

UNIVERSITY OF MARYLAND
Department of Physics
College Park, Maryland

PHYSICS Ph.D. QUALIFYING EXAMINATION
PART II

January 24, 2020

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.)**

**At the end of the exam, when you are turning in your papers,
please fill in a “no answer” placeholder form for the problem that
you skipped, so that the grader for that problem will have
something from every student.**

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

Problem II.1

Consider a one-dimensional potential of the form:

$$V(x) = U_0 a \sum_{n=-\infty}^{\infty} \delta(x - na) \quad (1)$$

- (a) [**5 points**] The electron wave function $\psi_I(x)$ in the region $0 < x < a$ may be written as

$$\psi_I(x) = Ae^{ikx} + Be^{-ikx} \quad \text{with} \quad k = \sqrt{\frac{2mE}{\hbar^2}} \quad (2)$$

Use the Bloch relation for a periodic potential: $\psi(x) = u(x)e^{iKx}$ and $u(x+a) = u(x)$ to write the wavefunction $\psi_{II}(x)$ in the region $a < x < 2a$ in terms of $A, B, a, k,$ and K

- (b) [**8 points**] What boundary conditions on the first derivatives $d\psi_I(x)/dx$ and $d\psi_{II}(x)/dx$ must be satisfied at $x = a$? Justify this from the time-independent Schrödinger equation.
- (c) [**8 points**] Using the boundary conditions at $x = a$ find the equations that A and B must satisfy.
- (d) [**4 points**] The equations from part (c) have the solution

$$P \frac{\sin ka}{ka} + \cos(ka) = \cos(Ka) \quad (3)$$

where $P = U_0 ma^2/\hbar^2$, K is the Bloch wave vector and must be real.

What are the allowed energies E for $U_0 \rightarrow \infty$? What is the physical significance of these solutions?

Problem II.2

Consider a hydrogen atom in a uniform weak electric field \vec{E} along the $+z$ axis, which exerts the electric force $F_z = eE = -|e|E$ on the electron. (To avoid confusion in notation, use the letter E for the magnitude of the perturbing electric field, \mathcal{E}_n for unperturbed energy eigenvalues, and let e be defined to be a negative charge.)

- (a) **[5 points]** Write down the Hamiltonian of the electron as $H = H_0 + H_I$, where H_0 is independent of F , and H_I depends on F . Ignore the spins of the electron and the proton, and assume that the proton has a fixed position at the origin.
- (b) **[5 points]** The energy eigenvalues and eigenstates of H_0 are denoted as \mathcal{E}_n and $|nlm\rangle$. Describe degeneracies of the energy levels \mathcal{E}_n , the values and the physical meaning of the quantum numbers n , l , and m , and their relation to the symmetries of H_0 .
- (c) **[5 points]** Now describe the symmetry of the full Hamiltonian H including the electric field. What are the good quantum numbers characterizing energy eigenstates? What are the symmetry-related degeneracies of the energy eigenstates?
- (d) **[5 points]** Treating H_I as a weak perturbation to H_0 , write a general formula for energy correction $\Delta\mathcal{E}_1$ to the ground state $n = 1$ to the lowest non-vanishing order in E . Is this correction positive or negative? Is it proportional to E or E^2 ?
- (e) **[5 points]** Obtain lower and upper bounds on the magnitude of $\Delta\mathcal{E}_1$, such that $|\Delta\mathcal{E}_{1\min}| < |\Delta\mathcal{E}_1| < |\Delta\mathcal{E}_{1\max}|$.

Show that keeping only the $n = 2$ contributions gives a lower bound on the energy shift. Identify non-zero matrix elements among those with $n = 2$, but do not attempt to calculate them.

Show that replacing each \mathcal{E}_n with \mathcal{E}_2 gives an upper bound on the energy shift. Find a way to use the completeness relation and the fact that $\langle 100|r^2|100\rangle = \langle 100|(x^2 + y^2 + z^2)|100\rangle = 3a^2$ (where a is the Bohr radius) to evaluate the resulting sum.

Problem II.3

A beam of electrons of mass m and energy $E = \hbar^2 k^2 / 2m$ scatters off a molecule consisting of two identical atoms, separated by the distance a . The molecule has a fixed position in space with a fixed vector \mathbf{a} connecting the two atoms.

