M.Phys Option in Theoretical Physics: C6. Problem Sheet 2

Question 11. Consider a fermion 'system' with just one single-particle orbital, so that the only states of the system are $|0\rangle$ (unoccupied) and $|1\rangle$ (occupied). Show that we can represent the operators a and $a^\dagger$ by the matrices

$$a^\dagger = \begin{pmatrix} 0 & 0 \\ C & 0 \end{pmatrix}, \quad a = \begin{pmatrix} 0 & C^* \\ 0 & 0 \end{pmatrix}.$$

You can do this by checking the values of aa, $a^\dagger a^\dagger$ and $a^\dagger a + aa^\dagger$. What values may the constant C take?

Question 12. A quantum-mechanical Hamiltonian for a system of an even number N of point unit masses interacting by nearest-neighbour forces in one dimension is given by

$$H = \frac{1}{2}\sum_{r=1}^{N}\left(p_r^2 + (q_{r+1} - q_r)^2\right),$$

where the Hermitian operators q_r, p_r satisfy the commutation relations $[q_r, q_s] = [p_r, p_s] = 0$, $[q_r, p_s] = \mathrm{i}\delta_{rs}$, and where $q_{r+N} = q_r$. New operators Q_k, P_k are defined by

$$q_r = \frac{1}{\sqrt{N}}\sum_k Q_k \mathrm{e}^{\mathrm{i}kr} \qquad \text{and} \qquad p_r = \frac{1}{\sqrt{N}}\sum_k P_k \mathrm{e}^{-\mathrm{i}kr},$$

where $k = 2\pi n/N$ with $n = -N/2+1, \ldots, 0, \ldots, N/2$.

Show that:

(a) $Q_k = \frac{1}{\sqrt{N}}\sum_{s=1}^{N} q_s \mathrm{e}^{-\mathrm{i}ks}$ and $P_k = \frac{1}{\sqrt{N}}\sum_{s=1}^{N} p_s \mathrm{e}^{\mathrm{i}ks}$

(b) $[Q_k, P_{k'}] = \mathrm{i}\delta_{kk'}$

(c) $H = \frac{1}{2}\left(\sum_k P_k P_{-k} + \omega^2 Q_k Q_{-k}\right)$, where $\omega^2 = 2(1-\cos k)$.

Similarly to the treatment of the simple harmonic oscillator in QM I we then define annihilation operators a_k by

$$a_k = \frac{1}{(2\omega_k)^{1/2}}(\omega_k Q_k + \mathrm{i}P_{-k}).$$

Show that the Hermitian conjugate operators are

$$a_k^\dagger = \frac{1}{(2\omega_k)^{1/2}}(\omega_k Q_{-k} - \mathrm{i}P_k),$$

and determine the canonical commutation relations for a_k and $a_p^\dagger$. Construct the Fock space of states and determine the eigenstates and eigenvalues of H.

Question 13. Bosonic creation operators are defined through their action on basis states in the occupation number representation as

$$c_l^\dagger|n_1 n_2 \ldots\rangle = \sqrt{n_l + 1}|n_1 n_2 \ldots n_l + 1 \ldots\rangle\ ,$$

a) Deduce from this how bosonic annihilation operators act.
b) Show that the creation and annihilation operators fulfil *canonical commutation relations*

$$[c_l, c_m] = 0 = [c_l^\dagger, c_m^\dagger]\ , \quad [c_l, c_m^\dagger] = \delta_{l,m}.$$

Question 14. Consider the N-particle interaction potential

$$\hat{V} = \sum_{i<j}^{N} V(\hat{\mathbf{r}}_i, \hat{\mathbf{r}}_j),$$

where $V(\hat{\mathbf{r}}_i, \hat{\mathbf{r}}_j) = V(\hat{\mathbf{r}}_j, \hat{\mathbf{r}}_i)$. Show that in second quantization it is expressed as

$$\hat{V} = \frac{1}{2}\int d^3\mathbf{r} d^3\mathbf{r}'\ V(\mathbf{r}, \mathbf{r}')\ c^\dagger(\mathbf{r})c^\dagger(\mathbf{r}')c(\mathbf{r}')c(\mathbf{r}).$$

