Do the multiple-choice tests first (but do not spend more than 1 hour on them!). Then solve one of the problems below (or more, if the first one was correct). Write out solution 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.

1 Spectrum of an half-harmonic oscillator

Consider an harmonic oscillator in one dimension:

$$H = \frac{p^2}{2m} + \frac{m\omega^2}{2}x^2$$

and its eigenvalues, ε_n, and eigenfunctions, $\phi_n(x)$.

Suppose that a rigid wall $[v(x) = +\infty$ for $x \leq 0$, $v(x) = 0$ for $x > 0]$ is then inserted at the origin, and consider now eigenvalues and eigenfunctions of the resulting asymmetric potential well.

i) What is the energy spectrum of this half-harmonic oscillator? Write the eigenfunction of its M-th excited state in terms of $\phi_n(x)$.

ii) Consider the expansion of this state in terms of eigenvectors of the original oscillator, $\phi_M^{half}(x) = \sum_{n=0}^{\infty} c_n \phi_n(x)$. Give the explicit expression for the expansion coefficients, c_n, on odd-numbered excited states of the original oscillator.

iii) From the expression for the energy of the eigenstate find a sum-rule that must be satisfied by even-numbered coefficients.

Suppose that the system is prepared in the ground state of the half harmonic oscillator and that at a given moment the delta-function potential is removed instantaneously.

iv) Is the probability for the system to be found at a later time on the ground state of the complete oscillator more or less than 25 % ?

2 Spinor rotations and phases

States of a spin-$\frac{1}{2}$ system are often represented in a 2-component formalism on the basis

$$|S_z \uparrow\rangle \quad \sim \quad \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad\qquad |S_z \downarrow\rangle \quad \sim \quad \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

The spin operator $\mathbf{S}$ is then represented with the help of the Pauli matrices:

$$\mathbf{S} = \frac{\hbar}{2}\boldsymbol{\sigma} \qquad \text{where} \qquad \sigma_x \sim \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y \sim \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z \sim \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

As well know, in this language, a generic rotation by an angle Φ about the axis defined by the versor $\hat{\mathbf{n}}$ is represented by

$$\mathcal{D}(\hat{\mathbf{n}}, \Phi) = \exp \frac{-i\mathbf{S}\cdot\hat{\mathbf{n}}\ \Phi}{\hbar} = \exp \frac{-i\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\ \Phi}{2} \sim \begin{pmatrix} \cos\frac{\Phi}{2} - in_z\sin\frac{\Phi}{2} & [-in_x - n_y]\sin\frac{\Phi}{2} \\ [-in_x + n_y]\sin\frac{\Phi}{2} & \cos\frac{\Phi}{2} + in_z\sin\frac{\Phi}{2} \end{pmatrix}$$

Using this 2-component notation, answer the following issues:

a. Calculate a spinor $|S_x \uparrow\rangle$ pointing in the positive $\hat{\mathbf{x}}$ direction, by applying a rotation $\mathcal{D}(\hat{\mathbf{y}}, \pi/2)$ of 90° around the $\hat{\mathbf{y}}$ axis, to the basis state $|S_z \uparrow\rangle$.

b. Let now the resulting spinor $|S_x \uparrow\rangle$ rotate around $\hat{\mathbf{z}}$ by a *suitable* angle, so that it finally points to the positive $\hat{\mathbf{y}}$ direction. Compute the resulting spinor $|S_y \uparrow\rangle$.

c. Complete the trip of our spinor, by rotating the result $|S_y \uparrow\rangle$ of point **b** around the $\hat{\mathbf{x}}$ axis by 90°. Write the resulting spinor $|\eta\rangle$.

d. Intuitively, the spinor $|\eta\rangle$ at the end of the loop should coincide with the starting state $|S_z \uparrow\rangle$. Verify that a *different* state is obtained instead. Compute the observables $\langle S_z \uparrow| S_z |S_z \uparrow\rangle$ and $\langle \eta| S_z |\eta\rangle$: are they equal or not?

e. Verify that the two states of points **b** and **c** are related by $|\eta\rangle = e^{i\alpha} |S_z \uparrow\rangle$, and compute the phase angle α.

f. Spinors are complex vectors: when taken around they acquire phases. "Trivial" gauge phases are removed by parallel transport, which corresponds to setting to zero the leading (linear) term in the phase change: $\langle \psi(\Phi)| \frac{d}{dt}\psi(\Phi)\rangle = 0$. Verify that along each of the paths of points **a**, **b** and **c**, our spinor is parallel-transported.

g. Geometric phases are obtained through parallel transport. By completing the demonstration of point **f**, you have shown that the angle α is a geometric phase. The candidate can demonstrate his culture by writing the name of the physicist generally associated with this kind of geometric phases.

3 Statistical Mechanics problem

A classical system can exist in N states $i = 1, ..., N$ with energies $E_1, ..., E_N$. Let $K_{i,j}$ be the transition rate from state j to state i and $P_i(t)$ the probability to be in state i at time t. If the time evolution is written in the form $dP/dt = -HP$

1. determine H in terms of K's.

