2.4.2 Answers

1. (a) Making use of the commutation relations for bosons, one finds

$$a^\dagger a a = a(a^\dagger a - 1), \qquad a^\dagger a a^\dagger = a^\dagger(1 + a^\dagger a)$$

from which the results follow. Using these results, one finds that, providing $a|\alpha\rangle \neq 0$,

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

(b) If $|\alpha\rangle$ is a normalised eigenstate of $a^\dagger a$ with eigenvalue α, the norm of state created by the action of the creation operator is given by

$$||a^\dagger|\alpha\rangle|| \equiv \sqrt{\langle\alpha|aa^\dagger|\alpha\rangle} = \sqrt{\langle\alpha|a^\dagger a + 1|\alpha\rangle} = \sqrt{\alpha + 1}.$$

Similarly, the norm of state created by the action of the annihilation operator is given by

$$||a|\alpha\rangle|| \equiv \sqrt{\langle\alpha|a^\dagger a|\alpha\rangle} = \sqrt{\alpha}.$$

Therefore, if we define $|\alpha + 1\rangle$ and $|\alpha - 1\rangle$ as the normalised eigenstates of the operator $a^\dagger a$ with eigenvalue $\alpha + 1$ and $\alpha - 1$ respectively, one finds

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

Defining as the vacuum $|\Omega\rangle$ the normalised state that is annihilated by the operator a, an application of the result above shows the state $|n\rangle = (1/\sqrt{n!})(a^\dagger)^n|\Omega\rangle$ to be a normalised eigenstate of $a^\dagger a$ with eigenvalue n.

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2. The kinetic energy operator is diagonal in the momentum basis. Following the analysis in the text, the corresponding second quantised one-body operator is given by $\hat{T} = \sum_p \frac{p^2}{2m} a_p^\dagger a_p$. Transforming to the coordinate representation, $a_p = L^{-1/2} \int_0^L dx e^{ipx/\hbar} a(x)$, one obtains

$$\hat{T} = \frac{1}{L} \sum_p \frac{p^2}{2m} \int_0^L dy \int_0^L dx e^{ip(x-y)/\hbar} a^\dagger(y) a(x).$$

Expressing factor p^2 as a derivative of the exponential factor, and integrating by parts, one obtains the required result.

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3. A Hamiltonian which is translationally invariant is easily diagonalised in the Fourier representation. Setting $c^\dagger_{\mathbf{m}\sigma} = \frac{1}{N^{d/2}}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{m}} c^\dagger_{\mathbf{k}\sigma}$, the Hamiltonian takes the form

$$\hat{H}^{(0)} = \sum_{\mathbf{k}}^{\text{B.Z.}} \sum_{\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma},$$

where $\epsilon_{\mathbf{k}} = -t\sum_{i=x,y,z} e^{i\mathbf{k}\cdot\hat{\mathbf{e}}_i} = -2t\sum_{i=x,y,z}\cos(\mathbf{k}\cdot\hat{\mathbf{e}}_i)$, with the sum running over neighbouring lattice vectors $\hat{\mathbf{e}}_i$, and the lattice spacing is taken to be unity.

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4. Substituting the definition of the spin raising and lowering operators using the Holstein-Primakoff transformation, the commutator is obtained as

$$\frac{1}{2S}[\hat{S}^+, \hat{S}^-] = \left(1 - \frac{a^\dagger a}{2S}\right)^{1/2} \overbrace{aa^\dagger}^{1+a^\dagger a} \left(1 - \frac{a^\dagger a}{2S}\right)^{1/2} - a^\dagger \left(1 - \frac{a^\dagger a}{2S}\right) a$$
$$= \left(1 - \frac{a^\dagger a}{2S}\right) + a^\dagger a \left(1 - \frac{a^\dagger a}{2S}\right) - a^\dagger a + \frac{a^\dagger a^\dagger a a}{2S} = 1 - \frac{a^\dagger a}{S}.$$

With $S^z = S - a^\dagger a$, we obtain the required commutation relation $[\hat{S}^+, \hat{S}^-] = 2S^z$.

