 1 \right) \approx \frac{\pi^2 n^2 \sigma}{4L} A_n^2 \cos^2(\omega_n t + \phi_n),$$

$$K_n \approx \int_0^L dx \frac{1}{2} \rho \dot{y}^2 = \frac{1}{4} \rho L A_n^2 \omega_n^2 \sin^2(\omega_n t + \phi_n)$$

and similarly in the  $z$  direction (any longitudinal or twisting motion is neglected).

- (A) (2 pts) Demonstrate that a vibrational mode with  $(n-1)$  nodes has frequency  $\omega_n = \omega_0 n$  and find  $\omega_0$ .

Assume below that the temperature is always such that  $T \gg \hbar \omega_0$ .

- (B) (4 pts) Find the partition function, free energy, and entropy for a single mode of vibration in plane  $(y, z)$  as function of temperature  $T$ .
- (C) (6 pts) Now find the entropy, heat capacity, and energy of free vibrations of the string. at high temperature  $T \gg \omega_0$ .
- (D) (4 pts) Calculate the mean squared *velocity* at the **midpoint** of the string  $\langle \dot{y}^2 + \dot{z}^2 \rangle_{x=L/2}$ .
- (E) (4 pts) Calculate the transverse fluctuation of the **midpont** of the string  $\langle y^2 + z^2 \rangle_{x=L/2}$ .

*Hint:* In parts (D) and (E), remember to average over both time and the statistical ensemble.

You may find the following formulas useful:

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

$$\sum_{n=1}^\infty \frac{1}{n^2} = \frac{\pi^2}{6}, \quad \sum_{n \text{ even}}^\infty \frac{1}{n^2} = \frac{\pi^2}{24}, \quad \sum_{n \text{ odd}}^\infty \frac{1}{n^2} = \frac{\pi^2}{8}.$$

# Statistical Mechanics 2

## Landau Diamagnetism

In a uniform magnetic field  $\vec{H} = H\hat{z}$ , the energy of electron motion in the  $(xy)$  plane is quantized:

$$\varepsilon(n, p_z) = \frac{e\hbar|H|}{m_e c} \left(n + \frac{1}{2}\right) + \frac{p_z^2}{2m_e}, \quad n = 0, 1, \dots, \quad (1)$$

which is known as Landau levels, while the motion along the magnetic field direction is unaffected. Assuming that the electron is confined into a box  $L_x \times L_y \times L_z$ , each Landau level  $n$  has degeneracy

$$g_{xy} = L_x L_y \frac{e|H|}{2\pi\hbar c} = \frac{L_x L_y}{\phi_e / |H|}, \quad \phi_e = \frac{2\pi\hbar c}{e}, \quad (2)$$

where  $\phi_e$  is a quantum of magnetic flux. Apart from the degeneracy  $g_e = 2$ , *the intrinsic spin of electrons is neglected in this problem*. Electromagnetic interactions between electrons are also neglected.

- (A) (4pt) Write expression for the grand potential  $\Omega(T, \mu, V, H)$  for the ensemble of electrons in magnetic field (1), without evaluating it.
- (B) (2pt) What is the condition on  $\mu$  and  $T$  for the system to be nondegenerate, i.e. the probability for each level to be occupied by an electron  $p_{\text{occ}}(\varepsilon) \ll 1$ ?
- (C) (4pt) Assuming that the system is nondegenerate as in part(B), calculate the approximate grand potential  $\Omega(T, \mu, V, H)$ .
- (D) (4pt) Compute the density of electrons  $N/V$ . How does the chemical potential  $\mu$  depend on magnetic field at constant temperature  $T$  and density  $N/V$ ? Compare to the case of an ideal gas.
- (E) (6pt) Assuming that the magnetic field is weak ( $|H| \ll \frac{m_e c T}{e\hbar}$ ), compute the magnetization of the gas  $M_z = -\left(\frac{\partial \Omega}{\partial H}\right)_{T, \mu, V}$  and its diamagnetic susceptibility  $\chi_{\text{dia}} = \left(\frac{\partial M_z}{\partial H}\right)_{T, N, V}$ . Explain qualitatively the negative sign of  $\chi_{\text{dia}}$ .

