# UNIVERSITY OF MARYLAND Department of Physics College Park, Maryland

# PHYSICS Ph.D. QUALIFYING EXAMINATION PART II

August 28, 2015

9:00 a.m. – 1:00 p.m.

Do any four problems. Each problem is worth 25 points. Start each problem on a new sheet of paper (because different faculty members will be grading each problem in parallel).

Be sure to write your Qualifier ID ("control number") at the top of each sheet — not your name! — and turn in solutions to four problems only. (If five solutions are turned in, we will only grade # 1 - # 4.) For whichever problem (or problems) you skip, fill in a placeholder form so that the grader for that problem will have something from every student.

You may keep this packet with the questions after the exam.

(a) [6 points] Consider a one-dimensional simple harmonic oscillator: a particle with mass m bound to a quadratic potential  $V = \frac{1}{2}kx^2$ . Show by explicit calculation that  $\langle u_n | \frac{1}{2m}p^2 | u_n \rangle = \langle u_n | \frac{1}{2}kx^2 | u_n \rangle$ 

holds for the eigenstates  $|u_n\rangle$ , which are normalized in the usual way.

- (b) [6 points] Write down the Hamiltonian for a system in which there are two nonidentical particles (of mass  $m_1$  and  $m_2$ ) moving in one dimension and interacting via a quadratic potential  $V = \frac{1}{2}k(x_2 - x_1)^2$ , where  $x_1$  is the position of the first particle and  $x_2$  is the position of the second particle. Find the energy of the ground state and its wavefunction in coordinate space.
- (c) [7 points] Explain how the energy and wavefunction of the ground state would be modified if the system in part (b) was composed of two *identical* spin  $\frac{1}{2}$  particles.
- (d) [6 points] Now add a spin-spin interaction between the identical spin  $\frac{1}{2}$  particles given by  $\alpha(x_2 - x_1)^4 \boldsymbol{\sigma_1} \cdot \boldsymbol{\sigma_2}$ , where  $\alpha$  is a small positive constant and  $\boldsymbol{\sigma} = \sigma_x \hat{\boldsymbol{x}} + \sigma_y \hat{\boldsymbol{y}} + \sigma_z \hat{\boldsymbol{z}}$ . Using perturbation theory, find the energy of the ground state to first order in  $\alpha$ .

Possibly useful information:  $\int_{-\infty}^{\infty} y^4 e^{-y^2} dx = 3\sqrt{\pi}/4.$  $a^{\dagger} = \sqrt{\frac{m\omega}{2\hbar}} (x - \frac{ip}{m\omega})$  $a = \sqrt{\frac{m\omega}{2\hbar}} (x + \frac{ip}{m\omega})$ 

Consider a linear triatomic molecule with ions constrained to move only along the axis of the molecule (which can be taken as the x-axis). The molecule consists of two ions of mass m and charge -e that are symmetrically located at either side of an ion of mass M = 2mand charge +2e at equilibrium. The complicated forces between the ions are approximated by two springs with spring constant k, and equilibrium length b, as shown in the figure.



- (a) [2 points] Write down the Hamiltonian for this system of three coupled masses.
- (b) [4 points] Show that the following transformation

$$x_1 = \frac{1}{2}(Q_B - \sqrt{2}Q_A)$$
$$x_2 = -\frac{1}{2}Q_B$$
$$x_3 = \frac{1}{2}(Q_B + \sqrt{2}Q_A)$$

simplifies both the kinetic and the potential energies and eliminates the center-of-mass motion.

(c) [8 points]  $Q_A$  and  $Q_B$  are normal-mode coordinates describing the internal vibrations of the molecule. These modes satisfy

$$Q_j(t) = Q_j(0)e^{i\omega_j t}, \quad j = (A, B).$$

Describe the motion of the ions in each of the normal modes. Determine the oscillation frequencies  $\omega_i$  and the electric dipole moments  $D_i$  for the two internal modes.

The molecule is actually a quantum mechanical system. Initially it is in its ground state; it is then subjected to a *weak* uniform electric field  $E_x(t) = E_0(\omega) \cos(\omega t)$ . The perturbing interaction between its dipole moment and the electric field is  $H' = -DE_x$ , where D is the electric dipole moment and  $E_x$  is the electric field component along the molecule. The transition probabilities  $P_j(\omega, t)$  for excitation of states with one quantum either in mode A or in mode B is

$$P_{0j}(\omega, t) = \frac{|V_{0j}|^2}{\hbar^2} \frac{\sin^2[(\omega_{0j} - \omega)t/2]}{(\omega_{0j} - \omega)^2},$$

where  $|V_{0j}|^2$  is the matrix element of the perturbing Hamiltonian, and in this case is  $|V_{0j}|^2 = |D_j E_0(\omega)|^2$  for mode j of frequency  $\omega_{0j}$ .

- (d) [3 points] Use the equation above to obtain expressions for  $P_{0A}(\omega, t)$  and  $P_{0B}(\omega, t)$ .
- (e) [8 points] Determine the transition rates  $R_j = \frac{d}{dt} \int d\omega P_{0j}(\omega, t)$ , for a uniform incoherent beam of radiation propagating in the z-direction and polarized along x, whose intensity per frequency interval is given by  $J(\omega) = \frac{1}{2}c\epsilon_0 |E_0(\omega)|^2$ , where c is the speed of light in vacuum and  $\epsilon_0$  is the permittivity of free space. Assume that  $J(\omega)$  depends weakly on frequency.

