FI 193 – Teoria Quântica de Sistemas de Muitos Corpos – Lista 1

01. P.1.8, Schwabl: Number operator.
A system of N interacting particles is described by the Hamiltonian

$$H = \sum_{i,j} \langle i|T|j\rangle a_i^\dagger a_j + \frac{1}{2} \sum_{i,j,k,l} \langle i\, j|V|k\, l\rangle a_i^\dagger a_j^\dagger a_l a_k.$$

(a) For a system of N interacting bosons, show that the Hamiltonian H commutes with the total particle-number operator $\hat{N} = \sum_i a_i^\dagger a_i$.

(b) For a system of N interacting fermions, show that $[H, \hat{N}] = 0$.

Hint: Identity $[AB, CD] = [A, C]BD + A[B, C]D + C[A, D]B + CA[B, D]$ and the equivalent in terms of anticommutators.

P.02. P.1.2, Miranda: Boson coherent states:
For the one-dimensional harmonic oscillator, the so-called coherent states $|\phi\rangle$ are defined as the eigenvectors of the non-Hermitian lowering operator a, (see, e.g., Sec. 10.7 from Merzbacher for a review)

$$a|\phi\rangle = \phi|\phi\rangle, \qquad \phi \in \mathcal{C}.$$

Similarly, one can also define coherent states for bosons. Let us consider boson operators $a_i^\dagger$ and a_i that, respectively, creates and annihilates a particle in the single-particle state $|i\rangle$, with $i = 1, 2, \ldots$. A boson coherent state is defined as

$$a_i|\phi\rangle = \phi_i|\phi\rangle, \qquad \phi_i \in \mathcal{C}, \qquad i = 1, 2, \ldots\ .$$

(a) It is interesting to expand a boson coherent state in the occupation number representation,

$$|\phi\rangle = \sum_{n_1, n_2, \ldots} C(n_1, n_2, \ldots)|n_1\, n_2\, \ldots\rangle,$$

where the vectors

$$|n_1\, n_2\, \ldots\rangle = \frac{(a_1^\dagger)^{n_1}}{\sqrt{n_1!}} \frac{(a_2^\dagger)^{n_2}}{\sqrt{n_2!}} \ldots |0\rangle,$$

with $|0\rangle$ being the vacuum state, form an orthonormal basis for the Fock space. Show that the coefficients $C(n_1, n_2, \ldots)$ are given by

$$C(n_1, n_2, \ldots) = \frac{(\phi_1)^{n_1}}{\sqrt{n_1!}} \frac{(\phi_2)^{n_2}}{\sqrt{n_2!}} \ldots = \prod_i \frac{1}{\sqrt{n_i!}} (\phi_i)^{n_i}.$$

(b) Show that a boson coherent state assumes the form

$$|\phi\rangle = \exp(\sum_i \phi_i a_i^\dagger)|0\rangle.$$

(c) Show that the action of the creation operator $a_i^\dagger$ on a boson coherent state is given by

$$a_i^\dagger|\phi\rangle = \frac{\partial}{\partial\phi_i}|\phi\rangle.$$

(d) Show that the overlap between two boson coherent states $|\phi\rangle$ and $|\theta\rangle = \exp(\sum_i \theta_i a_i^\dagger)|0\rangle$ is given by

$$\langle\theta|\phi\rangle = \exp(\sum_i \theta_i^* \phi_i).$$

(e) Show that the closure relation assumes the form

$$\frac{1}{\pi}\int \prod_i d\,\mathrm{Re}\phi_i \; d\,\mathrm{Im}\phi_i \, e^{-\sum_i \phi_i^*\phi_i}|\phi\rangle\langle\phi| = \hat{1}, \tag{1}$$

where $\hat{1}$ is the unit operator in the Fock space. The closure relation (1) indicates that, indeed, the boson coherent states form an overcomplete basis for the Fock space.

(f) For a given operator A, show that

$$\mathrm{Tr}A = \sum_{n_1,n_2,\ldots} \langle n_1\, n_2\, \ldots|A|n_1\, n_2\, \ldots\rangle = \frac{1}{\pi}\int \prod_i d\,\mathrm{Re}\phi_i \; d\,\mathrm{Im}\phi_i \, e^{-\sum_i \phi_i^*\phi_i}\langle\phi|A|\phi\rangle.$$

(g) Consider an operator $A(a_i^\dagger, a_i)$ that is expand in terms of the creation and annihilation operators and that is in normal order. Show that the matrix element between two boson coherent states $|\phi\rangle$ and $|\theta\rangle$ assumes the form

$$\langle\phi|A(a_i^\dagger, a_i)|\theta\rangle = A\,(\phi_i^*, \theta_i)\, e^{\sum_i \phi_i^*\theta_i}.$$

Obs.: It is possible to introduce coherent states for fermion operators. In this case, the eigenvalues of the annihilation operators are not complex numbers, but Grassmann numbers. For more details, see, e.g., Sec. 4.1 from Altland and Simons and Sec. 1.5 from Negele and Orland.

