1) Green function for noninteracting bosons: Consider noninteracting spinless bosons in a cube of volume V with periodic boundary conditions. The hamiltonian H is given by $H = \sum_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}}\, \epsilon_{\mathbf{k}}$.

a) Evaluate $[a_{\mathbf{k}}, H]$ and $[a_{\mathbf{k}}^{\dagger}, H]$.

b) Use your results from part (a) to obtain the Heisenberg operators $a_{\mathbf{k}}(t)$ and $a_{\mathbf{k}}^{\dagger}(t)$.

Define the noninteracting-boson Green function $G(\mathbf{p}, t, \mathbf{p}', t')$ through

$$G(\mathbf{p}, t, \mathbf{p}', t') = -i\langle 0|\, T\, a_{\mathbf{p}}(t)\, a_{\mathbf{p}'}^{\dagger}(t')\, |0\rangle,$$

where T is the time-ordering operator (which puts the later operator to the left).

c) Show that the $G(\mathbf{p}, t, \mathbf{p}', t')$ satisfies

$$i\partial_t G(\mathbf{p}, t, \mathbf{p}', t') = \hbar^{-1} \epsilon_{\mathbf{p}}\, G(\mathbf{p}, t, \mathbf{p}', t') + \delta(t - t')\, \delta_{\mathbf{p}\mathbf{p}'}.$$

d) **(optional)** By considering its definition, discuss the physical meaning of the Green function in terms of the inner product of two states, each built by adding a boson to the vacuum at some instant.

2) Hartree-Fock method – optional: For all but an extremely small set of cases, it is impossible to find the eigenstates and eigenfunctions for a system of interacting particles. Thus, to make progress, approximation schemes are required. The Hartree-Fock method is one such approximate method for finding energy eigenstates and eigenvalues for systems of interacting fermions. The essence of the method is to find a single-particle basis $\{|\mu\rangle\}$, and thus a set of single-particle creation operators $\{b_{\mu}^{\dagger}\}$, so that the state

$$|\Psi\rangle = b_1^{\dagger} b_2^{\dagger} \cdots b_N^{\dagger} |0\rangle$$

renders the expectation value of the hamiltonian stationary with respect to variations of the single-particle basis. Said another way, we are finding the unitary transformation (*e.g.*, from free particles) that best incorporates the effect of the interactions. You should regard $|\Psi\rangle$ as being a variational state vector with the variational parameters being the orthonormal set of single-particle states.

By following the steps outlined below we will explore the Hartree-Fock approximation. The hamiltonian that we shall consider is

$$\mathcal{H} = \sum_{\mu\nu} b_{\mu}^{\dagger}\, b_{\nu}\, \langle \mu|\mathcal{H}^0|\nu\rangle + \frac{1}{2} \sum_{\mu\nu\rho\sigma} b_{\mu}^{\dagger}\, b_{\nu}^{\dagger}\, b_{\rho}\, b_{\sigma}\, (\mu\nu|W|\sigma\rho)\,.$$

As usual, we shall search for stationary points by requiring that a first order variation vanishes (*c.f.* the calculus of variations). In this case, the variation is in each of the occupied single-particle states that are used to build up the many-particle ground state.

a) First we consider the independent variations of $|\Psi\rangle$. Show that under variations of the basis, the *independent* variations of $|\Psi\rangle$ are $|\delta\Psi_{\mu\nu}\rangle = \epsilon_{\mu\nu} b^\dagger_\mu b_\nu |\Psi\rangle$ with $\epsilon_{\mu\nu}$ complex, and $|\epsilon_{\mu\nu}| \ll 1$, and where $\mu = N+1, N+2, \ldots$ (*i.e.*, unoccupied) and $\nu = 1, 2, \ldots, N$ (*i.e.*, occupied).

b) Show that as $|\Psi\rangle \to |\Psi\rangle + |\delta\Psi_{\mu\nu}\rangle$ is norm-preserving, the condition that $\langle\Psi|\mathcal{H}|\Psi\rangle/\langle\Psi|\Psi\rangle$ be stationary implies that $\langle\delta\Psi_{\mu\nu}|\mathcal{H}|\Psi\rangle = 0$.

c) Show that, for the present system, the stationarity condition becomes

$$\langle\mu|\mathcal{H}^0|\nu\rangle + \sum\nolimits_\lambda \{(\mu\lambda|W|\nu\lambda) - (\mu\lambda|W|\lambda\nu)\} = 0,$$

where μ is an unoccupied state, ν is occupied, and $\sum_\lambda$ runs over occupied states.