To do so consider the action of $\hat{V}$ on a basis of N-particle position eigenstates

$$|\mathbf{r}_1 \ldots \mathbf{r}_N\rangle = \frac{1}{\sqrt{N! n_1! n_2! \ldots}} \sum_P (\pm 1)^{|P|} |\mathbf{r}_1\rangle \otimes |\mathbf{r}_2\rangle \otimes |\mathbf{r}_N\rangle = \frac{1}{\sqrt{n_1! n_2! \ldots}} \prod_{j=1}^{N} c^\dagger(\mathbf{r}_j)|0\rangle ,$$

where n_j is the occupation number of the j^{th} single-particle state. Argue that in an arbitrary basis of single-particle eigenstates $|l\rangle$ $\hat{V}$ can be expressed in the form

$$\hat{V} = \sum_{ll'mm'} \langle ll'|\hat{V}|mm'\rangle c_l^\dagger c_{l'}^\dagger c_{m'} c_m .$$

Question 15. Consider a system of fermions moving freely on a one-dimensional ring of length L, i.e. periodic boundary conditions are applied between $x = 0$ and $x = L$. The fermions are all in the same spin state, so that spin quantum numbers may be omitted. Fermion creation and annihilation operators at the point x are denoted by $\psi^\dagger(x)$ and $\psi(x)$.
a) Write down the complete set of anticommutation relation satisfied by $\psi^\dagger(x_1)$ and $\psi(x_2)$.
b) Write down the wave-functions of single-particle momentum eigenstates (make sure to take the boundary conditions into account!). What are the allowed values of momentum? Using this result, derive an expression for the momentum space creation and annihilation operators $\Psi_p^\dagger$ and Ψ_p in terms of $\psi^\dagger(x)$ and $\psi(x)$ (hint: use the general result for basis transformation obtained in the lecture notes).
c) Starting with your expression for the anticommutator $\{\psi^\dagger(x_1), \psi(x_2)\}$, evaluate $\{\Psi_p^\dagger, \Psi_q\}$.
d) Derive an expression for $\psi(x)$ in terms of Ψ_k.
e) The density operator $\rho(x)$ is defined by $\rho(x) = \psi^\dagger(x)\,\psi(x)$. The number operator is

$$N = \int_0^L dx\, \rho(x) .$$

Express $\rho(x)$ in terms of $\Psi_p^\dagger$ and Ψ_q, and show from this that

$$N = \sum_k \Psi_k^\dagger \Psi_k .$$

Let $|0\rangle$ be the vacuum state (containing no particles) and define $|\phi\rangle$ by

$$|\phi\rangle = A \prod_k (u_k + v_k \Psi_k^\dagger)|0\rangle,$$

where u_k and v_k are complex numbers depending on the label k, and A is a normalisation constant.

Evaluate (i) $|A|^2$, (ii) $\langle\phi|N|\phi\rangle$, and (iii) $\langle\phi|N^2|\phi\rangle$. Under what conditions is $|\phi\rangle$ an eigenstate of particle number?

Question 16. Consider a system of fermions in which the functions $\varphi_\ell(x)$, $\ell = 1, 2 \ldots N$, form a complete orthonormal basis for single particle wavefunctions.
a) Explain how Slater determinants may be used to construct a complete orthonormal basis for n-particle states with $n = 2, 3 \ldots N$. Calculate the normalisation constant for such a Slater determinant at a general value of n. How many independent n-particle states are there for each n?
b) Let $C_\ell^\dagger$ and C_ℓ be fermion creation and destruction operators which satisfy the usual anticommutation relations. The quantities a_k are defined by

$$a_k = \sum_{\ell=1}^{N} U_{k\ell} C_\ell,$$

where $U_{k\ell}$ are elements of an $N \times N$ matrix, U. Write down an expression for $a_k^\dagger$. Find the condition which must be satisfied by the matrix U in order that the operators $a_k^\dagger$ and a_k also satisfy fermion anticommutation relations.
c) Non-interacting spinless fermions move in one dimension in an infinite square-well potential, with position coordinate $0 \leq x \leq L$. The normalised single particle energy eigenstates are

$$\varphi_\ell(x) = \left(\frac{2}{L}\right)^{1/2} \sin\left(\frac{\ell \pi x}{L}\right) ,$$

and the corresponding fermion creation operator is $C_\ell^\dagger$.

Write down expressions for $C^\dagger(x)$, the fermion creation operator at the point x, and for $\rho(x)$, the particle density operator, in terms of $C_\ell^\dagger$, C_ℓ and $\varphi_\ell(x)$.

d) What is the ground state expectation value $\langle\rho(x)\rangle$ in a system of n fermions?