03. P.1.4, Mahan: Diagonalization of a bosonic Hamiltonian.
Consider a system of bosons described by the Hamiltonian

$$H = E_0 a^\dagger a + F\left(a + a^\dagger\right),$$

where E_0 and F are constants and a and $a^\dagger$ are boson operators. The Hamiltonian H can be diagonalized with the aid of the transformation

$$\bar{H} = e^S H e^{-S} \qquad \text{and} \qquad S = \lambda\left(a - a^\dagger\right),$$

where λ is a constant.

(a) Show that $\lambda = \lambda^*$ in order that $\bar{H}$ is Hermitian.

(b) Determine $\bar{H}$ with the aid of the Baker-Hausdorff identity and show that only a few terms of the series are finite.

(c) Determine the constant λ in terms of the E_0 and F in order to reduce H to a diagonal form. Also, determine the ground state energy E_{GS} in terms of E_0 and F.

(d) Show that the ground state of the Hamiltonian is a boson coherent state $|\phi\rangle$, where $a|\phi\rangle = \phi|\phi\rangle$.

P.04. P.1.3, Mahan: Canonical transformation for bosons I.
Consider a system of bosons described by the Hamiltonian

$$H = \epsilon a^\dagger a + \frac{1}{2}\Delta\left(a^\dagger a^\dagger + aa\right),$$

where ϵ and Δ are constants and a and $a^\dagger$ are boson operators.

(a) Show that the Hamiltonian H can be written as

$$H = E_0 + \frac{1}{2}\epsilon\left(a^\dagger a + aa^\dagger\right) + \frac{1}{2}\Delta\left(a^\dagger a^\dagger + aa\right) \tag{2}$$

and determine the constant E_0 in terms of the parameter ϵ.

(b) Express the boson operator a in terms of new bosons operators b and $b^\dagger$,

$$a = ub + vb^\dagger \qquad \text{and} \qquad a^\dagger = ub^\dagger + vb, \tag{3}$$

where u and v are real constants. Determine the condition that the constants u and v should satisfy in order that the new boson operators b and $b^\dagger$ satisfy the commutation algebra of bosons. Such a condition indicates that the relation (3) is a canonical transformation. Note also that such condition allows us to write $u = \cosh\xi$ and $v = \sinh\xi$.

(c) Substitute the transformation (3) into the Hamiltonian (2) and determine the constants u and v in terms of ϵ and Δ such that H is now diagonal.

(d) Determine the condition that ground state of the system $|\Psi_0\rangle$ should satisfy. Determine the ground state energy E_{GS} and the energy ω of the boson b in terms of ϵ and Δ.

(e) Show also that $|\Psi_0\rangle$ can be written as

$$|\Psi_0\rangle = e^{\alpha a^\dagger a^\dagger}|0\rangle,$$

where $|0\rangle$ is the vacuum state for the boson a, i.e., $a|0\rangle = 0$, and α is a constant to be determined.

P.05. P.1.6, Miranda: Canonical transformation for bosons II.
A system of bosons is described by the following Hamiltonian

$$H = \epsilon\left(a^\dagger a + b^\dagger b\right) + \Delta\left(a^\dagger b^\dagger + ba\right),$$

where ϵ and Δ are constants and a and b are boson operators.

(a) Consider the transformation

$$\begin{aligned} c &= ua + vb^\dagger \\ d^\dagger &= va + ub^\dagger, \end{aligned} \tag{4}$$

where u and v are real constants. Determine the condition that the constants u and v should satisfy in order that the new operators c and d satisfy the commutation algebra of bosons. Such a condition indicates that the relation (4) is indeed a canonical transformation. Note also that this condition allows us to write $u = \cosh\xi$ and $v = \sinh\xi$.

(b) Show that the Hamiltonian H can be written as

$$H = E_0 + \epsilon\left(a^\dagger a + b\, b^\dagger\right) + \Delta\left(a^\dagger b^\dagger + ba\right) \tag{5}$$

and determine the constant E_0 in terms of the parameter ϵ.

