SFI5711 - Solid State Physics (2020)
List of exercises #1

1. Bravais lattice and quasicrystals

(*a*) Show that a 2D Bravais lattice can have only rotational C_n symmetry axis with $n = 1$, 2, 3, 4, and 6.

(*b*) (Optional) What is the implication to 5-fold symmetry in 3D (or higer D)?

(*c*) In 1984, D. Shechtman and co-workers found that certain Al-Mn alloys display a x-ray diffraction pattern with icosahedral symmetry [Phys. Rev. Lett **53**, 1951 (1984)]: this was the discover of quasicrystals (Nobel Prize in Chemistry 2011). The puzzle is that icosahedral symmetry patterns are invariant under 5-fold rotations. Search the literature and explain in your words how this observation can be understood and modeled. Cite your references. (Be concise, and there is no need in going into technicalities and details.)

2. Kagome lattice

(*a*) The Kagome lattice (see Fig. 1) is widely studied in the context of frustrated magnetism. Describe it as a Bravais lattice with an appropriate basis. Give the primitive and basis vectors and the volume (in this case, area) of the unit cell.

(*b*) Draw the Wigner-Seitz unit cell of the Kagome lattice and calculate its area. Compare to the result found in the previous item.

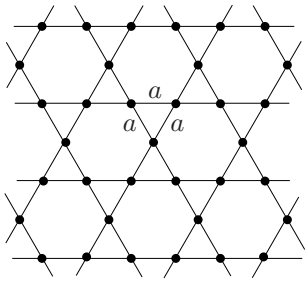

Figure 1: The Kagome lattice.

3. Debye-Waller factor

The potential describing the scattering of light off the lattice atoms is usually modeled by $\sum_j U(\mathbf{r} - \mathbf{R}_j)$, where $\mathbf{R}_j$ are the positions of the atoms on the lattice. At finite temperatures T, each atom actually oscillates around their equilibrium positions by a displacement $\boldsymbol{\delta}_j$. In this case, we have $\sum_j U(\mathbf{r} - \mathbf{R}_j - \boldsymbol{\delta}_j)$. These displacements are random and, in a simplified model, all components follow the same Gaussian probability distribution function

$$P(\delta_j^{(\alpha)}) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{1}{2}\left(\frac{\delta_j^{(\alpha)}}{\sigma}\right)^2\right], \text{ with } \alpha = x, y, z,$$

and σ is a constant which should be a function of T. Show that the x-ray scattering cross section at a transfered momentum equal to the reciprocal vector $\mathbf{G}$ is reduced by the so-called Debye-Waller factor $\exp\left(-\frac{1}{3}G^2\left\langle R^2\right\rangle\right)$, where $\left\langle R^2\right\rangle$ is the average square displacement of an atom.

4. DNA structure (adapted from Paul Crowell)

The DNA has a helical structure, which in principle can be probed by x-ray scattering. For this problem, consider that a helix is a one-dimensional crystal (in the z-direction) in which each unit cell contains one winding of the helix.

(*a*) Consider first that the helix is uniform, such that the electronic charge is distributed evenly along the helix, paramatrized by

$$x = R\cos\left(\frac{2\pi}{\lambda}z\right) \text{ and } y = R\sin\left(\frac{2\pi}{\lambda}z\right),$$

where R and λ are the radius and the pitch of the helix, respectively. Calculate the Fourier coefficient $\rho(\mathbf{k})$ of the electronic charge density $\rho(\mathbf{r})$ given above. Using this result, sketch the corresponding x-ray diffraction pattern in reciprocal space (recall that the x-ray intensity at the wave-vector $\mathbf{k}$ is proportional to $|\rho(\mathbf{k})|^2$).

(*b*) Consider now that the helix is non-uniform, with the density concentrated at atoms evenly distributed along the helix and separated by the distance a. Repeat the calculations from the previous item and discuss what happens as the ratio λ/a is changed. To simplify the calculations, model the electronic charge density of the non-uniform helix as the density of the uniform helix [given in item (a)] times a sum of delta functions $\sum_n \delta(z - na)$, with $n \in \mathbb{Z}$.

5. (Optional) **Structure factor** (from Ashcroft & Mermin)

It is often convenient to represent a face-centered cubic Bravais lattice as a simple cubic, with a cubic primitive cell of side a and a four-point basis $\mathbf{d}_j$.

(*a*) Show that the structure factor $S_\mathbf{G} = \sum_{j=1}^{n} e^{i\mathbf{G}\cdot\mathbf{d}_j}$ is either the same constant or 0 at all points of the simple cubic reciprocal lattice.

(b) Show that when points with zero structure factor are removed, the remaining points of the reciprocal lattice make up a body-centered cubic lattice with conventional cell of side $4\pi/a$. Why is this expected?

