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

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

[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

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

[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,

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

assumes a diagonal form. Here $\langle \mathbf{mn}\rangle$ 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,

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

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 α and $\alpha^\dagger$ are preserved by the Bogoluibov transformation,

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

How and why is this transformation related to the Lorentz transformation?

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

(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

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

where a denotes the lattice spacing. [Hint: in transferring to the continuum limit, apply a Taylor expansion to the spins viz. $S_{m+1} = S_m + a\partial S_m + \frac{a^2}{2}\partial^2 S_m + \cdots$.]

(c) Confirm that the equation of motion is solved by the *Ansatz*, $\mathbf{S}(x,t) = (c\cos(kx - \omega t), c\sin(kx - \omega t), \sqrt{S^2 - c^2})$, and determine the dispersion. Sketch a 'snapshot' configuration of the spins in the chain.

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

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

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 $|\Omega_\pm\rangle = \otimes\prod_{n=1}^{N/2}\frac{1}{\sqrt{2}}(|\uparrow\rangle_{2n}\otimes|\downarrow\rangle_{2n\pm1} - |\downarrow\rangle_{2n}\otimes|\uparrow\rangle_{2n\pm1})$, are exact ground states, i.e. $|\Omega_+\rangle$ 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 $\hat{\mathbf{J}}_n = \hat{\mathbf{S}}_{n-1} + \hat{\mathbf{S}}_n + \hat{\mathbf{S}}_{n+1}$, and consider what this representation implies.] Consider what would happen if the total number of sites was odd.

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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 π-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 **Peirels instability** (see Fig. 2.13b).

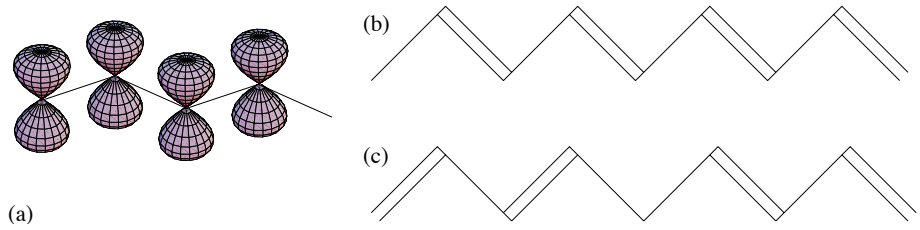

Figure 2.13: (a) Schematic diagram showing the π-bonding orbitals in long chain polyacetylene. (b) One of the configurations of the Peierls distorted chain. The double bonds represent the short links of the lattice. (c) A topological defect separating a two domains of the ordered phase.

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 Peierls 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).

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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

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

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

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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. $S_i^+ S_j^+ = S_j^+ S_i^+$, 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.

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

    Operationally, this seemingly complicated transformation 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

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

    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 $\epsilon_k = -J_\perp \cos ka$.