(c) Determine the inverse of the transformation (4). Substitute the inverse transformation into the Hamiltonian (5) and determine the constants u and v in terms of ϵ and Δ such that H is now diagonal.

(d) Determine the condition that ground state of the system $|\Psi_0\rangle$ should satisfy. Also, determine the ground state energy E_{GS} and the energies $\omega_c = \omega_d = \omega$ of the new bosons c and d in terms of ϵ and Δ.

(e) Show that the canonical transformation (4) and the Hamiltonian (5) can be written in a matrix form,

$$\Psi = \mathbf{U}\Phi \qquad \text{and} \qquad H = E_0 + \Phi^\dagger \mathbf{h} \Phi,$$

where $\mathbf{U}$ and $\mathbf{h}$ are 2×2 matrices, and

$$\Phi = \begin{pmatrix} a \\ b^\dagger \end{pmatrix} \qquad \text{and} \qquad \Psi = \begin{pmatrix} c \\ d^\dagger \end{pmatrix}.$$

Determine the matrix $\mathbf{U}$ in terms of the coefficients u and v and the matrix $\mathbf{h}$ in terms of the parameters ϵ and Δ.

(f) Determine the coefficients λ_i of the expansion of the 2×2 matrix $\mathbf{h}$ in terms of the identity matrix $\mathbf{1}$ and the Pauli matrices $\boldsymbol{\sigma}_1$, $\boldsymbol{\sigma}_2$, and $\boldsymbol{\sigma}_3$, i.e., $\mathbf{h} = \lambda_0 \mathbf{1} + \sum_{i=1}^{3} \lambda_i \boldsymbol{\sigma}_i$.

(g) Show that the matrix $\mathbf{U}$ satisfy the relation $\mathbf{U}^\dagger \sigma_3 \mathbf{U} = \sigma_3 \to \mathbf{U}^\dagger \sigma_3 = \sigma_3 \mathbf{U}^{-1}$.

For further details about the diagonalization of bosonic Hamiltonians, see
J. H. P. Colpa, Physica A **93**, 327 (1978).

P.06. P.1.5, Miranda and P.3.2, Coleman: Canonical transformation for fermions.
A system of fermions is described by the following Hamiltonian

$$H = \epsilon \left(a^\dagger a + b^\dagger b \right) + \Delta \left(a^\dagger b^\dagger + ba \right),$$

where ϵ and Δ are constants and a and b are fermion operators.

(a) Consider the transformation

$$\begin{aligned} c &= ua + vb^\dagger \\ d^\dagger &= -va + ub^\dagger, \end{aligned} \tag{6}$$

where u and v are real constants. Determine the condition that the constants u and v should satisfy in order that the new operators c and d satisfy the anticommutation algebra of fermions. Such a condition indicates that the relation (4) is indeed a canonical transformation. Note also that this condition allows us to write $u = \cos\xi$ and $v = \sin\xi$.

(b) Show that the Hamiltonian H can be written as

$$H = E_0 + \epsilon \left(a^\dagger a + b\, b^\dagger \right) + \Delta \left(a^\dagger b^\dagger + ba \right) \tag{7}$$

and determine the constant E_0 in terms of the parameter ϵ.

(c) Determine the inverse of the transformation (6). Substitute the inverse transformation into the Hamiltonian (7) and determine the constants u and v in terms of ϵ and Δ such that H is now diagonal.

(d) Determine the condition that ground state of the system $|\Psi_0\rangle$ should satisfy. Also, determine the ground state energy E_{GS} and the energies $\omega_c = \omega_d = \omega$ of the new fermions c and d in terms of ϵ and Δ.

(e) Show that the inverse of the canonical transformation (6) and the Hamiltonian (7) can be written in a matrix form (Nambu spinor formulation),

$$\Psi = \mathbf{U}\Phi \qquad \text{and} \qquad H = E_0 + \Phi^\dagger \mathbf{h} \Phi,$$

where $\mathbf{U}$ and $\mathbf{h}$ are 2×2 matrices, and the Nambu spinors are defined as

$$\Phi = \begin{pmatrix} a \\ b^\dagger \end{pmatrix} \qquad \text{and} \qquad \Psi = \begin{pmatrix} c \\ d^\dagger \end{pmatrix}.$$

Determine the matrix $\mathbf{U}$ in terms of the coefficients u and v and the matrix $\mathbf{h}$ in terms of the parameters ϵ and Δ. Also, determine the coefficients λ_i of the expansion of the 2×2 matrix $\mathbf{h}$ in terms of the identity matrix $\mathbf{1}$ and the Pauli matrices $\boldsymbol{\sigma}_1$, $\boldsymbol{\sigma}_2$, and $\boldsymbol{\sigma}_3$.

