SISSA ISAS

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April 2010 - Entrance Examination: Condensed Matter

Solve at least one of the following problems. Write out solutions clearly and concisely. State each approximation used. Diagrams welcome. Number page, problem, and question clearly. Do not write your name on the problem sheet, but use extra envelope.

Problem 1: Resurrecting a Hamiltonian

A certain one electron problem in one dimension has a ground state wavefunction $\psi(x) = C\exp(-|x|/a)$, where C and a are positive constants.

1. Specify if $\psi(x)$ is a bound state or a scattering state.
2. Derive the Hamiltonian $H = T + V(x)$ that has $\psi(x)$ as its exact ground state (here T is the kinetic energy).
3. Calling zero the value of the potential $V(x)$ far away from $x = 0$, determine the binding energy of state $\psi(x)$.
4. Describe the symmetry of the Hamiltonian H obtained, and specify the symmetry of the state $\psi(x)$ with respect to parity.
5. Write down a tentative trial wavefunction $f(x)$ of parity opposite to that of $\psi(x)$.
6. Identify, e.g. using the variational theorem if necessary, the lowest energy eigenstate of the Hamiltonian H with the symmetry of $f(x)$.
7. Specify — without doing any more calculations — the answer to all questions (1) - (6), for the similar wavefunction $\psi(\mathbf{r}) = C\exp(-|r|/a)$, now in three dimensions, instead of one dimension.

Problem 2: Structural phase transitions in crystals

It is found that a solid can exist in two different crystal structures, say α and β. A computer simulation gives the following approximate expressions for the Helmholtz free energies per unit mass of the two structures at ambient temperature (in some units):

$$\begin{aligned} f_\alpha(V) &= (V-1)^2 + 0.2 \\ f_\beta(V) &= 2(V-1.25)^2 \end{aligned}$$

1. Find the equilibrium structure and volume at zero pressure.
2. Calculate the Gibbs free energy of the two structures.
3. Find the equilibrium structure and volume at the pressure $P = 1$ (in units consistent with the Helmholtz free energies given above).
4. Find if there exists a pressure at which the structure which is more stable at ambient conditions becomes unstable, and predict the volume change, if any.

Problem 3: Diamagnetic contribution to the magnetic susceptibility of an hydrogenic atom

An hydrogenic atom is composed by a nucleus of charge Ze and an electron of charge $-e$.

1. Write its non relativistic Hamiltonian, assuming a fixed nucleus. Show that the wavefunction
$$\psi(\mathbf{r}) = \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \exp\left(-Zr/a_0\right) \tag{1}$$
is an eigenfunction and find its eigenvalue. $a_0 = \frac{(4\pi\epsilon_0)\hbar^2}{me^2}$ is the Bohr radius, m the electron mass, $\hbar$ the Planck constant and ϵ_0 the vacuum permittivity constant. $r = |\mathbf{r}|$ is the modulus of $\mathbf{r}$.

2. Now consider an external magnetic field $\mathbf{B} = (0, 0, B)$. This magnetic field can be written in terms of a vector potential $\mathbf{A} = -\frac{1}{2}\mathbf{r} \times \mathbf{B}$. Making the substitution of the momentum operator $\mathbf{p} \to \mathbf{p} + e\mathbf{A}$, write the Hamiltonian of the atom inside the magnetic field.

3. The Hamiltonian at point [2.] has a term linear in B and a term quadratic in B. Write down these two terms.

Now let us focus on the term quadratic in B. We want to calculate its contribution to the magnetic susceptibility of the atom in the ground state.

4. Using first order perturbation theory, find the shift ΔE of the ground state eigenvalue due to the term quadratic in B.

5. Calculate the effect of this shift on the magnetic susceptibility $\chi_m = -\frac{d^2 \Delta E}{dB^2}$. Which is its sign? Which is its Z dependence?

Problem 4: Localized phonons in one dimension

Consider a one-dimensional crystal composed almost entirely of atoms with mass M, except for one impurity atom with mass M'. We may approximate the interactions as nearest-neighbor harmonic potentials with a spring constant K. We want to explore localized phonons modes that may possibly arise in this situation.

- Write down the equations of motion. Consider periodic-boundary conditions and put the impurity in the origin.
- Determine the range of M/M' for which localized phonon modes exist.

  [Hint: try the test functions $u_n = e^{-\lambda\,|n|} e^{i(q\,n - \omega\,t)}$.

  1. Find the allowed values of q.
  2. Find the relation between λ and M/M'.
  3. Find the expression of ω in terms of K and M/M'.
  4. Give the expression of u_n in terms of M/M' and discuss the limit of $M' \to M$.]