2. Is probability conservation preserved by time evolution?

If $K_{i,j} = K_{j,i}$

3. show that the eigenvalues of H can not be negative.

4. Is there always a zero eigenvalue and when is it unique?

If the system is in contact with a thermal bath at temperature T and detail balance is satisfied

5. determine the similarity transformation which makes H symmetric.

6. Under which conditions $P_i(t)$ reaches its equilibrium value at large times?

7. Calculate the time evolution for a 2-state system with arbitrary initial conditions and the time dependence of the average energy.

4 Phase separation in a simple model

N boson particles are defined in a one dimensional lattice, namely their positions x are restricted to assume discrete values $i = 1, \cdots L$. The "hard core boson" condition is assumed, i.e. each site cannot host more than one boson. The particles can hop from each site i to nearest neighbor sites $i \pm 1$ with matrix elements $-t < 0$, If two bosons are nearest neighbors the gain in energy is given by $-V < 0$. The Hamiltonian can be formally written in second quantized notation as:

$$H = -t \sum_{i=1}^{L-1} (b_i^\dagger b_{i+1} + h.c.) - V \sum_{i=1}^{L-1} n_i n_{i+1}$$

where $b_i^\dagger$ creates a hard core boson at site i and $n_i = b_i^\dagger b_i$ is the boson occupation number at site i, $n_i = 0, 1$ from the hard core boson condition. *(Warning! do not try to solve the model for arbitrary N and L.)*

1) Write down the explicit matrix elements of H for $N = 0, 1, 2$ particles and $L = 2$ in the basis where particles have fixed positions (e.g. for $N = 1$ there are two states where the particle is localized at $i = 1$ or at $i = 2$).

2) Generalize to arbitrary L the simple ground states for **a.** $N = L$ and **b.** $N = 1$. (Case **b.** is a one-dimensional tight-binding model: optionally use periodic boundary conditions if you are not familiar with open boundary conditions).

3) Use the results (2) to evaluate the condition for which the particles cluster together even for $N < L$. Hint: evaluate the expectation value of the Hamiltonian over the state with all particles at position $i \leq N$. Then compute the energy cost to evaporate one particle from the particle rich region $i \leq N$ to the particle empty one $i > N$. At what value of V/t it is convenient to form a phase separated ground state in the thermodynamic limit (for $L \to \infty$ at fixed density $\rho = N/L$) ?

4) *Optional*: the phase-separated ground state is determined in (3) with a variational calculation. How rigorously can it be proved that phase separation shows up in the ground state of the model for large enough V/t ? (Hint: try to show that the exact ground state energy per site coincides in the thermodynamic limit with the variational one of the phase separated state, this without solving explicitly the model but using upper and lower bounds for the exact energy.)

5 Image-charge bound states

Consider an electron in vacuum, a distance z above a plane surface of a medium with very large dielectric constant. The dielectric has two effects: a) it provides a positive polarization charge below the surface; b) it also provides an infinite barrier against electron penetration at $z < 0$. The attraction at $z > 0$ between the electron and the polarization charge, plus the barrier for $z < 0$, form a potential well where the electron can be bound, while still moving freely along x, y, parallel to the surface. Since the potential due to the polarization can be reproduced by an image charge, these bound states go under the name of "image-charge states". The scope of this exercise will be to determine their properties.

1. Specify the magnitude, sign, and position of the image charge of the electron, and from this establish the force between electron and image (assume infinitely large dielectric constant as in a metal to simplify the result). Integrate the force to obtain the potential, and compare the result with that for two real charges a distance $2z$ apart.

2. Quantize the electron motion in this image charge potential well, by writing Schroedinger's equation, separating z from (x, y) motion, and solving each separately by direct identification with other well known standard problems (free motion and 3D hydrogen atom for $L = 0$). Write out at the end the eigenvalues, for the lowest states, as a function of the appropriate quantum numbers, namely n for z-motion, and (k_x, k_y) for x, y motion. Knowing that 1 Rydberg= $\frac{me^4}{2\hbar^2}$= 13.6 eV, what is the lowest state energy in eV?

3. Describe the lowest image state eigenfunctions and its extension along z. Knowing that 1 Bohr radius $= \frac{\hbar^2}{me^2}$= 0.529 Å, how many Angstroms does the lowest image charge state extend along z?

4. Plot out the few lowest image-charge state eigenvalues for increasing k_x, and find the critical values of k_x where they will cross the energy zero. Interpret the critical k_x value in terms of the z-extension discussed above. Find the corresponding critical x-velocity in cm/sec of the electron in the lowest image charge state, which is that velocity where the associated x-kinetic energy exactly compensates the z-binding energy, so that given a possibility to scatter the image charge state electron will cease to be bound.

