

INTERNATIONAL SCHOOL FOR ADVANCED STUDIES 1993
ENTRANCE EXAMINATION: CONDENSED MATTER

Solve one or more of the problems below (the order is irrelevant). Write out solution clearly and concisely. State each approximation used. Diagrams welcome.

Problem 1

Hydrogen atom and molecule

1. What is the first excitation energy for the hydrogen atom? How can it be observed?
2. What is the degeneracy, and symmetry, of that first excited state? Suggest ways to lift the degeneracy.
3. Starting from the neutral H atom, imagine forming the positive ion H^+ , or the negative ion H^- . Do both of them exist? Try to estimate, even if crudely, the energy Δ involved in forming the ions starting from the neutral H atom minus (or plus) an electron of zero energy (specify sign of Δ minus if energy is needed, plus if energy is emitted).
4. Consider the H_2 molecule, and describe its singlet ground state, and triplet excited state wave functions. Do that in the Molecular Orbital approximation, and also in the Valence Bond approximation. Discuss merits and drawbacks of each of them.
5. Assume the singlet-triplet excitation energy $E_T(r_o)$ at the equilibrium $H-H$ distance r_o to be approximately twice the singlet dissociation energy, $E_D = 4.7\text{eV}$. Assume also some crude but reasonable behavior for the triplet state of energy $E_T(r)$ for $r > r_o$ taking the asymptotic behavior $E_T(r \rightarrow \infty)$ from simple physical considerations. Using classical mechanics, provide a rough estimate of the time needed for the $H-H$ distance to increase from r_o by one Bohr radius, if the H_2 molecule is kept artificially in the triplet state.

Problem 2

Electron in a constant field

Consider the one-dimensional Schrödinger equation:

$$-\frac{\partial^2}{\partial x^2}\psi + Ex\psi = i\frac{\partial}{\partial t}\psi.$$

(1) Show that the time evolution of the wavefunction

$$\psi(x, 0) = e^{ipx}$$

is of the form

$$\psi(x, t) = e^{i(p-Et)x} e^{-i\phi},$$

where ϕ is a phase factor. Find explicitly $\phi = \phi(E, p, t)$.

(2) Calculate the current of this state as a function of time.

(3) Consider the gauge where the scalar potential is zero and the vector potential is $A(t) = -cEt$: we call $\tilde{\psi}(x, t)$ the wavefunctions in this new gauge. Find the time evolution of $\tilde{\psi}(x, 0) = \psi(x, 0)$, (i.e. same initial condition as above).

(4) What happens to the current in the new gauge?

Problem 3

Equilibrium properties of the H_2^+ molecule

The interaction between the two protons which constitute an H_2^+ molecule can be approximately described by the Morse potential:

$$V(r) = -D \left(2e^{-\beta(r-r_0)} - e^{-2\beta(r-r_0)} \right),$$

where $D = 2.795$ eV, $r_0 = 2.0$ a.u., and $\beta = 0.6678$ (a.u.)⁻¹.

(1) Calculate the equilibrium interatomic distance and the dissociation energy of the H_2^+ molecule.

(2) Discuss the dependence of the interatomic distance and dissociation energy upon the nuclear masses, and give a quantitative estimate of their variation for H_2^+ , HD^+ , and D_2^+ .

Problem 4

Harmonic and anharmonic oscillators

There is a model of thermal behaviour of crystalline solids, according to which each of the N atoms of the solid behaves like three independent harmonic oscillators. The $3N$ harmonic oscillators (which are on distinguishable sites) all have the same frequency, ω_0 . Their possible energy levels are

$$\epsilon_n = \hbar\omega_0 \left(n + \frac{1}{2} \right) \quad (n = 0, 1, 2, \dots)$$

a. Show that the free energy of the solid is given by

$$F = 3Nk_B T \log [1 - \exp(-\hbar\omega_0/k_B T)] + \frac{3}{2} N \hbar\omega_0$$

Where you have used the fact that the oscillators are on distinguishable sites?

b. Find the heat capacity, C , as a function of temperature and sketch a plot of C versus T .

c. Now introduce a weak cubic anharmonicity, imagining each oscillator to be characterized by a potential $\frac{1}{2}kx^2 - ax^3$, with a sufficiently small to permit a perturbative treatment. Find an expression for the thermal increase of $\langle x \rangle$ at very high temperature, where classical Boltzmann statistics is acceptable

Problem 5

One dimensional Schrödinger equation

The one dimensional Schrödinger equation is written in the following way:

$$-\frac{d^2}{dx^2}\psi(x) + gU(x)\psi(x) = E\psi(x)$$

where g is a physical coupling constant. Find how the ground state energy depends on g (regardless of multiplicative constants) if:

- i) the harmonic potential $U(x) = x^2$
- ii) the linear symmetric potential $U(x) = |x|$
- iii) what happens to the lowest energy if $U(x) = x$ simply?
- iv) If $U(x) = |x| + x^2$, what is the leading behaviour of the energy for $g \rightarrow 0$ or $g \rightarrow \infty$, as compared with cases (i) and (ii)? (Use of simple physical arguments is welcome).

Problem 6

Rotation of two classical particles

Two identical classical particles with mass m interact with each other by a potential

$$V(r) = \begin{cases} \cos\left(4\pi\frac{r}{r_c}\right) - 1 + 4\pi\left(\frac{r}{r_c} - 1\right) & \text{if } r < r_c \\ 0 & \text{if } r \geq r_c \end{cases} \quad (1)$$

where r is the interparticle distance.

1. Find the equilibrium condition when the two particles are at rest.
2. Assume that the two particles are rotating around an axis orthogonal to the line connecting them, and passing through the center of mass, with an angular momentum L . Discuss in qualitative terms (that is, without carrying out exact calculations) the equilibrium conditions as a function of L . In particular, sketch a diagram of the equilibrium distance(s) versus L .
3. Estimate the maximum value of the angular momentum L_{max} compatible with a bound state.