d) Suppose that there exists a basis $\{|i\rangle\}$ in which W is diagonal, *i.e.*, $(ij|W|kl) = W_{ij}\,\delta_{ik}\,\delta_{jl}$. Show that your solution to part (c) can be construed as expressing the orthogonality of the eigenkets of the effective one-particle eigenproblem $\tilde{\mathcal{H}}|\nu\rangle = \epsilon_\nu|\nu\rangle$, where the effective Hartree-Fock hamiltonian $\tilde{\mathcal{H}}$ is given by

$$\tilde{\mathcal{H}} = \mathcal{H}^0 + \sum_\lambda \sum_{ij} |i\rangle\langle\lambda|j\rangle V_{ij}\langle j|\lambda\rangle\langle i| - \sum_\lambda \sum_{ij} |i\rangle\langle\lambda|j\rangle V_{ij}\langle i|\lambda\rangle\langle j|,$$

and where $\sum_\lambda$ runs over occupied states only.

e) Thus, show that

$$\begin{aligned}\epsilon_\nu &= \langle\nu|\tilde{\mathcal{H}}|\nu\rangle \\ &= \langle\nu|\mathcal{H}^0|\nu\rangle + \sum_\lambda \sum_{ij}\langle\nu|i\rangle\langle\lambda|j\rangle V_{ij}\langle j|\lambda\rangle\langle i|\nu\rangle - \sum_\lambda \sum_{ij}\langle\nu|i\rangle\langle\lambda|j\rangle V_{ij}\langle i|\lambda\rangle\langle j|\nu\rangle.\end{aligned}$$

Notice that the Hartree-Fock energy $\langle\Psi|\mathcal{H}|\Psi\rangle$ is *not* simply the sum of the Hartree-Fock one-particle energies ϵ_ν. Thus, it is not necessarily true that the Hartree-Fock ground state will correspond to the occupation of N lowest values of ϵ_ν.

f) To see this, show that the expectation value of the energy in the Hartree-Fock state, *i.e.*, the Hartree-Fock energy, is given by

$$E_{\mathrm{HF}} = \langle\Psi|\mathcal{H}|\Psi\rangle = \sum_{\lambda=1}^{N} \epsilon_\lambda - \frac{1}{2}\sum_{\lambda,\sigma=1}^{N} \{(\lambda\sigma|W|\lambda\sigma) - (\lambda\sigma|W|\sigma\lambda)\}\,.$$

3) Cooper pairs: Let us explore Cooper's problem, the problem of one-pair of electrons interacting with one another outside a *quiescent* Fermi sea. The only role played by the Fermi sea is that, via the Pauli exclusion principle, it blocks the two electrons of the pair from occupying any of the single-particle states within the sea. Dynamical interactions involving one or more electrons in the Fermi sea are neglected. Our aim is to solve the corresponding energy eigenproblem

We shall take the interaction between the members of the pair to be translationally invariant and spin-independent. Thus, the eigenstates can be characterized by sharp values of the total momentum and total spin. Let us focus on the spin-singlet state, which is antisymmetric in spin indices; the corresponding orbital factor must then be symmetric in orbital coordinates.

a) Explain why the orbital factor $\Psi(\mathbf{r}_1, \mathbf{r}_2)$ can be taken to have the form

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \Phi_{\mathbf{Q}}(\mathbf{r}) \exp i\mathbf{Q} \cdot \mathbf{R}\,,$$

where the relative coordinate $\mathbf{r}$ is $\mathbf{r}_1 - \mathbf{r}_2$, the centre of mass $\mathbf{R}$ is $(\mathbf{r}_1 + \mathbf{r}_2)/2$, and the total momentum is $\mathbf{Q}$.

Let us express the relative orbital factor $\Phi_{\mathbf{Q}}(\mathbf{r}_1 - \mathbf{r}_2)$ in terms of the amplitudes $A_{\mathbf{k}}(\mathbf{Q})$:

$$\Phi_{\mathbf{Q}}(\mathbf{r}) = \sum_{\mathbf{k}(k>k_{\mathrm{F}})} A_{\mathbf{k}}(\mathbf{Q}) \exp i\mathbf{k} \cdot \mathbf{r}\,.$$

b) Focusing on the $\mathbf{Q} = \mathbf{0}$ eigenstate, show that the amplitudes $a_{\mathbf{k}}$ $[\equiv A_{\mathbf{k}}(\mathbf{0})]$ obey the energy eigenproblem