Suppose one atom produces a spherically-symmetrical potential $U_0(r)$, where r is the distance from the center of the atom. Then, the potential produced by the two atoms in the molecule is

$$U(\mathbf{r}) = U_0(r) + U_0(|\mathbf{r} - \mathbf{a}|). \quad (1)$$

This problem asks you to express scattering properties of the two-atom system in terms of the scattering properties of the single-atom potential using the Born approximation. You may ignore complicating factors such as molecular recoil, vibration, rotation, and excitation, and the electron spin.

The Born approximation formula for the scattering amplitude $f_0(q)$ on the single-atom potential $U_0(r)$ is

$$f_0(q) = -\frac{m}{2\pi\hbar^2} \int e^{-i\mathbf{q}\cdot\mathbf{r}} U_0(r) d^3r.$$

where $\mathbf{q} = \mathbf{k}' - \mathbf{k}$ is the change of the electron wavevector from \mathbf{k} to \mathbf{k}' upon scattering, $q = |\mathbf{k}' - \mathbf{k}| = 2k \sin(\theta/2)$ and θ is the scattering angle.

- (a) **[5 points]** Obtain a formula for the scattering amplitude $f(\mathbf{q})$ on the two-atom potential (1) in the Born approximation in terms of $f_0(q)$ and \mathbf{a} .
- (b) **[5 points]** Express the differential cross-section of scattering on the molecule, $d\sigma/d\Omega$, in terms of the corresponding cross-section $d\sigma_0/d\Omega$ for a single atom in the Born approximation.
- (c) **[5 points]** Assume that electrons have low energy, so that $ka \ll 1$, but the Born approximation is still applicable. Express $d\sigma/d\Omega$ in terms of $d\sigma_0/d\Omega$ in this limit. Also, how will the total cross sections compare in this limit?
- (d) **[5 points]** Now consider the high-energy limit where $ka \gg 1$. Express $d\sigma/d\Omega$ in terms of $d\sigma_0/d\Omega$ in this limit. Also, how will the total cross sections compare in this limit? (If necessary you may assume that the range of the potential $U_0(r)$ is much shorter than the interatomic distance.)
- (e) **[5 points]** The orientation of the molecular axis is determined by the unit vector $\mathbf{n} = \mathbf{a}/a$. So far, we assumed that the vector \mathbf{n} has a fixed orientation. Now assume that the molecular axis orientations are random, and different orientations appear with equal probability. Average the differential cross-section of scattering over random orientations of \mathbf{n} and obtain the averaged cross-section $\overline{d\sigma/d\Omega}$. Does it matter in the high energy limit whether the orientation of the molecule is fixed or random?

Problem II.4

Selection rules govern which transitions are allowed and which are disallowed. In this problem you will determine the selection rules for several reactions based upon angular momentum and parity conservation, and the spin-statistics theorem.

In what follows f is a spin-1/2 fermion with intrinsic parity +1, \bar{f} is the corresponding spin-1/2 anti-fermion with intrinsic parity -1, and ϕ is a spin zero scalar particle with parity +1.

(a) **[10 points]**

Consider the decay $\phi \rightarrow f\bar{f}$. Assuming the interaction conserves parity and angular momentum, what values of the orbital angular momentum quantum number ℓ are allowed for the final state?

(b) **[5 points]** Next consider the annihilation of a fermions into a pair of identical scalars

$$f\bar{f} \rightarrow \phi\phi \tag{1}$$

What are the allowed values of ℓ in the final state?

(c) **[8 points]** If parity and angular momentum are conserved in the interaction in Eq. 1, what values of ℓ are allowed for the initial state?

(d) **[2 points]** Among the allowed values of ℓ for the initial state and final state, which do we expect would give the largest reaction rate?