(f) Show that the matrix $\mathbf{U}$ is unitary, i.e., the canonical transformation (6) is unitary.

(g) Show that

$$H = E_0 + \Psi^\dagger \mathbf{U}\mathbf{h}\mathbf{U}^\dagger \Phi \equiv E_0 + \Psi^\dagger \mathbf{h}' \Phi.$$

Determine the matrix $\mathbf{h}'$ in terms of ϵ, Δ, and the coefficients u and v and verify that $\mathbf{h}'$ is diagonal once the conditions determined in item (c) are satisfied.

For further details about the diagonalization of bosonic Hamiltonians, see
J. H. P. Colpa, Physica A **93**, 327 (1978).

07. P.1.6, Mahan: Tight-binding model I.
Consider a system of $N_e = N$ free spinless electrons hopping on the sites of a square lattice and described by the tight-binding model

$$H = -t \sum_{\langle i,j \rangle} \left(c_i^\dagger c_j + c_j^\dagger c_i \right) = -t \sum_{i,\delta} \left(c_i^\dagger c_{i+\delta} + c_{i+\delta}^\dagger c_i \right),$$

where t is the nearest-neighbor hopping energy, $c_i^\dagger$ and c_i respectively creates and destroys an electron on site i of the square lattice, and $\delta = a\hat{x}$ and $a\hat{y}$ are the nearest-neighbor vectors with a being the lattice spacing.

(a) Show that the fermion operators $c_{\mathbf{k}}^\dagger$ and $c_{\mathbf{k}}$, defined via the Fourier transform

$$c_i^\dagger = \frac{1}{N_s^{1/2}} \sum_{\mathbf{k} \in BZ} e^{-i\mathbf{k}\cdot\mathbf{R}_i} c_{\mathbf{k}}^\dagger,$$

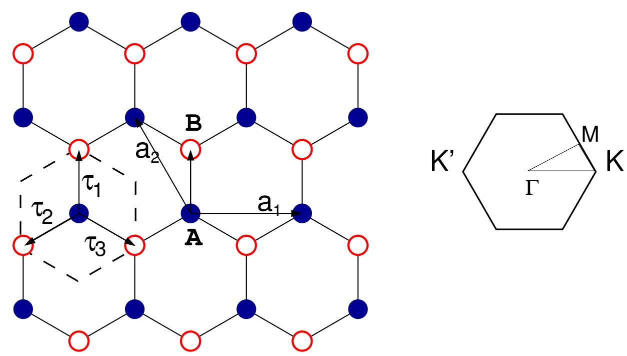
where $N_S = N$ is the number of sites of the square lattice and $\mathbf{R}_i$ is a vector of the square lattice, obey fermion anticommutation algebra.

(b) Show that the Hamiltonian H can be diagonalized with the aid of the above Fourier transform, i.e.,

$$H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}} c_{\mathbf{k}},$$

and determine the energy $\epsilon_{\mathbf{k}}$ of the electrons.
Hint: Identity $\sum_i e^{-i\mathbf{k}\cdot\mathbf{R}_i} = N_s \delta_{\mathbf{k},0}$.

P.08. P.1.6, Mahan: Tight-binding model for graphene.
Graphene is a single atomic layer of carbon arranged in a two-dimensional honeycomb lattice. The primitive vectors of the underline triangular lattice are $\mathbf{a}_1 = a(\sqrt{3}, 0)$ and $\mathbf{a}_2 = a\sqrt{3}/2(-1, \sqrt{3})$, where the carbon-carbon distance $a = 0.142\,\mathrm{nm}$, and the hexagonal unit cell [see dashed lines in the Fig. below] has two carbon atoms. In this atomic arrangement, the carbon atoms are connected by strong covalent σ-bonds, derived from the sp^2 hybridization of the atomic orbitals. The remaining p_z orbitals (perpendicular to the plane) have a weak overlap and form a narrow band, the so-called π-band, which crosses the Fermi level.



Consider that the kinetic energy of the π-electrons on the honeycomb lattice is described by the tight-binding model

$$H = \sum_i \left(\epsilon_A a^\dagger_i a_i + \epsilon_B b^\dagger_i b_i \right) + t \sum_i \sum_\tau \left(a^\dagger_i b_{i+\tau} + b^\dagger_{i+\tau} a_i \right), \tag{8}$$

where a_i and b_j are electron operators respectively associated with (triangular) sublattices A and B, t is the nearest-neighbor hopping amplitude, ϵ_A and ϵ_B are on-site energies of the sublattices A and B, respectively, and the index τ indicates the nearest-neighbor vectors $\boldsymbol{\tau}_1$, $\boldsymbol{\tau}_2$, and $\boldsymbol{\tau}_3$. [For more details, see, e.g., Goerbig, Rev. Mod Phys. **83**, 1193 (2011) and Kotov *et al.*, Rev. Mod. Phys. **84**, 1067 (2012)].