Possibly useful information:  $\int_{-\infty}^{\infty} \frac{\sin^2 x}{x^2} dx = \pi.$ 

Consider diffraction of quantum particles of wavevector  $\mathbf{k}_i$  on a system of N identical scatterers located a distance b apart along the direction of incidence  $\hat{\mathbf{z}}$ , as shown in the figure below.



Each individual scatterer is characterized by a potential  $U_0(r)$  and the corresponding Born amplitude of scattering  $f_0(\theta)$ , which is assumed to be a smooth, featureless function.

- (a) [3 points] First consider the case of only one scatterer (N = 1). In the Born approximation, express the amplitude  $f_0(\theta)$  and the differential cross section  $d\sigma_0/d\Omega$  of scattering in terms of  $U_0(r)$  and k.
- (b) [6 points] Now consider N scatterers. The total potential is

$$U(\boldsymbol{r}) = \sum_{n=0}^{N-1} U_0(|\boldsymbol{r} - nb\hat{\boldsymbol{z}}|),$$

where  $\hat{z}$  is the unit vector along the z axis.

In the Born approximation, calculate the amplitude  $f(\theta)$  and the differential cross section  $d\sigma/d\Omega$  of scattering in terms of  $f_0(\theta)$ , k, b, and N.

Explore the answer obtained in Part (b) for various values of kb as follows:

(c) [4 points] What are  $f(\theta)$  and  $d\sigma/d\Omega$  in the limit  $Nbk \ll 1$ ? Interpret the result.

In the case of  $kb \ge 1$  and  $N \gg 1$ , answer the following questions and give geometrical interpretations of your results:

- (d) [4 points] Sketch  $d\sigma/d\Omega$  as a function of  $\theta$ . Calculate the angles  $\theta_n$  at which  $d\sigma/d\Omega$  has strong maxima.
- (e) [4 points] What is the total number of strong maxima for a given value of kb?
- (f) [4 points] Discuss how the height and the width of a strong maximum depend on  $N \gg 1$ . The width  $\Delta \theta_n = 2\delta \theta_n$  is determined by the angles  $\theta_n \pm \delta \theta_n$  where  $d\sigma/d\Omega$  vanishes.

Useful formula:

$$\sum_{n=0}^{N-1} a^n = \frac{a^N - 1}{a - 1}.$$

Two particles interact via a spin-spin Hamiltonian term  $AS_1 \cdot S_2$ , where A is a positive constant and  $S_{1,2}$  are the spin angular momenta of the two particles. Particle 1 has spin 1 and magnetic moment  $\mu_1 = -\frac{\mu_B}{\hbar}S_1$ , whereas particle 2 has spin  $\frac{1}{2}$  and zero magnetic moment.

- (a) [6 points] What are the energy levels of this system and the degree of degeneracy of the levels?
- (b) [8 points] Write down the energy eigenstates corresponding to the different energy levels in part (a), as linear superpositions of products of single-particle spin states.

Now consider what happens when the system is in a magnetic field of strength B.

- (c) [4 points] What are the approximate energy eigenstates and eigenvalues if  $B \gg \frac{A\hbar^2}{\mu_B}$ ?
- (d) [7 points] Sketch the approximate energy eigenvalues as functions of  $0 < B \leq \frac{A\hbar^2}{\mu_B}$ , and label the appropriate states. Do not neglect the spin-spin interaction term from parts (a) and (b).

Possibly useful information:  $J_{\pm}|j,m\rangle = \sqrt{j(j+1) - m(m\pm 1)}|j,m\pm 1\rangle$ 

The notion of negative absolute temperature is unusual but it can occur in, for example, quantum spin systems. To see this, consider a quantum system of N noninteracting magnetic dipoles each with spin 1/2, having a magnetic moment  $\mu_B$ , placed in a magnetic field **B**. Assume a canonical ensemble description of this spin system with a temperature  $T = 1/(k\beta)$ , where k is Boltzmann's constant.

- (a) [3 points] Write down the energy  $\epsilon$  of this two-level system in terms of  $\mu_B$  and B (the magnitude of the magnetic field). Determine the partition function  $Z_N$  in terms of  $\beta\epsilon$ .
- (b) [9 points] Calculate the free energy F, the entropy S, and the internal energy U of this system as a function of N and  $\beta$ .

A schematic plot of  $s \equiv \frac{S}{Nk}$  versus  $u \equiv \frac{U}{N\epsilon}$  is provided in the figure below to aid you in answering the following questions:



- (c) [4 points] What is the temperature T of the magnetic system in terms of quantities you obtained in part (b)? Indicate in the figure: (i) the places where T = 0, (ii) the region where negative temperature T < 0 appears, (iii) indicate with one arrow on each branch the direction of increasing T, and (iv) what is the temperature at the global maximum of that curve?
- (d) [6 points] Plot the temperature parameter  $\theta = kT/\epsilon$  on the vertical axis versus u (from -1 to +1) on the horizontal axis. (i) place an arrow along the curves indicating the directions of decreasing temperature. (ii) Explain what energy state the system is in at T = 0. (iii) If a system of this nature at T = -300K somehow interacts with an identical system at T = 300K, what is the final equilibrium temperature?
- (e) [3 points] Name two necessary conditions for a system to manifest negative temperature.