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, $\left[a, a^\dagger\right] = 1$, show that

$$[a^\dagger a, a] = -a, \qquad [a^\dagger a, a^\dagger] = a^\dagger.$$

Using this result, show that, if $|\alpha\rangle$ represents an eigenstate of the operator $a^\dagger a$ with eigenvalue α, $a|\alpha\rangle$ 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 α for all $\alpha \geq 0$, show that

$$\begin{aligned} a|\alpha\rangle &= \sqrt{\alpha}|\alpha - 1\rangle \\ a^\dagger|\alpha\rangle &= \sqrt{\alpha + 1}|\alpha + 1\rangle \end{aligned}$$

Defining as the normalised vacuum $|\Omega\rangle$ the normalised state that is anniliated by the operator a, show that $|n\rangle = (1/\sqrt{n!})(a^\dagger)^n|\Omega\rangle$ is a normalised eigenstate of $a^\dagger a$ with eigenvalue n.

---

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

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

[Hint: Remember that the representation is most easily obtained from the basis in which the operator is diagonal.]

---

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

$$\hat{H}^{(0)} = -\sum_{\langle \mathbf{mn} \rangle} t_{\mathbf{mn}} c^\dagger_{\mathbf{m}\sigma} c_{\mathbf{n}\sigma},$$

where the matrix elements $t_{\mathbf{mn}}$ take the positive real value t between neighbouring sites and zero otherwise.

---

4. Starting with the definition

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

confirm the validity of the Holstein-Primakoff transformation by explicitly checking the commutation relations of the spin raising and lowering operators.

---

5. †**Frustration**: On a bipartite lattice (i.e. one in which the neighbours of one sublattice belong to the other sublattice), the ground state (known as a Néel state) of a classical antiferromagnet can adopt a staggered spin configuration in which the exchange energy is maximised. Lattices which can not be classified in this way are said to be frustrated — the maximal exchange energy associated with each bond can not be recovered. *Using only symmetry arguments*, specify one of the possible ground states of a classical three site triangular lattice antiferromagnet. (Note that the invariance of the Hamiltonian under a global rotation of the spins means that the there is manifold of continuous degeneracy in the ground state.) Using this result, construct one of the classical ground states of the infinite triangular lattice.

---

6. Confirm that the bosonic commutation relations of the operators a and $a^\dagger$ are preserved by the Bogoluibov transformation,

$$\begin{pmatrix} \alpha \\ \alpha^\dagger \end{pmatrix} = \begin{pmatrix} \cosh\theta & \sinh\theta \\ \sinh\theta & \cosh\theta \end{pmatrix} \begin{pmatrix} a \\ a^\dagger \end{pmatrix}.$$

---

7. (a) Making use of the spin commutation relation, $[S_i^\alpha, S_j^\beta] = i\delta_{ij}\epsilon^{\alpha\beta\gamma} S_i^\gamma$, apply the identity

$$i\dot{\mathbf{S}}_i = [\hat{\mathbf{S}}_i, \hat{H}]$$

to express the equation of motion of a spin in a nearest neighbour spin S one-dimensional Heisenberg ferromagnet.

(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

$$\dot{\mathbf{S}} = Ja^2 \mathbf{S} \times \partial^2 \mathbf{S},$$

where a denotes the lattice spacing. [Hint: Going to the continuum limit, apply a Taylor expansion to the spins viz. $S_{i+1} = S_i + a\partial S_i + a^2 \partial^2 S_i/2 + \cdots$.]

(c) Confirm that the equation of motion is solved by the *Ansatz*,

$$\mathbf{S} = \left(c\cos(kx - \omega t), c\sin(kx - \omega t), \sqrt{S^2 - c^2}\right),$$

and determine the dispersion. Sketch a ‘snapshot’ configuration of the spins in the chain.

---

8. †**Valence Bond Solid**: Starting with the spin 1/2 **Majumdar-Ghosh Hamiltonian**

$$\hat{H}_{\mathrm{MG}} = \frac{4|J|}{3}\sum_{n=1}^{N}\left(\hat{\mathbf{S}}_n\cdot\hat{\mathbf{S}}_{n+1} + \frac{1}{2}\hat{\mathbf{S}}_n\cdot\hat{\mathbf{S}}_{n+2}\right) + \frac{N|J|}{2},$$

where the total number of sites N is even, and $\hat{\mathbf{S}}_{N+1} = \hat{\mathbf{S}}_1$, show that the two dimer or valence bond states

$$|\Omega_{\pm}\rangle = \prod_{n=1}^{N/2}\frac{1}{\sqrt{2}}\left(|\uparrow_{2n}\rangle\otimes|\downarrow_{2n\pm1}\rangle - |\downarrow_{2n}\rangle\otimes|\uparrow_{2n\pm1}\rangle\right),$$

are exact eigenstates. [Hint: Try to recast the Hamiltonian in terms of the total spin of a triad $\hat{\mathbf{J}}_n = \hat{\mathbf{S}}_{n-1} + \hat{\mathbf{S}}_n + \hat{\mathbf{S}}_{n+1}$, and consider what this representation implies.] In fact these states represent the ground states of the Hamiltonian. Suggest what would happen if the total number of sites was odd.