$$2\epsilon_{\mathbf{k}}\, a_{\mathbf{k}} + \sum_{\mathbf{k}'(k'>k_{\mathrm{F}})} V_{\mathbf{k},\mathbf{k}'}\, a_{\mathbf{k}'} = E\, a_{\mathbf{k}}\,,$$

where the interaction between the pair is characterized by the scattering matrix elements $V_{\mathbf{k},\mathbf{k}'} = (\mathbf{k}, -\mathbf{k}|V|\mathbf{k}', -\mathbf{k}')$, the quantity $\epsilon_{\mathbf{k}}$ is the free-particle dispersion relation, and E is the energy eigenvalue.

c) To obtain a solvable situation, let us take the interaction to be factorizable:

$$V_{\mathbf{k},\mathbf{k}'} = \Lambda\, U_{\mathbf{k}}\, U^*_{\mathbf{k}'}\,.$$

Show that the energy eigenvalues obey

$$\frac{1}{\Lambda} = \sum_{\mathbf{k}(k>k_{\mathrm{F}})} \frac{|U_{\mathbf{k}}|^2}{E - 2\epsilon_{\mathbf{k}}}\,.$$

d) Recall that the system is large but finite, so that the single-particle energy levels are discrete. By sketching the left and right hand sides of this equation as a function of the eigenvalue E, show that attractive ($\Lambda < 0$) interactions lead to a bound (negative energy) state, split off from the spectrum, whereas repulsive ($\Lambda > 0$) interactions do not.

e) Let us further take the interaction to be confined to a limited range of energies:

$$U_{\mathbf{k}} = \begin{cases} 1, & \text{for } E_{\mathrm{F}} < \epsilon_{\mathbf{k}} < E_{\mathrm{F}} + \epsilon_{\mathrm{c}}, \\ 0, & \text{otherwise,} \end{cases}$$

where ϵ_{c} parametrizes the range. Show that the bound-state energy is given by

$$E = 2E_{\mathrm{F}} - \frac{2\epsilon_{\mathrm{c}}}{\exp[2/|\Lambda|N(E_{\mathrm{F}})] - 1} \approx 2E_{\mathrm{F}} - 2\,\epsilon_{\mathrm{c}}\,\mathrm{e}^{-2/|\Lambda|N(E_{\mathrm{F}})},$$

where $N(E_{\mathrm{F}})$ is the density of states at the Fermi energy, which we assume varies slowly on the scale ϵ_{c}, and the approximate result occurs for the weak-coupling case, $|\Lambda|N(E_{\mathrm{F}}) \ll 1$. Discuss briefly why this result cannot be obtained via perturbation theory

It can be shown that the energy $E_{\mathbf{Q}}$ of the bound state with nonzero momentum $\mathbf{Q}$ varies, for small $\mathbf{Q}$, as

$$|E_{\mathbf{Q}}| = |E_{\mathbf{0}}| - \frac{1}{2} v_{\mathrm{F}} \hbar\, |\mathbf{Q}|,$$

where v_{F} is the Fermi velocity. Note that this is a linear rise in the energy, with Q. Assuming $E_{\mathbf{0}}$ to be of order $k_{\mathrm{B}}T_{\mathrm{c}}$ (where k_{B} is Boltzmann's constant and T_{c} is the superconducting transition temperature), the bound state has lost most of its binding energy when $Q \sim k_{\mathrm{B}}T_{\mathrm{c}}/\hbar v_{\mathrm{F}}$. This gives a length-scale $\xi_0 \sim \hbar v_{\mathrm{F}}/k_{\mathrm{B}}T_{\mathrm{c}} \sim E_{\mathrm{F}}/k_{\mathrm{B}}T_{\mathrm{c}}$, the superconducting coherence length, which gives the size-scale of the Cooper wave function. For $T_{\mathrm{c}} \approx 2\,\mathrm{K}$ and $v_{\mathrm{F}} \approx 10^6\,\mathrm{m\,s^{-1}}$, one finds $\xi_0 \sim 10^{-6}\,\mathrm{m}$.

4) Weakly interacting boson gas – optional: The purpose of this question is to follow Bogoliubov's approach to the issue of Bose-Einstein condensation in a weakly interacting boson gas. Although this approach is only of qualitative value for the context in which is was developed, namely the superfluidity of ^{4}He, it has quantitative validity for the context of Bose-Einstein condensation in atomic gases.

