INTERNATIONAL SCHOOL FOR ADVANCED STUDIES 1994
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. A single well-solved problem is better, than many half-solved ones.

Problem 1
Electron motion in a simple one-dimensional potential

Consider the one-dimensional motion of an electron in an attractive delta-function potential

$$V_1(x) = -vl\delta(x)$$

where l is the length unit, and $v > 0$ has the dimension of an energy.

1) Find the ground state energy and eigenfunction for the electron.
Consider next the same electron in a new potential with *two* attractive delta-functions, a distance d apart

$$V_2(x) = vl[\delta(x) + \delta(x - d)]$$

2) Construct, for d not too small, the approximate ground state and first excited state, using linear combination of the single δ-function solution, found earlier. Discuss in particular the splitting between the two states for large d.
3) Imagine an electron initially in the ground state of V_1 and turn on the potential V_2 at $t = 0$. Use Schrödinger's time-dependent equation to find the time evolution of the electron. Restrict to the two states found in 2), and discuss the physical significance of the result.
4) Consider finally two non-interacting electrons, in the potential V_2. Describe the singlet ($S = 0$) and triplet ($S = 1$) configurations of these two electrons, and their relative energies.

Problem 2
Vibrations of a classical linear chain

Consider a linear chain of classical particles with mass m in one dimension, interacting with each other through the potential

$$V(r) = \frac{1}{\lambda^2 - 1} e^{-\lambda(r - r_\circ)} - \frac{\lambda^2}{\lambda^2 - 1} e^{-\frac{1}{\lambda}(r - r_\circ)}$$

where r is the interparticle distance, and $r_\circ$ and λ are parameters of the potential ($\lambda > 1$). Assume interactions only between first neighbors, and Born-von Karman (periodic) boundary conditions for all the questions except the last.

1. At $T = 0$, find
   (a) the equilibrium lattice spacing $a_\circ$
   (b) the cohesive energy of the lattice
   (c) its compression modulus $B = L(\partial^2 E/\partial L^2)$, where L is the total length of the chain and E is its total energy
   (d) within the harmonic approximation, the density of states $n(\omega)$. Make use of the formula for the dispersion relation of a first-neighbor chain
   $$\omega(k) = 2\sqrt{\frac{C}{m}} \left| \sin \frac{k a_\circ}{2} \right|$$
   where $C = (\partial^2 V/\partial r^2)|_{r=a_\circ}$ is the force constant between neighboring atoms.
2. Discuss which physical properties of this system you expect to be affected by λ.
3. Describe (in terms of the atomic displacements) the vibrational mode(s) that will be excited by applying to the system an external perturbation with angular frequency $\omega_e = 2\sqrt{C/m}$.
4. (Optional) Suppose that the two extremes of the chain are kept fixed by two external supports, so that the lattice spacing is fixed at $a = a_\circ$. An external perturbation at the above frequency ω_e is applied, inducing atomic vibrations following the mode discussed above, with a peak displacement u_m (assumed to be much smaller than a). Calculate the direction and the amplitude of the force exerted by the chain to the two external supports.

Problem 3
Electron bound to a surface
An electron is located at a distance $z > 0$ from the surface of a perfect metal.
1) Using the method of images, determine the force $F(z)$ acting on the electron, and derive the corresponding electrostatic potential $V(z)$.

Consider then the one-dimensional hamiltonian

$$H = \frac{p_z^2}{2m} + V(z), z > 0$$

with $V(z) = +\infty$ if $z < 0$, and neglect motion of the electron on the plane parallel to the surface. In order to obtain a variational estimate of the ground state wavefunction and energy, one may try, in analogy with the hydrogen atom, the following variational trial functions ($z > 0$):

1) $\phi_1(z) = A_1 e^{-\alpha z}$

2) $\phi_2(z) = A_2 z e^{-\alpha z}$

3) $\phi_3(z) = A_3(z^2 - z)e^{-\alpha z}$

where $A_{1,2,3}$ are normalization factors, and α is the variational parameter.
2) Choose the more appropriate (giving a short motivation of your choice) and determine the value of α which minimizes the expectation value of the energy.

[Useful integral: $\int_0^\infty z^n e^{-z} dz = n!$]

Problem 4
A model for the Jahn-Teller effect
Consider a system of N non interacting electrons in 2 dimensions, confined to a rectangular box whose edges have lengths a and b.
1) Write down the value of the ground state energy of the system for N=1,2,3, and discuss the corresponding degeneracy for $a = b$ and $a \neq b$.
Suppose now that the lengths a and b are variable and that a classic elastic energy $E_{elastic}(a, b) = \frac{1}{2}(a^2 + b^2)$ is associated to the box.
2) Find the minimum total energy of the system (classical elastic plus quantum electronic) for N=1,2, and 3, and show that the equilibrium shape of the box is a square for N=1,2, while it is a rectangle for N=3.

Problem 5

Lattice gas

A lattice gas is a collection of atoms whose positions can take on only discrete values, corresponding to the sites of a regular lattice.

Assume the lattice is simple cubic, that each site is occupied at most by one atom, that the kinetic energy is negligible, that the energy of a pair of nearest neighbour atoms is $-\epsilon$ (with $\epsilon > 0$) and that the energy per atom is $-\mu$ (= chemical potential).

1) Derive the equation of state and describe the phase diagram in the mean field approximation (also known as Bragg–Williams or molecular field approximation).

2) Discuss the type of singularities appearing near the critical point.

3) Perform an exact calculation of the equation of state in a one dimensional lattice.

Problem 6

One dimensional free particle wavefunction in a finite box

1) Find the spectrum and the eigenfunctions of a free particle with mass m confined in a one dimensional region with coordinate x restricted to $x_l < x < x_r$, and with $L = x_r - x_l$ being the size of the linear region.

2) Consider the ground state of the system for $x_l = 0$ and $x_r = L$. Find the overlap of this state with the approximate state obtained by joining the ground states of the two subsystems of size $L/2$ ($[x_l = 0\ ,\ x_r = L/2]$ with $[x_l = L/2\ ,\ x_r = L]$), obviously after normalization of the two states.

How good is the approximation ? Plot the approximate two-subsystem ground state against the exact one of the entire system.

3) Discuss if there may be any efficient method to approximate the ground state of a system of size L by the knowledge of some excited states of the two subsystems of size $L/2$.