A18533H1

Honour School of Mathematical and Theoretical Physics Part C
Master of Science in Mathematical and Theoretical Physics

Quantum Matter

Trinity Term 2025

Thursday 24th April 9:30-11:30am

This exam paper consists of two questions, each marked out of 25. You must answer both questions.
You must start a new booklet for each question which you attempt. Indicate on the front sheet the numbers of the questions attempted. A booklet with the front sheet completed must be handed in even if no question has been attempted.

The numbers in the margin indicate the weight that the Examiners anticipate assigning to each part of the question

Do not turn this page until you are told that you may do so

1. In this question we consider electrons hopping on a one-dimensional tight binding chain with M sites and periodic boundary conditions. The interaction is between nearest-neighbor sites and is only nonzero when the spins between two electrons are aligned either both spin-up or both spin-down. We write the Hamiltonian more formally as

$$H = \sum_{j=1}^{M} \sum_{\sigma=\uparrow,\downarrow} \left[-t \left(c^\dagger_{\sigma,j+1} c_{\sigma,j} + c^\dagger_{\sigma,j} c_{\sigma,j+1} \right) + V n_{\sigma,j} n_{\sigma,j+1} \right] \quad ,$$

where $n_{\sigma,j} = c^\dagger_{\sigma,j} c_{\sigma,j}$, and because of the periodic boundary conditions we understand site $j = M + 1$ to be the same as site $j = 1$. The coefficients V and t may have either sign. We can assume the number of sites M is large.

(a) [3 marks] Explain briefly (two sentences or less) what the Hartree-Fock approximation is for a ground state wavefunction.

Define the Fourier transform of the $c^\dagger_{\sigma,j}$ creation operators as

$$\tilde{c}^\dagger_{\sigma,k} = \frac{1}{\sqrt{M}} \sum_{j=1}^{M} e^{ikj} c^\dagger_{\sigma,j} \quad . \tag{1}$$

(b) [7 marks] Determine the possible values of k in Eq. 1. Rewrite the Hamiltonian in terms of the $\tilde{c}^\dagger_{\sigma,k}$ operators and the corresponding annihilation operators.

(c) [6 marks] Fill a noninteracting Fermi sea with $N_\uparrow$ spin-up electrons and $N_\downarrow$ spin-down electrons. We use this state as a trial wavefunction here and in part (d) below. Determine the expectation of H as a function of $N_\uparrow$ and $N_\downarrow$.

(d) [5 marks] Let the total number of electrons be the same as the number of sites in the system, $N = N_\uparrow + N_\downarrow = M$. Let $x = N_\uparrow / N$ be the fraction of spin-up electrons, and calculate the total energy of the system as a function of x. Determine which values of $V/|t|$ result in $x = 0$ being a local minimum. Show that $x = \frac{1}{2}$ is always a local extremum. Determine which values of $V/|t|$ result in $x = \frac{1}{2}$ being a local minimum. Sketch x in the ground state as a function of $V/|t|$ within this approximation.

(e) [4 marks] Again assuming $N = M$, consider the limit of $V/|t| \gg 1$. Explain why a Fermi sea trial state is extremely inaccurate in this limit. Describe the actual ground states. You may assume M is even.

2. Consider N spinless bosons of mass m in two dimensions in a harmonic trapping potential $V(\mathbf{r}) = \frac{1}{2}\kappa|\mathbf{r}|^2$ with $\kappa > 0$. The non-interacting boson Hamiltonian is given by

$$H_0 = \sum_{j=1}^{N} \left[\frac{\mathbf{p}_j^2}{2m} + \frac{1}{2}\kappa|\mathbf{r}_j|^2 \right] \qquad ,$$

where $\mathbf{p}_j$ and $\mathbf{r}_j$ are the momentum and position operators for particle j. The oscillation frequency is $\omega = \sqrt{\kappa/m}$. For this problem, N can be assumed to be large, and the density of states can be approximated as $D(E) = E/(\hbar\omega)^2$ states per unit energy for $E \geqslant 0$ (and $D(E) = 0$ for $E < 0$). The ground state single-particle wavefunction is given by $(\ell\sqrt{\pi})^{-1}\exp[-|\mathbf{r}|^2/(2\ell^2)]$ with $\ell^2 = \hbar/\sqrt{\kappa m}$.

(a) [5 marks] Show that this system undergoes a Bose-Einstein condensation transition. Write an expression that relates the density of bosons to the critical temperature T_c. Determine how many bosons are in the condensate as a function of temperature. The integral provided below might be useful.

(b) [7 marks] Let $\psi^\dagger(\mathbf{r})$ and $\psi(\mathbf{r})$ be boson creation and annihilation operators respectively. Calculate the correlation function $\langle\psi^\dagger(\mathbf{0})\psi(\mathbf{r})\rangle$ at zero temperature. Sketch this correlation function as a function of $|\mathbf{r}|$ for temperature $T = 0$. Sketch this correlation function for $0 < T < T_c$, and for $T > T_c$. You do not need to do a complete calculation, but you should be as accurate as you can with your sketch. What is the interpretation of the value of this correlation function at $\mathbf{r} = 0$? For $T \gg T_c$ what is the approximate width of the peak?

We now add an interaction term U and a chemical potential μ. Let $H = H_0 + U - \mu\hat{N}$ where

$$U = \sum_{i<j} g\,\delta(\mathbf{r}_i - \mathbf{r}_j) \qquad .$$

Here $\hat{N}$ is the number operator, $\delta()$ is a two-dimensional delta function, and $g > 0$ is an interaction strength.

(c) [5 marks] Consider a normalized single-particle orbital $\phi(\mathbf{r})$ which we fill with N bosons. Write an appropriate many-boson wavefunction. Write an expression for the expectation value of H as a functional of the orbital ϕ. By varying with respect to ϕ, or otherwise, derive a Gross-Pitaevskii equation (or nonlinear Schroedinger equation) for ϕ.

(d) [4 marks] Assume that the kinetic term of the Gross-Pitaevskii equation can be dropped. Solve for the density as a function of position. At what radius does the density drop to zero? Solve for the relationship between the chemical potential μ and the density N. At what radius is the approximation of dropping the kinetic energy most accurate? At what radius is this approximation the worst?

(e) [4 marks] Sketch $\langle\psi^\dagger(\mathbf{0})\psi(\mathbf{r})\rangle$ for the solution to the Gross-Pitaevskii equation at zero temperature. Your result is only an approximation of the exact correlation function for this interacting system. What does your result get wrong, and why? Show on your sketch how a more accurate calculation might change your result.

Useful integral:

$$\int_0^\infty dx \frac{x}{e^x - 1} = \frac{\pi^2}{6}$$