Consider a large cubic container of volume V, containing a large number N of identical, non-interacting, free, spinless, bosons, each of mass m. Impose periodic boundary conditions on the box. Choose the set of momentum eigenstates $\{|\mathbf{p}\rangle\}$ as the set of single-particle state vectors from which is built a basis for the space of physical many-boson states.

a) Write down the wave functions $\langle \mathbf{r}|\mathbf{p}\rangle$ corresponding to the single-particle state vectors $|\mathbf{p}\rangle$. What values can the momenta take?

b) What extra requirement must the state vector for a system of many bosons satisfy if the bosons are identical?

c) Write down the hamiltonian for this system of free bosons in terms of the creation and annihilation operators $a^\dagger_{\mathbf{p}}$ and $a_{\mathbf{p}}$.

d) What commutation relations do these creation and annihilation operators satisfy?

f) Write down the normalised ground state vector for the system of bosons in terms of occupation number representation kets; and

g) Write it down in terms of operators acting on the vacuum state vector.

h) Write down the many-body wave function in real space for this normalised ground state.

i) Write down the energy of this normalised many-body ground state.

j) Write down the occupation number of the *lowest* single-particle state when the many-boson system is in this non-interacting ground state.

k) Write down the occupation numbers for the remaining single-particle states.

For the non-interacting system, the elementary excitation spectrum is defined as the collection of possible values by which the total energy of an N-boson state is raised above the N-boson ground state when two occupation numbers each differ by unity from those of the N-boson ground state.

l) Give the elementary excitation spectrum for the present system.

Now consider the effect of a weak repulsion between pairs of bosons. Our aim is to describe the effect of this interaction on the ground state and the elementary excitation spectrum of this N-boson system. Note that you do not need any prior knowledge about interacting boson systems, Bose-Einstein condensation, or superfluidity to address this problem.

m) Write down the most general operator describing pairwise boson interactions, in terms of the creation and annihilation operators, carefully defining any symbols you introduce.

A simplified model of interacting bosons is described by the hamiltonian $\mathcal{H}$ that includes, in addition to your answer to part (c), a term describing boson-boson repulsion:

$$\mathcal{H}_{\text{int}} = \frac{U}{2V} \sum_{\substack{\mathbf{p}_1\,\mathbf{p}_2\,\mathbf{p}_3\,\mathbf{p}_4 \\ (\mathbf{p}_1+\mathbf{p}_2=\mathbf{p}_3+\mathbf{p}_4)}} a^\dagger_{\mathbf{p}_4}\, a^\dagger_{\mathbf{p}_3}\, a_{\mathbf{p}_2}\, a_{\mathbf{p}_1}.$$

n) What form should the interaction matrix elements take in order to reproduce this term?

o) Explain the physical content of the constraint on the summation over momenta?

To investigate the impact of this interaction term we shall make two related assumptions:

[i] that the ground state of the *interacting system* is similar to that of the non-interacting system, in the sense that the fraction of bosons occupying the single-particle ground state remains close to unity whilst the total fraction occupying all the remaining single-particle states is small; and

[ii] that as the occupation of the ground state is a large number, of order N, we may treat the creation and annihilation operators associated with the lowest single-particle state as *commuting variables rather than quantum mechanical operators*.

To use these assumptions, recall that $a^\dagger_{\mathbf{0}} a_{\mathbf{0}} = N_{\mathbf{0}}$, and make the replacement

$$\begin{aligned} a^\dagger_{\mathbf{0}} &\rightarrow \sqrt{N_{\mathbf{0}}}, \\ a_{\mathbf{0}} &\rightarrow \sqrt{N_{\mathbf{0}}}, \end{aligned}$$

where $N_{\mathbf{0}}$ is the occupation of the lowest single-particle state in the many-boson ground state.

p) What physical assumption are we making about the quantum mechanical fluctuations in this state of the observable $a^\dagger_{\mathbf{0}} a_{\mathbf{0}}$?

q) In the given interaction term $\mathcal{H}_{\text{int}}$ eliminate the operators $a^\dagger_{\mathbf{0}}$ and $a_{\mathbf{0}}$ in favour of the (as yet unknown) occupation of the lowest single-particle state $N_{\mathbf{0}}$ using $a^\dagger_{\mathbf{0}} \rightarrow \sqrt{N_{\mathbf{0}}}$ and $a_{\mathbf{0}} \rightarrow \sqrt{N_{\mathbf{0}}}$, *retaining only terms of order $N_{\mathbf{0}}$ or greater*. Write down the complete hamiltonian that you obtain using this scheme.