(a) Show that, after a Fourier transformation,

$$a_i^\dagger = \frac{1}{N_A^{1/2}} \sum_{\mathbf{q}\in BZ} e^{-i\mathbf{q}\cdot\mathbf{R}_i} a_{\mathbf{q}}^\dagger \qquad \text{and} \qquad b_i^\dagger = \frac{1}{N_B^{1/2}} \sum_{\mathbf{q}\in BZ} e^{-i\mathbf{q}\cdot\mathbf{R}_i} b_{\mathbf{q}}^\dagger,$$

where the number of sites of the sublattices A and B are $N_A = N_B = N$, the Hamiltonian (8) assumes the form

$$H = \sum_{\mathbf{q}} \left(a_{\mathbf{q}}^\dagger \, b_{\mathbf{q}}^\dagger\right) \begin{pmatrix} \epsilon_A & \gamma_{\mathbf{q}} \\ \gamma_{\mathbf{q}}^* & \epsilon_B \end{pmatrix} \begin{pmatrix} a_{\mathbf{q}} \\ b_{\mathbf{q}}^\dagger \end{pmatrix}, \tag{9}$$

with $\gamma_{\mathbf{q}} \equiv \sum_{\tau} \exp(i\mathbf{k}\cdot\boldsymbol{\tau})$.

(b) The Hamiltonian (9) can be diagonalized with the aid of the following transformation

$$a_{\mathbf{q}} = u_{\mathbf{q}}^\dagger c_{\mathbf{q}} + v_{\mathbf{q}} d \qquad\qquad \text{and} \qquad\qquad b_{\mathbf{q}} = v_{\mathbf{q}}^\dagger c_{\mathbf{q}} - u_{\mathbf{q}} d, \tag{10}$$

where the coefficients $u_{\mathbf{q}}$ and $v_{\mathbf{q}}$ are complex quantities. Determine the condition that the coefficients $u_{\mathbf{q}}$ and $v_{\mathbf{q}}$ should satisfy in order that the operators c and d satisfy the anticommutation algebra of fermions.

(c) Instead of the Hamiltonian (9), let us consider a general 2×2 fermionic Hamiltonian,

$$H = \sum_{\mathbf{q}} \Phi_{\mathbf{q}}^\dagger \mathbf{h}_{\mathbf{q}} \Phi_{\mathbf{q}}, \qquad \Phi_{\mathbf{q}}^\dagger = \left(a_{\mathbf{q}}^\dagger \;\; b_{\mathbf{q}}^\dagger\right), \qquad \mathbf{h}_{\mathbf{q}} = \lambda_{0,\mathbf{q}}\mathbf{1} + \sum_{i=1}^{3} \lambda_{i,\mathbf{q}}\boldsymbol{\sigma}_i, \tag{11}$$

with $\mathbf{1}$ being the identity matrix and $\boldsymbol{\sigma}_1$, $\boldsymbol{\sigma}_2$, and $\boldsymbol{\sigma}_3$ being the Pauli matrices. Show that the Hamiltonian (11) can be diagonalized by the canonical transformation (10) once the coefficients $u_{\mathbf{q}}$ and $v_{\mathbf{q}}$ are given by

$$|u_{\mathbf{q}}|^2, |v_{\mathbf{q}}|^2 = \frac{1}{2}\left(1 \pm \hat{\lambda}_3(\mathbf{q})\right), \qquad u_{\mathbf{q}} v_{\mathbf{q}}^\dagger = \frac{1}{2}\left(\hat{\lambda}_1(\mathbf{q}) + i\hat{\lambda}_2(\mathbf{q})\right),$$

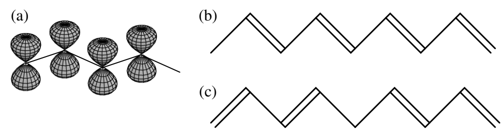
with $\hat{\lambda}_i(\mathbf{q}) = \lambda_i(\mathbf{q})/\sqrt{\lambda_1^2(\mathbf{q}) + \lambda_2^2(\mathbf{q}) + \lambda_3^2(\mathbf{q})}$. Determine the energies $\omega_c(\mathbf{q})$ and $\omega_d(\mathbf{q})$ of the fermions c and c in terms of the coefficients $\lambda_i(\mathbf{q})$.
Hint: It is useful to employ the matrix formalism discussed in Problem 06.

