2.4 Problem Set

2.4.1 Questions on the Second Quantisation

1. (a) Starting with the commutation relation for bosonic creation $a^\dagger$ and annihilation operators $a$, $[a,a^\dagger]_- = 1$, show that

$$[a^\dagger a, a]_- = -a, \quad [a^\dagger a, a^\dagger]_- = a^\dagger.$$  

Using this result, show that, if $|\alpha\rangle$ represents an eigenstate of the operator $a^\dagger a$ with eigenvalue $\alpha$, $a|\alpha\rangle$ is also an eigenstate with eigenvalue $(\alpha - 1)$ (unless $a|\alpha\rangle = 0$). Similarly, show that $a^\dagger |\alpha\rangle$ is an eigenstate with eigenvalue $(\alpha + 1)$.

(b) If $|\alpha\rangle$ represents a normalised eigenstate of the operator $a^\dagger a$ with eigenvalue $\alpha$ for all $\alpha \geq 0$, show that

$$a|\alpha\rangle = \sqrt{\alpha}|\alpha - 1\rangle, \quad a^\dagger |\alpha\rangle = \sqrt{\alpha + 1}|\alpha + 1\rangle.$$  

[Hint: consider the norm of the state.] Defining $|\Omega\rangle$ the normalised vacuum state, annihilated by the operator $a$, show that $|n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger)^n|\Omega\rangle$ is a normalised eigenstate of $a^\dagger a$ with eigenvalue $n$.

As an additonal exercise, consider the generalisation of parts (a) and (b) to the case of fermionic operators $a$.

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2. Starting from first principles, show that the second quantised representation of the one-body kinetic energy operator is given by

$$\hat{T} = \int_0^L dx \, a^\dagger(x) \frac{p^2}{2m} a(x).$$

[Hint: it may be helpful to start with the Fourier representation in which the one-body kinetic energy operator is diagonal and carefully transform to the real space basis.]

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3. Transforming to the Fourier basis, show that the non-interacting three-dimensional cubic lattice tight-binding Hamiltonian,

$$\hat{H}^{(0)} = -t \sum_{\langle mn \rangle} \left( c^\dagger_{m\sigma} c_{n\sigma} + \text{h.c.} \right),$$

assumes a diagonal form. Here $\langle mn \rangle$ denotes the sum over all neighbouring sites and h.c. is short-hand for the Hermitian conjugate.

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4. Show that the Holstein-Primakoff transformation,

$$\hat{S}^- = a^\dagger \left( 2S - a^\dagger a \right)^{1/2}, \quad \hat{S}^+ = (\hat{S}^-)^\dagger, \quad \hat{S}^z = S - a^\dagger a,$$

is consistent with the quantum spin algebra $[\hat{S}^+, \hat{S}^-] = 2\hat{S}^z$. [Hint: you may prove this result without explicitly expansion of the square root!]

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5. Confirm that the bosonic commutation relations of the operators $\alpha$ and $\alpha^\dagger$ are preserved by the Bogoliubov transformation,
\[
\begin{pmatrix} \alpha \\ \alpha^\dagger \end{pmatrix} = \begin{pmatrix} \cosh \theta & -\sinh \theta \\ -\sinh \theta & \cosh \theta \end{pmatrix} \begin{pmatrix} \alpha \\ \alpha^\dagger \end{pmatrix}.
\]
How and why is this transformation related to the Lorentz transformation?

6. (a) Making use of the spin commutation relation, $[\hat{S}_m^a, \hat{S}_n^b] = i\delta_{mn}c^{ab}\hat{S}_m^a$ ($\hbar = 1$), apply the identity $i\dot{\hat{S}}_i = [\hat{S}_i, \hat{H}]$, to express the equation of motion of a spin in a nearest neighbour spin $S$ one-dimensional Heisenberg ferromagnet, $\hat{H} = -J\sum_m \hat{S}_m \cdot \hat{S}_{m+1}$.

(b) Interpreting the spins as classical vectors, and taking the continuum limit, show that the equation of motion of the hydrodynamic modes takes the form
\[
\dot{\hat{S}} = Ja^2\nabla^2 \hat{S},
\]
where $a$ denotes the lattice spacing. [Hint: in transferring to the continuum limit, apply a Taylor expansion to the spins viz. $\hat{S}_m^a = \hat{S}_1^a + a\partial S^a_m + \frac{a^2}{2} \partial^2 S^a_m + \cdots$.]