The next step is to eliminate the unknown occupation number $N_{\mathbf{0}}$ in favour of the known total particle-number N. To do this, recall that

$$N = N_{\mathbf{0}} + \sum\nolimits'_{\mathbf{p}} a^\dagger_{\mathbf{p}} a_{\mathbf{p}},$$

where the prime on the sum denotes the omission of the $\mathbf{p} = \mathbf{0}$ term.

r) Use this equation to eliminate $N_{\mathbf{0}}$ from the hamiltonian that you have given as the answer to part (q). In doing this, treat N and $N_{\mathbf{0}}$ as *large quantities*, and their difference as *a small quantity*, consistent with assumption (i). By retaining only terms of order N or greater, show that the hamiltonian that results is

$$\mathcal{H} = \frac{UN^2}{2V} + \sum\nolimits_{\mathbf{p}}' \left(\frac{p^2}{2m} + \frac{UN}{V}\right) a^\dagger_{\mathbf{p}} a_{\mathbf{p}} + \frac{UN}{2V} \sum\nolimits_{\mathbf{p}}' \left(a^\dagger_{\mathbf{p}} a^\dagger_{-\mathbf{p}} + a_{\mathbf{p}} a_{-\mathbf{p}}\right).$$

Discuss the nature of the terms in this hamiltonian. Are there interactions? Is the problem a single- or a many-particle problem?

Finally, we make a transformation (known as a Bogoliubov transformation) to diagonalise the hamiltonian given in part (r). To do this we introduce new operators $b_{\mathbf{p}}$ and $b^\dagger_{\mathbf{p}}$ such that

$$\begin{aligned} a_{\mathbf{p}} \quad &\equiv u_{\mathbf{p}} b_{\mathbf{p}} + v_{\mathbf{p}} b^\dagger_{-\mathbf{p}} \\ a^\dagger_{\mathbf{p}} \quad &\equiv u_{\mathbf{p}} b^\dagger_{\mathbf{p}} + v_{\mathbf{p}} b_{-\mathbf{p}}. \end{aligned}$$

The parameters $u_{\mathbf{p}}$ and $v_{\mathbf{p}}$ are real, satisfy $u_{\mathbf{p}} = u_{-\mathbf{p}}$ and $v_{\mathbf{p}} = v_{-\mathbf{p}}$, and otherwise are as-yet arbitrary.

s) If the operators $b^\dagger_{\mathbf{p}}$ and $b_{\mathbf{p}}$ also create and annihilate bosons, what constraint must $u_{\mathbf{p}}$ and $v_{\mathbf{p}}$ satisfy?

t) Show that by choosing $u_{\mathbf{p}}$ and $v_{\mathbf{p}}$ to satisfy

$$\left(\frac{p^2}{2m} + \frac{UN}{V}\right) u_{\mathbf{p}} v_{\mathbf{p}} + \left(\frac{UN}{2V}\right)\left(u^2_{\mathbf{p}} + v^2_{\mathbf{p}}\right) = 0$$

the hamiltonian acquires the diagonal form

$$\mathcal{H} = E_0 + \sum\nolimits_{\mathbf{p}}' \hat{\epsilon}(\mathbf{p})\, b^\dagger_{\mathbf{p}} b_{\mathbf{p}}.$$

State the appropriate forms of E_0 and $\hat{\epsilon}(\mathbf{p})$ in terms of $u_{\mathbf{p}}$ and $v_{\mathbf{p}}$.

u) By introducing $t_{\mathbf{p}} \equiv v_{\mathbf{p}}/u_{\mathbf{p}}$ show that the condition on $u_{\mathbf{p}}$ and $v_{\mathbf{p}}$ given in part (t) amounts to choosing

$$t_{\mathbf{p}} = -1 - \frac{(p^2/2m)}{UN/V} + \frac{\epsilon(\mathbf{p})}{UN/V},$$

where

$$\epsilon(\mathbf{p}) = \sqrt{\left(\frac{p^2}{2m}\right)^2 + \left(\frac{p^2}{m}\right)\left(\frac{UN}{V}\right)}.$$

v) Show that $\hat{\epsilon}(\mathbf{p}) = \epsilon(\mathbf{p})$. Discuss the nature of the elementary excitation spectrum for this system of interacting bosons, and compare it with that of noninteracting bosons.