# Statistical Mechanics 3

## Hydrogen and Deuterium molecules

Deuterium ( $D$ ) is a heavy isotope of hydrogen ( $H$ ) with the a proton and neutron nucleus,  $d = pn$ . This nucleus is a boson with spin 1 and is approximately two times heavier compared to the hydrogen nucleus, the proton with spin- $\frac{1}{2}$ . To a good approximation, the electronic state energies and wave functions are the same in the three molecules  $H_2$ ,  $D_2$ ,  $HD$ , and *will be assumed identical* in this problem.

- (A) (1point) Assuming that r.m.s. distance between atoms in all three cases is the same,  $R = 7.4 \times 10^{-11}$  m, express the moments of inertia of  $HD$  and  $D_2$  in unints of  $I_0 = I_{H_2}$ .  
In the  $HD$  molecule, the two nuclei  $p$  and  $d$  are not identical and there are no constraints on its rotational wave function.

- (B) (3 points) Show that the spin-rotational of  $HD$  is given by the formula

$$Z_{\text{spin-rot}}^{HD} = (2 \cdot 3) \sum_{L=0}^{\infty} (2L+1) \exp\left(-\frac{\hbar^2 L(L+1)}{2I_{HD}T}\right) \quad (1)$$

(explain the integer factors in front of the sum) and compute it for high temperature  $T \gg \hbar^2/I_{HD}$ .

However, the rotational partition functions for  $H_2$  and  $D_2$  are different due to the particle statistics of the nuclei. Depending on the combined spin of the nuclei  $S$  (not counting electrons), their orbital angular momenta (OAM)  $L$  is constrained to be  $L = 0, 2, 4, \dots$  (even) or  $L = 1, 3, 5 \dots$  (odd):

	spin-symmetric	spin-antisymmetric
$H_2$	$S = 1, L = \text{odd}$	$S = 0, L = \text{even}$
$D_2$	$S = 0 \text{ or } 2, L = \text{even}$	$S = 1, L = \text{odd}$

- (C) (3 points) Explain the constraints on OAM in the table and count the number of combined nuclear spin  $S$  orientations for each case.

*Hint:* for the nucleus made of identical fermions, the total (spin  $\times$  rotational) wave function must be antisymmetric, while for the nucleons made of identical bosons it must be symmetric.

- (D) (4 points) With these constraints, calculate the spin-rotational partition functions  $Z^{\text{spin-rot}}$  for  $H_2$  and  $D_2$  gases at high temperature  $T \gg \hbar^2/I_0$ :

$$Z_{HH}^{\text{spin-rot}} = N_{HH,L=\text{odd}}^{\text{spin}} \sum_{L=\text{odd}} (\dots) + N_{HH,L=\text{even}}^{\text{spin}} \sum_{L=\text{even}} (\dots), \quad (2)$$

$$Z_{DD}^{\text{spin-rot}} = N_{DD,L=\text{odd}}^{\text{spin}} \sum_{L=\text{odd}} (\dots) + N_{DD,L=\text{even}}^{\text{spin}} \sum_{L=\text{even}} (\dots) \quad (3)$$



Now consider the equilibrium in the mixed gas of diatomic molecules  $H_2 + D_2 \leftrightarrow 2HD$ .

(E) (4 points) Show that the relation between molecular densities is

$$\frac{(N_{HD})^2}{N_{H_2} N_{D_2}} = \frac{(Z_{HD})^2}{Z_{H_2} Z_{D_2}} = \left[ \frac{(Z_{HD}^{\text{trans}})^2}{Z_{H_2}^{\text{trans}} Z_{D_2}^{\text{trans}}} \right] \cdot \left[ \frac{(Z_{HD}^{\text{spin-rot}})^2}{Z_{H_2}^{\text{spin-rot}} Z_{D_2}^{\text{spin-rot}}} \right] \cdot \left[ \frac{(Z_{HD}^{\text{osc}})^2}{Z_{H_2}^{\text{osc}} Z_{D_2}^{\text{osc}}} \right] \quad (4)$$

where the factors in the r.h.s. correspond to translational, rotational and oscillational motions of the molecules.

(F) (5 points) Compute the translational partition functions of the gases and estimate the ratio of  $N_{HD}^2/(N_{H_2} N_{D_2})$  at room temperature  $T \approx 300$  K *ignoring oscillations*. Are the formulas for spin-rotational partition functions derived above applicable at this temperature?