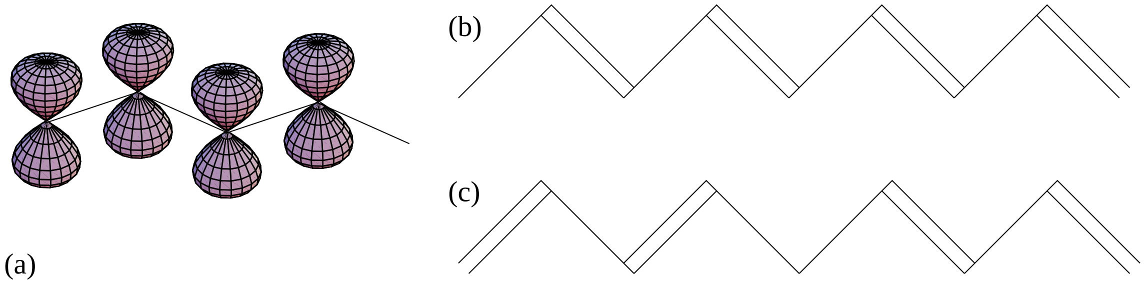


Figure 2.13: (a) Schematic diagram showing the π-bonding orbitals in long chain polyacetylene. (b) One of the configurations of the Peirels distorted chain. The double bonds represent the short links of the lattice. (c) A topological defect separating a two domains of the ordered phase.

9. **Su-Shrieffer-Heeger Model:**[25] 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

[25] Alan J. Heeger: 2000 Nobel Laureate in Physics with Alan G. MacDiarmid, and Hideki Shirakawa for the discovery and development of conductive polymers.

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 π-conduction band (cf. the benzene molecule) — 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 **Peirels instability** (see fig. 2.13b). One can think of an enhanced probability of finding the π 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

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

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, $u_n = (-1)^n\alpha$, 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 Peirels distortion. To complete this calculation, you will need the approximate formula for the (elliptic) integral,

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

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).

10. In the **Schwinger boson representation**,[26] the quantum mechanical spin is expressed in terms of two bosonic operators a, and b in the form

$$\hat{S}^+ = a^\dagger b, \qquad \hat{S}^- = (\hat{S}^+)^\dagger, \qquad \hat{S}^z = \frac{1}{2}\left(a^\dagger a - b^\dagger b\right).$$

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

(b) Using the bosonic commutation relations, show that

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

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

$$\{|n_a, n_b\rangle : n_a + n_b = 2S\}.$$

---

11. †**The Jordan-Wigner Transformation**: So far we have shown how the algebra of quantum mechanical spin can be expressed using boson operators — cf. the Holstein-Primakoff transformation and the Schwinger representation. In this problem we show that a representation for spin 1/2 can be obtained in terms of Fermion operators. Specifically, let us formally represent an up spin as a particle and a down spin as the vacuum $|0\rangle$, viz.

$$|\uparrow\rangle \equiv |1\rangle = f^\dagger|0\rangle,$$
$$|\downarrow\rangle \equiv |0\rangle = f|1\rangle.$$

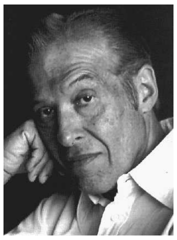
In this representation the spin raising and lowering operators are expressed in the form $\hat{S}^+ = f^\dagger$ and $\hat{S}^- = f$, while $\hat{S}^z = f^\dagger f - 1/2$.

(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.

$$S_i^+ S_j^+ = S_j^+ S_i^+, \qquad \text{but} \quad f_i^\dagger f_j^\dagger = -f_j^\dagger f_i^\dagger.$$

[26] Julian Schwinger: 1965 Nobel Laureate in Physics with Sin-Itiro Tomonaga and Richard P. Feynman, for their fundamental work in quantum electrodynamics, with deep-ploughing consequences for the physics of elementary particles.



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.

$$\hat{S}_l^+ = f_l^\dagger e^{i\pi \sum_{j<l} \hat{n}_j}, \qquad \hat{S}_l^- = e^{-i\pi \sum_{j<l} \hat{n}_j} f_l, \qquad \hat{S}_l^z = f_l^\dagger f_l - \frac{1}{2}.$$

Operationally, this seemingly complicated transformation is straightforward: 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

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

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

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

(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

$$\epsilon(k) = -J_\perp \cos ka$$