(c) Confirm that the equation of motion is solved by the Ansatz,
\[
\hat{S}(x, t) = \begin{pmatrix} c \cos(kt) \\ c \sin(kt) \\ p \end{pmatrix},
\]
determine the dispersion. Sketch a ‘snapshot’ configuration of the spins in the chain.

7. †Valence Bond Solid: Starting with the spin 1/2 Majumdar-Ghosh Hamiltonian
\[
\hat{H}_{MG} = \frac{4|J|}{3} \sum_{n=1}^{N} \left( \hat{S}_n \cdot \hat{S}_{n+1} + \frac{1}{2} \hat{S}_n \cdot \hat{S}_{n+2} \right) + \frac{N|J|}{2},
\]
where the total number of sites $N$ is even, and $\hat{S}_{N+1} = \hat{S}_1$, show that the two dimer or valence bond states $|\Omega_{\pm}\rangle = \otimes \prod_{n=1}^{N/2} \frac{1}{\sqrt{2}} (|\uparrow\rangle |\downarrow\rangle + |\downarrow\rangle |\uparrow\rangle |\downarrow\rangle |\downarrow\rangle + 1)_{2n+1}$, are exact ground states, i.e. $|\Omega_{\pm}\rangle$ describes the state where neighbouring spins on sites $2n$ and $2n+1$ are in a total spin singlet ($S = 0$) state. [Hint: recast the Hamiltonian in terms of the total spin of a triad $J_n = \hat{S}_{n-1} + \hat{S}_n + \hat{S}_{n+1}$, and consider what this representation implies.] Consider what would happen if the total number of sites was odd.

8. Su-Shrieffer-Heeger Model: Polyacetylene consists of bonded CH groups forming an isomeric long chain polymer. According to molecular orbital theory, the carbon atoms are expected to be sp$^2$ hybridised suggesting a planar configuration of the molecule. An unpaired electron is expected to occupy a single p-orbital which points out of the plane. The weak overlap of the p-orbitals delocalise the electrons into a $\pi$-conduction band (cf. benzene) — see Fig. 2.13a. Therefore, according to the nearly free electron theory, one might expect the half-filled conduction band of a polyacetylene chain to be metallic. However, the energy of a half-filled band of a one-dimension system can always be lowered by imposing a periodic lattice distortion known as the Peierls instability (see Fig. 2.13b).
One can think of an enhanced probability of finding the $\pi$ electron on the short bond where the orbital overlap is stronger — the “double bond”. The aim of this problem is to explore the instability.

(a) At its simplest level, the conduction band of polyacetylene can be modelled by a simple Hamiltonian, due to Su-Shrieffer-Heeger, in which the hopping matrix elements of the electrons are modulated by the lattice distortion of the atoms. Taking the displacement of the atomic sites from the equilibrium separation $a \equiv 1$ to be $u_n$, and treating their dynamics as classical, the effective Hamiltonian takes the form

$$\hat{H} = -t \sum_{n=1}^{N} \sum_{\sigma} (1 + u_n) \left[ c_{n\sigma}^\dagger c_{n+1\sigma} + \text{h.c.} \right] + \sum_{n=1}^{N} \frac{k_s}{2} (u_{n+1} - u_n)^2,$$

where, for simplicity, the boundary conditions are taken to be periodic. The first term describes the hopping of electrons between neighbouring sites with a matrix element modulated by the periodic distortion of the bond-length, while the last term represents the associated increase in the elastic energy. Taking the lattice distortion to be periodic, $u_n = (-1)^n a$, and the number of sites to be even, diagonalise the Hamiltonian. [Hint: the lattice distortion lowers the symmetry of the lattice. The Hamiltonian is most easily diagonalised by distinguishing the two sites of the sublattice — i.e. doubling the size of the elementary unit cell — and transforming to the Fourier representation.] Show that the Peierls distortion of the lattice opens a gap in the spectrum at the Fermi level of the half-filled system.

(b) By estimating the total electronic and elastic energy of the half-filled band (i.e. an average of one electron per lattice site), show that the one-dimensional system is always unstable towards the Peierls distortion. To complete this calculation, you will need the approximate formula for the (elliptic) integral,

$$\int_{-\pi/2}^{\pi/2} dk \left( 1 - (1 - \alpha^2) \sin^2 k \right)^{1/2} \simeq 2 + (a_1 - b_1 \ln \alpha^2) \alpha^2$$

where $a_1$ and $b_1$ are (unspecified) numerical constants.