6   Magnetic susceptibility of a Fermi gas

The Hamiltonian to compute the spin susceptibility of an homogeneous fermionic system at zero temperature in a magnetic field, ignoring any orbital effects, is given by

$$H = H_0 - \mu \sum_i \vec{\sigma}_i \cdot \vec{B} . \tag{1}$$

where μ is the magnetic moment and $\vec{\sigma}$ are the Pauli matrices. The susceptibility per particle is defined as

$$\chi = -\rho \frac{\partial^2 E_0(B)}{\partial B^2}\bigg|_{B=0} , \tag{2}$$

where ρ is the density of the system and E_0 is the ground state energy per particle at a given field B.

Pauli expanded the energy per particle as a function of the polarization p

$$E(p) = E(0) - \mu_B \, p + \frac{1}{2} p^2 E''(0) . \tag{3}$$

1) Write the spin susceptibility in terms of $E(p)$.

2) Calculate $E(p)$ for the free gas, and verify that gives the usual Pauli spin susceptibility χ_p.

Suppose that you want to compute χ for a real system, like for instance neutron matter at $\rho = 0.32$ fm^{-3} (for a neutron, the magnetic moment is $\mu = 9.66 \times 10^{-27}$ J/T $= 6.03 \times 10^{-18}$ MeV/Gauss, and the constant combination $\frac{\hbar^2}{2m} = 3.320 \times 10^{-42}$ J m$^2 =$ 20.72 MeV fm^2). You have at your disposal a code which gives you the ground state energy for a given polarization p and a given magnetic field B for a finite number of particles (take ~ 60) in a periodic box.

3) Which values you would choose for the number of particle with spin up and particle with spin down ? Which are the values of the box size L for each couple of $N \uparrow, N \downarrow$ considered ?

4) Choose one of the above cases and write the energy as a function of B considering the fermions as non–interacting.

5) With the guide of the non–interacting fermions, describe a strategy on how to use the code to get an estimate of χ/χ_p within $20 \div 30\%$. In particular give an estimate of the value of B you need to use in the calculation.

7   Two-dimensional electrons in a perpendicular magnetic field

Consider a single electron moving in the two-dimensional $(x_1 - x_2)$-plane and in the presence of a magnetic field in the z-direction, i.e. $\vec{B} = (0, 0, B)$. The Hamiltonian is

$$H = \frac{1}{2m} \vec{\Pi} \cdot \vec{\Pi}, \tag{4}$$

where the two-dimensional vector

$$\vec{\Pi} = \vec{p} + \frac{e}{c} \vec{A},$$

being $\vec{p}$ the conjugate momentum of the coordinate $\vec{x}$, and $\vec{A}$ the vector potential satisfying $\vec{\nabla} \times \vec{A} = \vec{B}$.

Classically the electron moves along circular orbits centered at position $\vec{R}$ which depends on the $t = 0$ initial values of $\vec{x}$ and $\vec{p}$.

1. Find $\vec{R}$ as function of the $t = 0$ values of $\vec{x}$ and $\vec{p}$.

In quantum mechanics, $\vec{\Pi}$ as well as $\vec{R}$, as functions of $\vec{x}$ and $\vec{p}$, become operators.

2. Calculate the following commutation relations: $[\Pi_i, \Pi_j]$, $[R_i, \Pi_j]$, and $[R_i, R_j]$, where $i = 1, 2$ labels the components of the two dimensional vectors.

3. Find the eigenvalues and eigenfunctions of the Hamiltonian (4), using preferably the representation in terms of the above introduced Π_1, Π_2, R_1 and R_2. (*Hints*: Write Π_i and R_i ($i = 1, 2$) in terms of conjugate variables X_Π, P_Π, X_R, and P_R, where $[X_\Pi, P_\Pi] = [X_R, P_R] = i\hbar$, being all the other commutators zero. Then, rewrite the Hamiltonian in terms of these variables. Alternatively, fix the gauge and solve directly the Schrœdinger equation)

4. Show that each energy level is degenerate such that there is one state per $\hbar c/(eB) = 0.6582 \times 10^{-16}$ Tesla$/B$ square centimeters.

Now, introduce an electric field in the x_2-direction by adding to the Hamiltonian the term

$$\delta H = -eEx_2. \tag{5}$$

5. Find eigenvalues and eigenvectors of $H + \delta H$;

6. Calculate the average over the ground state of the transverse current operator $-e\dot{x}_1$.

Optional: Add to the Hamiltonian $H + \delta H$ an unrealistic barrier of the form
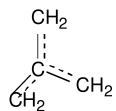
$$U\delta(R_1).$$

Show that the wave function is perfectly transmitted across this barrier apart from a simple phase-shift.

8 Bio-simulation exercise:

PROBLEM

1–Classify the following molecules according to their point group symmetry.

cis–1,2–dichloroethylene, *trans*–1,2dichloroethylene, trimethylenemethane (

), and 1,1–dicloro– trimethylenemethane

2– Using group theory, establish whether these molecules *may* possess a permanent electric dipole moment.

3– Calculate the resonance energy of trimethylenemethane using Hückel MO theory.