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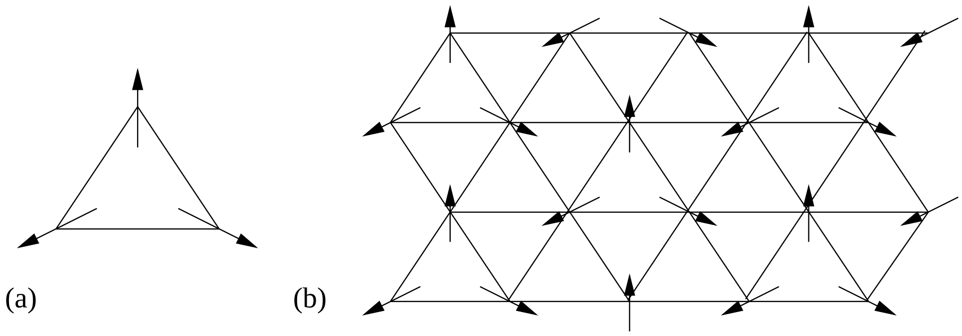
5. By symmetry, the maximal exchange energy that can be recovered is obtained when the spins are maximally anti-aligned, i.e. at 120^o to each other. Using the spin



orientation of a single triangle, the two-dimensional triangular lattice can be tessilated with all spins aligned at 120^o to the neighbours. Notice that this configuration represents just one of an infinite degenerate manifold of ground states obtained by global rotation of the spins.

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6. To confirm the validity of the Bogoluibov transformation let us consider the commutation relations of α:[27]

$$\begin{aligned}\left[\alpha,\alpha^\dagger\right] &= \left[\cosh\theta\ a+\sinh\theta\ a^\dagger,\cosh\theta\ a^\dagger+\sinh\theta\ a\right]\\ &= \cosh^2\theta\left[a,a^\dagger\right]+\sinh^2\theta\left[a^\dagger,a\right]=\cosh^2\theta-\sinh^2\theta=1.\end{aligned}$$

as required.

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7. (a) Making use of the equation of motion $i\dot{\mathbf{S}}_i = [\hat{\mathbf{S}}_i,\hat{H}]$, and the commutation relation $[S_i^\alpha,S_j^\beta]=i\delta_{ij}\epsilon^{\alpha\beta\gamma}S_i^\gamma$, we obtain

$$i\dot{\mathbf{S}}_i = Ji\hat{\mathbf{S}}_i\times\left(\hat{\mathbf{S}}_{i+1}+\hat{\mathbf{S}}_{i-1}\right)$$

(b) Interpreting the spins as classical vectors, and applying the Taylor expansion $\mathbf{S}_{i+1}=\mathbf{S}_i+a\partial\mathbf{S}_i+(a^2/2)\partial^2\mathbf{S}_i+\cdots$, we obtain the classical equation of motion

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

Substituting, we find that $\mathbf{S}=\left(c\cos(kx-\omega t),c\sin(kx-\omega t),\sqrt{S^2-c^2}\right)$, satisfies the equation of motion with $\omega=J(ka)^2\sqrt{S^2-c^2}$.

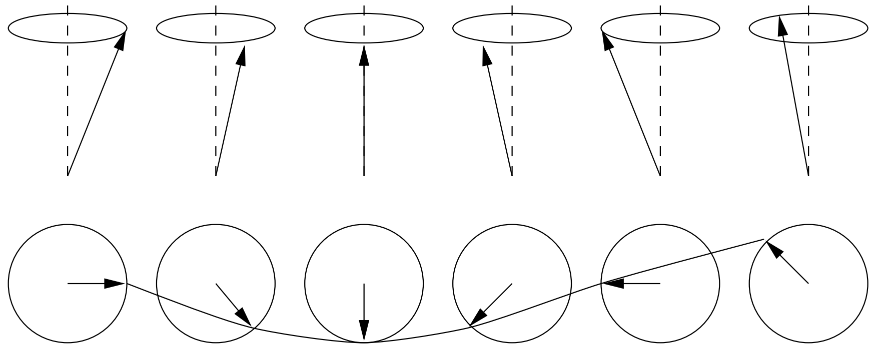

Figure 2.14: Spin-wave dispersion.

(c) The corresponding spin wave solution has the precessional form shown in Fig. 2.14.

