

Department of Physics, Princeton University

**Graduate Preliminary Examination
Part II**

Friday, January 12, 2007

9:00 am - 12:00 noon

Answer TWO out of the THREE questions in Section A (Quantum Mechanics) and TWO out of the THREE questions in Section B (Thermodynamics and Statistical Mechanics).

Work each problem in a separate booklet. Be sure to label each booklet with your name, the section name, and the problem number.

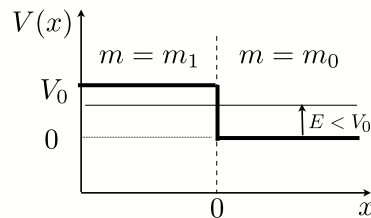
Section A. Quantum Mechanics

1. Consider a non-relativistic mass- m particle with coordinate x in one dimension that is subject to an attractive delta-function potential at $x = 0$, *i.e.*, a potential $V(x) = -V_0\delta(x/a)$, with $V_0 > 0$.
 - (a) The ground state of the particle is a bound state. Find its wave function and binding energy.
 - (b) The particle is now perturbed by a weak time-dependent potential $V(x, t) = Fx \cos(\omega t)$. Find the transition rate from the bound state to the continuum. (It may help to confine the particle in a large box $|x| < L/2$ and then take the limit $L \rightarrow \infty$.)

2. An electron is moving in one dimension in a potential $V(x) = 0$ for $x > 0$ and $V(x) = V_0 > 0$ for $x < 0$. The region $x > 0$ is empty space, where the electron mass is the usual bare mass m_0 , but in the region $x < 0$ it has a modified “effective mass” m_1 . When the mass of a non-relativistic particle depends on its position, the Hamiltonian should be written in the operator-ordered form

$$H = \frac{1}{2}p(m(x))^{-1}p + V(x)$$

where $[x, p] = i\hbar$.



- (a) The standard continuity conditions (continuity of $\Psi(x)$ and $\Psi'(x) \equiv d\Psi(x)/dx$) only apply at $x = 0$ if $m_1 = m_0$. Derive the modified continuity conditions that apply at points where the mass is discontinuous.
- (b) The (unnormalized) wavefunction of an eigenstate of the Hamiltonian with an energy $E < V_0$ is given by $\Psi(x) = A \sin k(x - x_0)$ for $x > 0$. Find k , x_0 and $\Psi(x)$ for $x < 0$. Make a sketch of the function $\Psi(x)$, indicating its essential features.

3. If a Na atom is represented by a singly-occupied 3s orbital, the molecular orbitals of the triangular Na₃ *molecule* are given by the eigenstates $\psi_\nu(i) = \langle i|\psi_\nu\rangle$ of the one-electron Hamiltonian

$$h(\mathbf{t}) = \sum_{i=1}^3 \varepsilon_0 |i\rangle\langle i| - \sum_{i \neq j} t_{ij} |i\rangle\langle j|, \quad t_{ij} = t_{ji}, \quad \langle i|j\rangle = \delta_{ij}.$$

with all t_{ij} real and positive, where $|i\rangle$, $i = 1, 2, 3$, is the 3s orbital on atom i . $\mathbf{t} = (t_{12}, t_{23}, t_{31})$ is a coordinate in a three-dimensional parameter space characterizing the molecular shape. For general values of \mathbf{t} , $h_{ij} = \langle i|h(\mathbf{t})|j\rangle$ is a generic 3×3 matrix, but when two or more of the t_{ij} are equal, symmetries of the eigenvectors make it easy to diagonalize (it is also easily diagonalized when any t_{ij} vanish).

- (a) Find the three molecular orbitals $\psi_\nu(i)$ when $\mathbf{t} = (t, t, \lambda t)$. Classify them by symmetry, and sketch the energy levels $\varepsilon_\nu(\lambda)$ as a function of $\lambda > 0$. How are they occupied in the Na₃ molecule ground state? What is special when $\lambda = 1$ (when all three Na atoms are equivalent)?