(d) Considering $\epsilon_A = \epsilon_B = 0$, determine the energies $\omega_c(\mathbf{q})$ and $\omega_d(\mathbf{q})$ of the π-electrons in graphene. Expand the dispersion relation in the vicinity of the K and K' points of the first Brioullin zone, show that $\omega_{c,d}(K+\mathbf{q}) \approx \pm v_F q$, and determine the Fermi-velocity v_F in terms of t and a. Here,

$$\boldsymbol{\tau}_1 = a(0,1), \qquad \boldsymbol{\tau}_2 = \frac{a}{2}(-\sqrt{3},-1), \qquad \boldsymbol{\tau}_3 = \frac{a}{2}(\sqrt{3},-1),$$

$$K, K' = \frac{4\pi}{(3\sqrt{3}a)}(\pm 1, 0).$$

09. P.2.x, Altland and Simons: Su-Shrieffer-Heeger (SSH) model for polyacetylene.
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 hybridized suggesting a planar configuration of the molecule. An unpaired electron is expected to occupy a single π-orbital which is oriented perpendicular to the plane. The weak overlap of the π-orbitals delocalize the electrons into a narrow conduction band. 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-dimensional system can always be lowered by imposing a periodic lattice distortion known as the Peierls instability. The aim of this problem is to explore such instability.



(a) At its simplest level, the conduction band of the polyacetylene chain can be modelled by a simple Hamiltonian (SSH model), where the hopping matrix elements of the electrons are modulated by the lattice distortion of the atoms. Taking the displacement for the atomic sites to be u_n, and treating their dynamics as classical, the effective Hamiltonian takes the form

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

where, for simplicity, the boundary conditions are taken to be periodic, and summation over the spins σ is assumed. The first term describes the hopping of electrons between neighbouring sites with a matrix element modulated by the periodic distortion of the bond-length. The last term represents the associated increase in the elastic energy. Taking the lattice distortion to be periodic, $u_n = (-1)^n \alpha$, the Hamiltonian assumes the form

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

Considering the number of sites to be even, diagonalize the Hamiltonian. Show that the Peierls distortion of the lattice opens a gap in the spectrum at the Fermi level of the half-filled system.
Hint: The Hamiltonian is most easily diagonalized by distinguishing the two sites of the sublattice, i.e., doubling the size of the elementary unit cell.

(b) By estimating the total electronic energy of the half filled band (which is just the sum over the eigenvalues of the first part, i.e., $\sum_k \epsilon_k \sim \int dk\ \epsilon_k$) and its elastic energy, show that the one-dimensional system is always unstable towards the Peierls distortion. To complete this calculation, you will need the approximate formula $\int_{-\pi/2}^{\pi/2} dk \sqrt{1 - (1-\alpha^2)\sin^2 k} \simeq 2 + (a_1 - b_1 \ln \alpha^2)\alpha^2 + O(\alpha^2 \ln \alpha^2)$, where a_1 and b_1 are (unspecified) numerical constants.

10. P.1.16, Mahan: Spin-wave theory for a Heisenberg ferromagnet.
Consider a ferromagnetic system of N localized spins S described by the Heisenberg model

$$H = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j,$$

where $\mathbf{S}_i$ is a spin operator associated with a spin S localized at site i of the lattice, the exchange constant $J > 0$, and $\langle i,j \rangle$ indicates that the sum is restricted to nearest-neighbor sites. The ferromagnetic Heisenberg model can be studied with the aid of the so-called the Holstein-Primakoff transformation,

$$S_i^+ = (2S - \hat{n}_i)^{1/2} a_i, \qquad S_i^- = a_i^\dagger (2S - \hat{n}_i)^{1/2}, \qquad S_i^z = S - \hat{n}_i,$$

where $S_i^\pm = S_i^x \pm i S_i^y$ and $\hat{n}_i = a_i^\dagger a_i$.

(a) Show that the commutation relations for the spin operators,

$$[S_i^z, S_j^+] = \delta_{i,j} S_i^+, \qquad [S_i^z, S_j^-] = -\delta_{i,j} S_i^-, \qquad [S_i^+, S_j^-] = 2\delta_{i,j} S_i^z,$$

are satisfied by the above bosonic representation.

(b) Express the Heisenberg Hamiltonian in terms of the boson operators a_i.