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[27] More formally, one may prove the relation as follows: Suppose we define a two component operator $\mathbf{a}=(a,a^\dagger)$. If a obeys bosonic commutation relations, $[a_\mu,a_\nu^\dagger]=g_{\mu\nu}$ where the diagonal matrix has elements $g=\mathrm{diag}(1,-1)$. If we define an operator transformation Λ such that $\alpha_\mu=\Lambda_{\mu\nu}a_\nu$ (summation convention implied), then the condition that the commutation relations are preserved requires

$$g_{\mu\nu}\stackrel{!}{=}[\alpha_\mu,\alpha_\nu^\dagger]=\Lambda_{\mu\eta}\Lambda^*_{\nu\gamma}[a_\eta,a_\gamma^\dagger]=\Lambda_{\mu\eta}\Lambda^*_{\nu\gamma}g_{\eta\gamma},$$

i.e. the admissable transformations fulfil the condition that $g_{\mu\nu}=\Lambda_{\mu\eta}\Lambda^*_{\nu\gamma}g_{\eta\gamma}$. Such transformations, that preserve the "metric" $g=\mathrm{diag}(1,-1)$, belong to the group of Lorentz transformations. In the context of bosonic operators, they are termed Bogoluibov transformations. Note that, for fermionic systems, with $\mathbf{c}=(c,c^\dagger)$, $[c_\mu,c_\nu^\dagger]=\delta_{\mu\nu}$. In this case, we require that $\delta_{\mu\nu}=\Lambda_{\mu\eta}\Lambda^*_{\nu\gamma}\delta_{\eta\gamma}$, i.e. Λ belongs the class of Unitary transformations: $\Lambda^\dagger\Lambda=\mathbf{1}$

8. Defining the total spin on a triad $\hat{\mathbf{J}}_n = \hat{\mathbf{S}}_{n-1} + \hat{\mathbf{S}}_n + \hat{\mathbf{S}}_{n+1}$, the Hamiltonian can be recast in the form

$$\hat{H}_{\rm MG} = |J| \sum_{n=1}^{N} \hat{\mathcal{P}}_{3/2}(n-1, n, n+1),$$

where $\hat{\mathcal{P}}_{3/2}(n-1,n,n+1) = (\hat{\mathbf{J}}_n^2 - 3/4)/3$ annihilates any state with total spin $J = 1/2$ of the triad. Since in any three sites, two of the spins are in a singlet, there can be no components of $J = 3/2$ on any triad. Therefore the dimer states are eigenstates of zero energy. Now since $\hat{\mathcal{P}}_{3/2}$ is positive definite, these states must be the ground states.

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9. (a) Since each unit cell is of twice the dimension of the original lattice, we begin by recasting the Hamiltonian in the sublattice form

$$\hat{H} = -t \sum_{m=1,\sigma}^{N/2} \left\{(1+\alpha)\left[a^\dagger_{m\sigma} b_{m\sigma} + \text{h.c.}\right] + (1-\alpha)\left[b^\dagger_{m\sigma} a_{m+1\sigma} + \text{h.c.}\right]\right\} + \frac{Nk_s\alpha^2}{2}.$$

Switching to the Fourier basis, $a_m = \sqrt{2/N}\sum_k e^{-2ikm} a_k$ (similarly b_m), where k takes $N/2$ values uniformly on the interval $[-\pi/2, \pi/2]$, the Hamiltonian takes the form

$$\begin{aligned}\hat{H} = {} & \frac{Nk_s a^2}{2}\alpha^2 \\ & -t\sum_{k\sigma} \begin{pmatrix} a^\dagger_{k\sigma} & b^\dagger_{k\sigma}\end{pmatrix} \begin{pmatrix} 0 & (1+\alpha)+(1-\alpha)e^{-2ik} \\ (1+\alpha)+(1-\alpha)e^{2ik} & 0 \end{pmatrix} \begin{pmatrix} a_{k\sigma} \\ b_{k\sigma}\end{pmatrix}.\end{aligned}$$

Diagonalising the 2×2 Hamiltonian, we obtain the spectrum

$$\epsilon(k) = \pm 2t\left[\cos^2 k + \alpha^2 \sin^2 k\right]^{1/2}.$$

Reassuringly, in the limit $\alpha \to 0$, we obtain the cosine spectrum of the undistorted problem, while in the limit $\alpha \to 1$, pairs of monomers become decoupled and we obtain a massively degenerate bonding and antibonding spectrum.