Problem II.5

The Debye model of lattice vibrations in an isotropic three-dimensional N -atom crystal postulates an excitation spectrum of the form $\epsilon(\mathbf{k}) = \hbar|\mathbf{k}|v = \hbar\omega$ for $\omega \leq \omega_D$, where ω_D is the Debye frequency and v is the speed of sound. In the Debye model, one assumes that the density of states $\rho(\omega)$ behaves like a power law in ω up to the so-called Debye frequency ω_D , above which $\rho(\omega)$ vanishes. At this frequency the integrated density of states includes the correct number of normal or vibrational (simple harmonic oscillator) modes. However, some materials, such as graphite, exhibit a layered crystalline structure for which the restoring forces parallel to each layer are much larger than those perpendicular to the layers. For such an anisotropic system, it is tempting to consider an artificial, oversimplified model by separating the lattice vibrations into two-dimensional modes in which atoms vibrate within each layer, characterized by Debye frequency ω_{D2} , and one-dimensional modes in which atoms vibrate perpendicular to the layers, characterized by Debye frequency ω_{D1} , where $\omega_{D2} > \omega_{D1}$. [Note: ω_{Dn}^n means $(\omega_{Dn})^n$ throughout.] Likewise, we expect the in-plane sound velocity $v_2 \gg v_1$, the sound velocity perpendicular to the layers.

- (a) **[6 points]** The density of states for n -dimensional vibrations (with isotropic dispersion) has the form

$$\rho_n(\omega) = \begin{cases} b_n N (\omega^{n-1} / \omega_{Dn}^n) & , \quad \omega \leq \omega_{Dn} \\ 0 & , \quad \omega > \omega_{Dn} \end{cases}$$

- (i) Starting with the density of states in reciprocal (\mathbf{k} -) space, show that this equation is correct for $n = 2$. *For simplicity we assume* (i.e. pretend) *throughout that there is only one polarization per normal mode* (per \mathbf{k}), as for sound. Find the value of the dimensionless constant b_2 .
- (ii) By integrating $\rho_1(\omega)$, show that $b_1 = b_2/2$.
- (b) **[6 points]** Show that the total heat capacity for an n -dimensional Debye crystal has the form

$$C_n(T) = N k_B b_n x_n^{-n} f_n(x_n), \quad \text{for } n = 1, 2$$

i.e., explicitly, $C_1(T) = N k_B b_1 x_1^{-1} f_1(x_1)$ and $C_2(T) = N k_B b_2 x_2^{-2} f_2(x_2)$

where $x \equiv \hbar\omega/(k_B T)$ and $x_n \equiv \hbar\omega_{Dn}/(k_B T)$ are dimensionless reduced inverse temperatures with respect to arbitrary ω and the Debye frequency ω_{Dn} , respectively; $f_n(x_n)$ is a dimensionless definite integral in the expression for $C_n(T)$, with x_n as one of its limits. You cannot to evaluate analytically the integral, but should determine the explicit form of $f_n(x_n)$.

- (c) **[5 points]** Obtain explicit expressions for the [leading-order] temperature dependence of the heat capacity C_n in the limits:

$$(i) \quad k_B T \ll \hbar\omega_{Dn}$$

$$(ii) \quad k_B T \gg \hbar\omega_{Dn}$$

being careful to show your intermediate steps. (Reminders: for non-negative integer m , $\int_0^\infty e^{-x} x^m dx = m!$; for $|x| \ll 1$, $e^{-x} = 1 - x + x^2/2 + \dots$)

- (d) **[8 points]** (i) **[2]** Sketch on the same graph (i.e., co-plot) the temperature dependencies of the heat capacities $C_2(T)$ and $C_1(T)$ for the same N and using $\omega_{D1}/\omega_{D2} \approx 0.05$.
- (ii) **[2]** Based on this graph and the preceding analysis, describe qualitatively the features of the total heat capacity $C_1(T) + C_2(T)$ for low temperature, high temperature, and in the crossover region.
- (iii) **[2]** Experiments on materials like graphite do not display this behavior at low temperature. Which of our approximations is the worst in our crude model in terms of analyzing qualitatively the thermal dependence of $C(T)$ at low T ?
- (A) $v_1 < v_2$.
 - (B) Neglecting transverse vibration modes.
 - (C) Describing low-energy modes perpendicular to the layers as 1D phonons.
 - (D) Describing low-energy modes within the layers as 2D phonons.
- (iv) **[2]** How, very briefly, does one measure the heat capacity experimentally? (What steps are necessary? Not what equipment is used.)