6. Counting states

(*10 points*) Consider a one-particle quantum mechanical system with a Hilbert space spanned by three orthonormal states $|n\rangle$, with $n = 1, 2, 3$. Three non-interacting particles occcupy these states. Determine how many distinct physical states there are if these particles are: (a) three identical fermions, (b) three identical bosons, (c) two identical fermions and one boson, (d) two identical bosons and one fermion, (e) three distinct fermions, and (f) three distinct bosons.

7. (Optional) **Exchange interaction - the Hydrogen molecule**

The purpose of this problem is to understand the mechanism that gives stability to the Hydrogen molecule and the covalent bond. (Use first quantization.)

(a) Write the complete Hamiltonian H of the Hydrogen molecule.

(b) In the limit the two protons are $R \gg a_0$ faraway from each other with a_0 being the Bohr radius, write $H = H_0 + H_1$ with H_0 and H_1 being the nonperturbed Hamiltonian and its perturbation, respectively. Justify your choice of H_0 and H_1.

(c) Now, use the limit in which the protons are much heavier than the electrons. What is the physical meaning of this limit? Moreover, consider the protons being classical particles (thus, R becomes a parameter in the problem) and treat the electrons as indistinguishable spin-1/2 quantum particles. Write the simplified H_0 and H_1.

(d) Write down the ground-state wavefunctions of H_0 (do not forget the spin and the normalization). What is the degeneracy of the ground state? Discuss the permutation properties of the ground-state wavefunctions. Make a sketch of these wavefunctions in the plane $r_1 \times r_2$, where r_i is the distance of the i-th electron to the first proton (which you can conviniently set as the orign).

(e) In first order of perturbation theory, compute the correction to the ground-state energy ΔE due to H_1, and analyze how the degeneracy is lifted. (Do not compute the integrals. Just analyze how they can lift the degeneracy.)

(f) Which is the new ground state? Discuss its symmetry properties and the role of the parameter R. (As the integrals in (e) were not computed, you cannot decide for which one. Thus, discuss all the possible outcomes. Alternatively, you can give a physical insight in order to guess if the integral is positive or negative)

(f.α) Compute the integrals. (All of them, but one, can be computed analytically. The final one is important. Either you can perform it numerically or quote in the literature. Cite the corresponding reference.)

(g) What is the condition that ΔE must satisfy in order to guarantee the stability of the Hydrogen molecule?

(h) Notice that the degeneracy of the ground state is lifted in a way that the new spectrum can be represented by the effective hamiltonian $H_{\text{eff}} = \text{const} + J\mathbf{S}_1 \cdot \mathbf{S}_2$, where $\mathbf{S}_i$ is the spin operator of the i-th electron. Give the expression for the exchange coupling J. (Do not compute any integral.)

(i) Notice that $J\mathbf{S}_1 \cdot \mathbf{S}_2$ is a magnetic type interaction (two dipoles interacting). However, the Hamiltonian H is purely electric. Discuss which physical principle (or principles) is (are) involved in order to give an effective magnetic interaction from "purely" electric interactions.

8. Free fermions

Consider a system of noninteracting N spin-1/2 particles which are free to move in a smooth one-dimentional ring of length L. The one-particle wavefunctions are

$$\langle x, \sigma | \psi \rangle = \psi_{n,\sigma}(x),$$

with $\sigma = \uparrow, \downarrow$ representing the spin, and n a quantum number to be defined. Assume that $N/2$ is an odd integer.

(a) Write down the one-particle states wavefunctions $\psi_{\sigma,n}(x)$ which obey the boundary condition given above. What is the meaning of the quantum number n?

(b) Use the fermionic field operators $a^\dagger_\sigma(x)$ and $a_\sigma(x)$ in position space (which create/annihilate a fermion in with spin σ at position x) to write the Hamiltonian of this free fermion system in the Fock space. Do the same now for the operators in momentum space.

(c) Compute the anticommutators $\left\{\tilde{a}_\sigma(p), \tilde{a}^\dagger_\tau(q)\right\}$ and $\{\tilde{a}_\sigma(p), \tilde{a}_\tau(q)\}$.

(d) Construct the many-particle ground state $|G\rangle$ for this system in the Fock space. Compute the Fermi energy E_F, namely the energy of the topmost occupied state. How many single-particle states are present in $|G\rangle$?

(e) Show that the wavefunction of the ground state is an $N \times N$ Slater determinant. In addition, show this determinant can be factorized to the product of two $\frac{N}{2} \times \frac{N}{2}$ determinants. (*Hint*: Notice that $\langle x_{i,\sigma} | \psi_{n,\tau} \rangle = \delta_{\sigma,\tau} \psi_{n,\tau}(x_{i,\sigma})$, where $x_{i,\sigma}$ is the position of the i-th particle with spin σ.)