(b) According to the formula given in the text, the total shift in energy is given by

$$\delta\epsilon = -2t(a_1 - b_1 \ln\alpha^2)\alpha^2 + \frac{Nk_s\alpha^2}{2}$$

Maximising the energy gain with respect to α, one finds that the stable configuration is found when

$$\alpha^2 = \exp\left[\frac{a_1}{b_1} - 1 - \frac{Nk_s}{4tb_1}\right]$$

(c) If the number of sites is odd, the Peirels distortion is inevitably frustrated — a configuration that starts ABABAB must finish as BABABA. The result is that the polymer chain must accommodate a **topological excitation**. The excitation is said to be topological because the defect can not be removed by a smooth continuous deformation — it is like a dislocation line in a crystal. Its effect on the spectrum of the model is to introduce a state that lies within the band gap of the material.

The consideration of an odd number of sites forces a topological defect into the system. However, even if the number of sites is even, one can create low energy topological excitations of the system either by doping (see fig. 2.13c), or by the creation of **excitons**, particle-hole excitations of the system. Indeed, such topological excitations can dominate the transport properties of the system.

As a footnote, one should add that the particular model considered above is somewhat over-simplified. It seems likely that Coulomb interactions play a dominant role in driving the Peirels instability in Polyacetylene. However, the qualitative interpretation of the existence of topological excitations is born out by experiment.

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10. (a) Using the commutation relation for bosons, one finds.

$$\begin{aligned}[\hat{S}^+, \hat{S}^-] &= a^\dagger b\, b^\dagger a - b^\dagger a\, a^\dagger b = a^\dagger a b b^\dagger - a a^\dagger b^\dagger b \\ &= a^\dagger a(b^\dagger b + 1) - (a^\dagger a + 1) b^\dagger b = a^\dagger a - b^\dagger b = 2\hat{S}^z.\end{aligned}$$

(b) Using the identity

$$\begin{aligned}\hat{\mathbf{S}}^2 &= (\hat{S}^z)^2 + \frac{1}{2}\left(\hat{S}^+\hat{S}^- + \hat{S}^-\hat{S}^+\right) = \frac{1}{4}\left(\hat{n}_a - \hat{n}_b\right)^2 + \frac{1}{2}\left(a^\dagger b\, b^\dagger a + b^\dagger a\, a^\dagger b\right) \\ &= \frac{1}{4}\left(\hat{n}_a - \hat{n}_b\right)^2 + \hat{n}_a\hat{n}_b + \frac{1}{2}\left(\hat{n}_a + \hat{n}_b\right),\end{aligned}$$

one finds that

$$\hat{\mathbf{S}}^2|S,m\rangle = \left[m^2 + (S+m)(S-m) + S\right]|S,m\rangle = S(S+1)|S,m\rangle$$

as required. Similarly, one finds

$$\begin{aligned}\hat{S}^z|S,m\rangle &= \frac{1}{2}(n_a - n_b)|n_a = S+m, n_b = S-m\rangle \\ &= \frac{1}{2}\left[(S+m) - (S-m)\right]|S,m\rangle = m|S,m\rangle,\end{aligned}$$

showing $|S,m\rangle$ to be an eigenstate of the operator $\hat{S}^z$ with eigenvalue m.

As with the Holstein-Primakoff representation, the Schwinger boson represents yet another representation of quantum mechanical spin. Which representation is most convenient for the analysis of quantum spin models depends sensitively on the nature of the microscopic Hamiltonian.

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11. (a) Using the fermionic anticommutation relations, one finds

$$\begin{aligned}[\hat{S}^+, \hat{S}^-]_- &= [f^\dagger, f]_- = f^\dagger f - f f^\dagger \\ &= 2f^\dagger f - 1 = 2\hat{S}^z.\end{aligned}$$

(b) Using the fact that the number operators on different sites commute, one finds

$$\hat{S}^+_m \hat{S}^-_{m+1} = f^\dagger_m e^{i\pi \sum_{j<m} n_j} e^{-i\pi \sum_{l<m+1} n_l} f_{m+1} = f^\dagger_m e^{-i\pi n_m} f_{m+1} = f^\dagger_m f_{m+1}$$

where here we have made use of the fact that, for fermionic particles $f^\dagger_m e^{-i\pi n_m} \equiv f^\dagger_m$.

(c) The fermion representation is simply obtained by substitution.

(d) With $J_z = 0$, the spin Hamiltonian assumes the form of a non-interacting tight-binding Hamiltonian

$$\hat{H} = -\frac{J_\perp}{2} \sum_n \left(f^\dagger_n f_{n+1} + \text{h.c.} \right).$$

This Hamiltonian, which has been encountered previously, is diagonalised in the Fourier space after which one obtains the cosine band dispersion.