(c) At low temperatures, the Hamiltonian derived in item (b) can be simplified since $n_i = \langle \hat{n}_i \rangle \ll 2S$. Derive an approximate expression for the Hamiltonian up to second order in terms of the boson operators a_i (harmonic approximation).

(d) Show that the approximate Hamiltonian derived in item (c) can be diagonalized via a Fourier transformation, i.e.,

$$H = E_0 + \sum_{\mathbf{k}} \omega_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}},$$

and determine the constant E_0 and the energy $\omega_{\mathbf{k}}$ of the bosons $a_{\mathbf{k}}$ (magnons). Determine the ground-state of the system $|\Psi_0\rangle$ and the ground-state energy E_{GS}.

P.11. P.3.1, Miranda: Spin-wave theory for a Heisenberg antiferromagnet.
Consider a antiferromagnetic system of N localized spins S described by the Heisenberg model

$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \tag{12}$$

where $\mathbf{S}_i$ is a spin operator associated with a spin S localized at site i of a bipartite lattice (e.g., a square lattice), the exchange constant $J > 0$, and $\langle i, j \rangle$ indicates that the sum is restricted to nearest-neighbor sites. Similarly to the ferromagnetic system, the Heisenberg model (12) can be studied with the aid of the Holstein-Primakoff transformation.

(a) Let us consider the (semiclassical) Néel state as a reference state, where the spins S of the A sublattice points in the $+z$ direction while the ones of the B sublattice points in the $-z$ direction. It is interesting to introduce two Holstein-Primakoff transformations, one for each sublattice,

$$\begin{aligned} S^+_{i\,A} &= \left(2S - a^\dagger_i a_i\right)^{1/2} a_i, \quad S^-_{i\,A} = a^\dagger_i \left(2S - a^\dagger_i a_i\right)^{1/2}, \quad S^z_{i\,A} = S - a^\dagger_i a_i, \\ S^+_{i\,B} &= b^\dagger_i \left(2S - b^\dagger_i b_i\right)^{1/2}, \quad S^-_{i\,B} = \left(2S - b^\dagger_i b_i\right)^{1/2} b_i, \quad S^z_{i\,B} = -S + b^\dagger_i b_i, \end{aligned} \tag{13}$$

where $S^\pm_i = S^x_i \pm i S^y_i$ and a_i and b_i are two independent set of boson operators. For the A sublattice, show that the algebra of the spin operators,

$$[S^z_i, S^+_j] = \delta_{i,j} S^+_i, \qquad [S^z_i, S^-_j] = -\delta_{i,j} S^-_i, \qquad [S^+_i, S^-_j] = 2\delta_{i,j} S^z_i,$$

is satisfied by the bosonic representation (13).

(b) With the aid of the representation (13), express the Hamiltonian (12) up to quadratic order in the boson operators a_i and b_i.

(c) Show that, after a Fourier transformation,

$$a^\dagger_i = \frac{1}{N_A^{1/2}} \sum_{\mathbf{q} \in BZ} e^{-i\mathbf{q}\cdot\mathbf{R}_i} a^\dagger_{\mathbf{q}} \qquad \text{and} \qquad b^\dagger_i = \frac{1}{N_B^{1/2}} \sum_{\mathbf{q} \in BZ} e^{-i\mathbf{q}\cdot\mathbf{R}_i} b^\dagger_{\mathbf{q}},$$

where the number of sites of the sublattices A and B are $N_A = N_B = N$, the Hamiltonian (12) assumes the form

$$H = E_0 + \sum_{\mathbf{q}} \left(a^\dagger_{\mathbf{q}} \; b^\dagger_{-\mathbf{q}} \right) \left(\begin{array}{cc} 1 & \gamma_{\mathbf{q}} \\ \gamma_{\mathbf{q}} & 1 \end{array} \right) \left(\begin{array}{c} a_{\mathbf{q}} \\ b^\dagger_{-\mathbf{q}} \end{array} \right). \tag{14}$$

Here $\gamma_{\mathbf{q}} \equiv (1/z) \sum_\delta \exp(-i\mathbf{k} \cdot \boldsymbol{\delta})$, with the index δ indicating the z nearest-neighbor vectors $\boldsymbol{\delta}$ (e.g., for the square lattice, $z = 4$, since $\boldsymbol{\delta} = \pm a\hat{x}, \pm a\hat{y}$, with a being the lattice spacing).