The Born-Oppenheimer (BO) approximation determines molecular shape by minimizing the electronic energy as a function of fixed nuclear coordinates of the atoms. Your results in (a) should imply that the BO energy has (at least) *three* distinct minima. Label them A, B, and C. Tunneling of the molecular shape degrees of freedom between these minima restores the symmetry of the molecule, in which all three Na atoms are equivalent.

- (b) Model the molecular orbitals of A, B and C by those of $(t, 0, 0)$, $(0, t, 0)$ and $(0, 0, t)$. The $\psi_\nu(i)$ can always be chosen real; if they change adiabatically as the shape evolves along the periodic path $A \rightarrow B \rightarrow C \rightarrow A$, $\psi_\nu(i) \rightarrow \eta_\nu \psi_\nu(i)$, $\eta_\nu = \pm 1$. Determine η_ν for each orbital. (You may assume that the path from A to B passes through the configuration $(t/2, t/2, 0)$, and use this to fix the sign of $\Psi_\nu(i)$ at B relative to that at A, *etc.*; only the *sign* (\pm or 0) of $\Psi_\nu(i)$ is important in this calculation.)

(Your results should imply that the BO ground state $|\Psi_0\rangle$ of the Na₃ molecule evolves to $-|\Psi_0\rangle$ along this path: this calculation was historically the first time that a “Berry phase” was encountered).

Section B. Statistical Mechanics and Thermodynamics

1. Consider an extremely dilute gas of partially ionized atomic hydrogen, such as occurred in the early universe. The binding energy of an electron and proton in the atomic ground state is $\epsilon \cong 13.6$ eV. Let this dilute plasma be neutral, with equal numbers of electrons and protons. Assume it is at equilibrium at a temperature T such that $\epsilon/(k_B T) = 100$.
 - (a) The fraction of the atoms ionized is $1/2$, so the densities of atoms, free electrons, and free protons are all equal. What is this density? Give it as a formula in terms of T , ϵ , and any fundamental constants or particle masses, and then, for $\epsilon/k_B T = 100$, give it as a numerical density, in units of m^{-3} , correct to the nearest order of magnitude. Make and justify any appropriate approximations that will simplify your calculation.
 - (b) At this density, estimate how much you need to lower the temperature to reduce the fraction of ionized atoms to $1/10$, so only 10% of the electrons are free, while the remainder are bound in atoms. Again, make and justify any reasonable approximations.

useful constants: $\hbar c \cong 2000$ eV-Å = 200 eV-nm ; $m_e c^2 \cong 500,000$ eV.

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2. Consider a dilute gas of diatomic molecules with number density n . Each molecule has a constant electric dipole moment μ . The temperature T is high enough so all degrees of freedom may be treated classically, and the correlations between molecules may be neglected.
- (a) Calculate, to leading non-vanishing order in the density n , the electric polarization density \mathbf{P} in an arbitrary external electric field \mathbf{E} .
- (b) What is the dielectric constant ϵ of this gas?

3. Consider spin waves in an isotropic ferromagnetically ordered crystal. These are waves in which the spins on each atom oscillate in space and time. Just as with sound waves, the spin waves can be quantized and they can store internal energy in a crystal lattice. However, these waves have a different relation between frequency and wave number than do sound waves. In particular, at low wavenumber,

$$\omega(k) = Ak^2$$

where A is a constant. Consider a crystal containing N spins in thermal equilibrium at temperature T .

- (a) What is the average energy in a spin-wave mode of frequency ω ? (Neglect the zero-point energy of the mode).
- (b) At low temperatures, the heat capacity of the spin wave system in the crystal is proportional to T^α . What is the numerical value of α ?
- (c) If the material is a metal, do the spin waves give the dominant contribution to the heat capacity in the low-temperature limit? What if the material is an insulator?. Explain both of your answers.