(f) Show that

$$\Psi\left(x_{1,\uparrow}, x_{1,\downarrow}, \ldots, x_{\frac{N}{2},\uparrow}, x_{\frac{N}{2},\downarrow}\right) = L^{-\frac{N}{2}} e^{-i\left(\frac{2\pi}{L}\right)\left(\frac{N-2}{4}\right)NX_{\mathrm{CM}}} \prod_{i<j=1}^{\frac{N}{2}} \left(z_{i,\uparrow} - z_{j,\uparrow}\right)\left(z_{i,\downarrow} - z_{j,\downarrow}\right),$$

where $z_{i,\sigma} = e^{i\frac{2\pi}{L}x_{i,\sigma}}$ and X_{CM} is the position of the center of mass of the system. (*Hint*: Recall the Vandermonde matrix.)

9. Two coupled bosons

Consider a system of two distinct bosonic particles (type A and B) in which only one mode of each is present:

$$H = \epsilon_{\mathrm{A}} a^\dagger a + \epsilon_{\mathrm{B}} b^\dagger b + V a^\dagger b + V^* b^\dagger a.$$

(a) Show that $c \equiv ua - vb$ and $d \equiv v^* a + u^* b$, with $|u|^2 + |v|^2 = 1$ are bosonic operators.

(b) Show that when $\epsilon_{\mathrm{A}} = \epsilon_{\mathrm{B}}$ and $V = V^*$, the choice $u = v = 1/\sqrt{2}$ decouples the system of bosonic particles C and D.

(c) Determine u and v that diagonalizes the system in the general case. Find the Eigenenergies and Eigenvectors of the system.

10. Two fermions

Consider a system of two spin-1/2 identical fermionic particles that can occupy three different states of energies E_i, $i = 1, 2, 3$. The matrix elements allowing the transitions between these states are M_{ij}.

(a) Write down the system Hamiltonian in terms of the criation and annihilation operators.

(b) Determine the equation that gives the Eigenenergies of the sytem.

(c) Diagonalize the system for the particular case $E_i = E$ and $M_{ij} = M$, and the spins of the particles are the same.

11. Grand-canonical ensamble

The Grand partition function is given by the trace

$$Z_{\mathrm{G}} = \mathrm{tr}\, e^{-\beta(H-\mu N)}, \text{ where } H = \sum_i \epsilon_i a_i^\dagger a_i \text{ and } N = \sum_i a_i^\dagger a_i,$$

and the constants β and μ are the inverse of temperature and the chemical potential, respectively. In the following compute the required quantities for both cases of identical bosonic and fermionic particles.

(a) Compute Z_{G}. (*Hint*: Use the trace in the Fock space: $\mathrm{tr}\, O = \sum_{n_i \ldots n_\infty} \langle n_1 \ldots n_\infty | O | n_1 \ldots n_\infty \rangle$, and recall that in the Grand-canonical ensamble the number of particles is not fixed.)

(b) Compute the average occupation number $\langle n_i \rangle$, such that $\mathcal{N} = \sum_i \langle n_i \rangle$. (*Hint*: Recall the thermodynamic Grand-potential $\Omega(T, V, \mu) = \beta^{-1} \ln Z_{\mathrm{G}}$, and that $\mathcal{N} = -\left(\frac{\partial \Omega}{\partial \mu}\right)_{T,V}$.)

(c) Show that the fractional deviation from the mean occupation number

$$\frac{\left\langle \left(n_i - \langle n_i \rangle\right)^2 \right\rangle}{\langle n_i \rangle^2} = e^{\beta(\epsilon_i - \mu)} = \frac{1}{\langle n_i \rangle} + \zeta,$$

with the $\zeta = \pm 1$ for bosons and fermions, respectively.

12. Simple Hubbard model

Consider a simple molecule made of 2 sites and 2 electrons descibed by

$$H = -t \sum_\sigma \left(c_{1,\sigma}^\dagger c_{2,\sigma} + c_{2,\sigma}^\dagger c_{1,\sigma} \right) + U \left(n_{1,\uparrow} n_{1,\downarrow} + n_{2,\uparrow} n_{2,\downarrow} \right),$$

with $\sigma = \uparrow$ or $\downarrow$, $c_{i,\sigma}$ ($c_{i,\sigma}^\dagger$) being the anihillation (creation) operator of electrons at site i with spin projection σ at the z-axis, $n_{i,\sigma} = c_{i,\sigma}^\dagger c_{i,\sigma}$, and $t > 0$ and $U > 0$ being constants.

(a) Write the spin operators $\mathbf{S}_1$ and $\mathbf{S}_2$ in terms of the operators $c_{i,\sigma}$ and $c_{i,\sigma}^\dagger$.

(b) Give a physical interpretation (orign) of each term in the Hamiltonian H.

(c) Write the matrix H in the basis $\{i, \sigma; j, \tau\}$, where i,j denotes the sites the electrons occupy and σ,τ denotes their spin projection.

(d) Diagonalize the matrix H. What is the ground state?

(e) Interpret and discuss your results in the limits $U \gg t$ and $U \ll t$.