(d) Diagonalize the Hamiltonian (14) with the aid of a canonical transformation and show that the energy of the excitations (spin waves) are given by

$$\omega_{\mathbf{q}} = 2JSz(1-\gamma_{\mathbf{q}}^2)^{1/2},$$

while the ground state energy assumes the form

$$E_{GS} = -2NzJS(S+1) + 2JSz\sum_{\mathbf{q}\in BZ}(1-\gamma_{\mathbf{q}}^2)^{1/2}.$$

Consider a cubic lattice ($z=6$), and expand $\omega_{\mathbf{q}}$ for small qa, where a is the lattice spacing, and compare the result with the equivalent for a ferromagnet.

(e) Determine the deviation of the maximum value of the sublattice magnetization,

$$\Delta S_a^z = NS - \langle\Psi_0|\sum_{i\in a} S_{i\,a}^z|\Psi_0\rangle,$$

with $a = A$, B, for the ground state $|\Psi_0\rangle$.
It is not necessary to calculate the sum, express ΔS_a^z as the ground state energy E_{GS}.

(f) Consider a three-dimensional system at low temperatures and determine the behaviour of the specific heat with the temperature T. In this case, it is interesting to replace the sum by a continuous integral.

12. P.1.3, Fetter and Walecka:
Given a homogeneous system of spin-zero particles interacting through a potential $V(\mathbf{r})$:

(a) Show that the expectation value of the Hamiltonian in the noninteracting ground state is

$$\frac{E^{(1)}}{N} = \frac{1}{2V}(N-1)V(0) \approx \frac{1}{2}nV(0), \qquad \text{where} \qquad V(\mathbf{q}) = \int d^3r V(\mathbf{r})e^{-i\mathbf{q}\cdot\mathbf{r}}$$

and $V(0)$ means $V(\mathbf{q}=0)$.

(b) Assume $V(r)$ is central and spin independent. If $V(|\mathbf{r}_1-\mathbf{r}_2|) < 0$ for all $|\mathbf{r}_1-\mathbf{r}_2|$ and $\int d^3r|V(r)| < \infty$, prove that the system will collapse.
Hint: Start from $E^{(1)}/N$ as a function of density.

(c) Show that the second-order contribution to the ground state energy is

$$\frac{E^{(2)}}{N} = -\frac{N-1}{2V}\int\frac{d^3q}{(2\pi)^3}\frac{|V(\mathbf{q})|^2}{\hbar^2q^2/m} \approx -\frac{n}{2}\int\frac{d^3q}{(2\pi)^3}\frac{|V(\mathbf{q})|^2}{\hbar^2q^2/m}.$$

Hint: see pg. 31, Fetter.

P.13. P.1.4, Fetter and Walecka:
Show that the second-order contribution to the ground state energy of an electron gas is given by

$$E^{(2)} = \frac{Ne^2}{2a_0}\left(\epsilon_2^r + \epsilon_2^b\right),$$

where

$$\epsilon_2^r = -\frac{3}{8\pi^5}\int \frac{d^3q}{q^4}\int_{|\mathbf{k}+\mathbf{q}|>1} d^3k \int_{|\mathbf{p}+\mathbf{q}|>1} d^3p\, \frac{\theta(1-k)\theta(1-p)}{\mathbf{q}^2+\mathbf{q}\cdot(\mathbf{k}+\mathbf{p})},$$

$$\epsilon_2^b = \frac{3}{16\pi^5}\int \frac{d^3q}{q^2}\int_{|\mathbf{k}+\mathbf{q}|>1} d^3k \int_{|\mathbf{p}+\mathbf{q}|>1} d^3p\, \frac{\theta(1-k)\theta(1-p)}{(\mathbf{q}+\mathbf{k}+\mathbf{p})^2[\mathbf{q}^2+\mathbf{q}\cdot(\mathbf{k}+\mathbf{p})]}.$$

Hint: see pg. 31, Fetter.

14. P.1.6, Fetter and Walecka:
Consider a polarized electron gas in which N_+ and N_- denote the number of electrons with spin-up and spin-down, respectively.

(a) Find the ground-state energy to first order in the interaction potential as a function of $N = N_+ + N_-$ and the polarization $\zeta = (N_+ - N_-)/N$.

(b) Prove that the ferromagnetic state ($\zeta = 1$) represents a lower energy than the unmagnetized state ($\zeta = 0$) if $r_s > (2\pi/5)(9\pi/4)^{1/3}(2^{1/3}+1) = 5.45$. Explain why this is so.

(c) Show that $\partial^2(E/N)/\partial\zeta^2|_{\zeta=0}$ becomes negative for $r_s > (3\pi^2/2)^{2/3} = 6.03$.

(d) Discuss the physical significance of the two critical densities. What happens for $5.45 < r_s < 6.03$?