(c) For an even number of sites, the Peierls instability has two degenerate configurations (see Fig. 2.13b) — ABABAB... and BABABA... Comment on the qualitative form of the ground state lattice configuration if the number of sites is odd (cf. Fig. 2.13c).
9. In the **Schwinger boson representation** quantum mechanical spin is expressed in terms of two bosonic operators, $a$ and $b$, in the form $\hat{S}^+ = a^\dagger b$, $\hat{S}^- = (\hat{S}^+)^\dagger$, $\hat{S}^z = \frac{1}{2}(a^\dagger a - b^\dagger b)$.

(a) Show that this definition is consistent with spin commutation relations $[\hat{S}^+ , \hat{S}^-] = 2\hat{S}^z$.

(b) Using the bosonic commutation relations, show that

$$|S,m\rangle = \frac{(a)^{\hat{S}+m}}{\sqrt{(S+m)!}} \frac{(b)^{\hat{S}^{-m}}}{\sqrt{(S-m)!}} |\Omega\rangle,$$

is compatible with the definition of an eigenstate of the total spin operator $\hat{S}^2$ and $\hat{S}^z$. Here $|\Omega\rangle$ denotes the vacuum of the Schwinger bosons, and the total spin $S$ defines the physical subspace $\{ |n_a, n_b\rangle : n_a + n_b = 2S \}$.

10. **The Jordan-Wigner Transformation**: So far we have shown how the algebra of quantum mechanical spin can be expressed using boson operators. Here we show that a representation for spin 1/2 can be obtained in terms of Fermion operators. Specifically, let us represent an up spin as a particle and a down spin as the vacuum $|0\rangle$, viz. $|\uparrow\rangle \equiv |1\rangle = f^\dagger |0\rangle$, and $|\downarrow\rangle \equiv |0\rangle = f |1\rangle$. In this representation the spin raising and lowering operators are expressed in the form $\hat{S}^+ = f^\dagger$ and $\hat{S}^- = f$, while $\hat{S}^z = f^\dagger f - 1/2$.

(a) With this definition, confirm that the spins obey the algebra $[\hat{S}^+, \hat{S}^-] = 2\hat{S}^z$.

However, there is a problem: spins on different sites commute while fermion operators anticommute, e.g. $\hat{S}_i^+ \hat{S}_j^+ = \hat{S}_j^+ \hat{S}_i^+$, but $f_i^\dagger f_j^\dagger = -f_j^\dagger f_i^\dagger$. To obtain a faithful spin representation, it is necessary cancel this unwanted sign. Although a general procedure is hard to formulate, in one dimension, this can be achieved by a non-linear transformation, viz.

$$\hat{S}^+_i = f_i e^{i\pi \sum_{j<i} n_j}, \quad \hat{S}^-_i = e^{-i\pi \sum_{j<i} n_j} f_i, \quad \hat{S}^z_i = f_i^\dagger f_i - \frac{1}{2}.$$

Operationally, this seemingly complicated transformation has a straightforward interpretation: in one dimension, the particles can be ordered on the line. By counting the number of particles ‘to the left’ we can assign an overall phase of +1 or −1 to a given configuration and thereby transmute the particles into a fermions. (Put differently, the exchange to two fermions induces a sign change which is compensated by the factor arising from the phase — the ‘Jordan-Wigner string’.)

(b) Using the Jordan-Wigner representation, show that $\hat{S}_m^+ \hat{S}_{m+1}^- = f_m^\dagger f_{m+1}$.

(c) For the spin 1/2 anisotropic quantum Heisenberg spin chain, the spin Hamiltonian assumes the form

$$\hat{H} = -\sum_n \left[ J_z \hat{S}^z_n \hat{S}^z_{n+1} + \frac{J_{\perp}}{2} \left( \hat{S}^+_n \hat{S}^-_{n+1} + \hat{S}^-_n \hat{S}^+_n \right) \right].$$

Turning to the Jordan-Wigner representation, show that the Hamiltonian can be cast in the form

$$\hat{H} = -\sum_n \left[ \frac{J_{\perp}}{2} \left( f_m^\dagger f_{m+1} + \text{h.c.} \right) + J_z \left( \frac{1}{4} - f_m^\dagger f_m + f_m^\dagger f_m f_{m+1}^\dagger f_{m+1} \right) \right].$$

(d) The mapping above shows that the one-dimensional quantum spin 1/2 XY-model (i.e. $J_z = 0$) can be diagonalised as a non-interacting theory of spinless fermions. In this case, show that the spectrum assumes the form $\epsilon_k = -J_{\perp} \cos ka$. 

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