In the limit $n \to \infty$, $L \to \infty$, taken at fixed average density $\rho_0 = n/L$, show that

$$\langle\rho(x)\rangle = \rho_0 \left[1 - \frac{\sin 2\pi\rho_0 x}{2\pi\rho_0 x}\right] .$$

Sketch this function and comment briefly on its behaviour for $x \to 0$ and $x \to \infty$.

Question 17. A magnetic system consists of two types of Heisenberg spin $\mathbf{S}^A$ and $\mathbf{S}^B$ located respectively on the two inter-penetrating sublattices of an NaCl crystal structure (i.e. a simple cubic structure with alternate A and B in any Cartesian direction). Its Hamiltonian is

$$H = J\sum_{i,j} \mathbf{S}_i^A \cdot \mathbf{S}_j^B$$

where the i, j are nearest neighbours, respectively on the A and B sublattices. J is positive. Show that the classical ground state has all the A spins ferromagnetically aligned in one direction and all the B spins ferromagnetically aligned in the opposite direction. Assume the quantum mechanical ground state is well approximated by the classical one. To a first approximation the spin operators are given in terms of boson operators a, b by

A sublattice	B sublattice
$S_i^z = S^A - a_i^\dagger a_i$	$S_j^z = -S^B + b_j^\dagger b_j$
$S_i^+ \equiv S_i^x + \mathrm{i}S_i^y \simeq (2S^A)^{1/2} a_i$	$S_j^+ \equiv S_j^x + \mathrm{i}S_j^y \simeq (2S^B)^{1/2} b_j^\dagger$
$S_i^- \equiv S_i^x - \mathrm{i}S_i^y \simeq (2S^A)^{1/2} a_i^\dagger$	$S_j^- \equiv S_j^x - \mathrm{i}S_j^y \simeq (2S^B)^{1/2} b_j$

Discuss the validity of this approximation. Use these relations to express the Hamiltonian in terms of the boson operators to quadratic order.

Transforming to crystal momentum space using (with N the number of sites on one sublattice)

$$a_i = N^{-1/2}\sum_{\mathbf{k}} \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}_i} a_{\mathbf{k}}, \quad b_j = N^{-1/2}\sum_{\mathbf{k}} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}_j} b_{\mathbf{k}}$$

show that your result can be expressed in the form

$$H = E_0 + \sum_{\mathbf{k}} \left[A_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + B_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + C_{\mathbf{k}}(a_{\mathbf{k}}^\dagger b_{\mathbf{k}}^\dagger + b_{\mathbf{k}} a_{\mathbf{k}})\right]$$

and determine the coefficients. Hence calculate the spectrum of excitations at low momenta. Consider both the cases with $S^A = S^B$ and $S^A \neq S^B$ and comment on your results.

Question 18. Consider the ideal Fermi gas at finite density N/V in a periodic 3-dimensional box of length L.

(a) Give an expression of the ground state in terms of creation operators for momentum eigenstates.

(b) Calculate the **single-particle Green's function**

$$\begin{aligned} G_{\sigma\tau}(\omega, \mathbf{q}) &= \int dt\, e^{i\omega(t-t')} \int d^3\mathbf{r}\, e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} G_{\sigma\tau}(t, \mathbf{r}; t', \mathbf{r}') , \\ G_{\sigma\tau}(t, \mathbf{r}; t', \mathbf{r}') &= -i\langle GS|T c_\sigma(\mathbf{r}, t)\, c_\tau^\dagger(\mathbf{r}', t')|GS\rangle, \end{aligned} \tag{1}$$

where T denotes time-ordering (i.e. $T\mathcal{O}(t_1)\mathcal{O}(t_2) = \theta(t_1 - t_2)\mathcal{O}(t_1)\mathcal{O}(t_2) - \theta(t_2 - t_1)\mathcal{O}(t_2)\mathcal{O}(t_1)$ for fermionic operators), and

$$c_\sigma(\mathbf{r}, t) \equiv e^{\frac{i}{\hbar}Ht} c_\sigma(\mathbf{r}) e^{-\frac{i}{\hbar}Ht}.$$

First express the creation/annihilation operators $c_\sigma^\dagger(\mathbf{r}, t)$, $c_\sigma(\mathbf{r}, t)$ in terms of creation/annihilation operators in momentum space $c_\sigma^\dagger(\mathbf{p}, t)$, $c_\sigma(\mathbf{p}, t)$. Then show that for annihilation operators in momentum space we have

$$c_\sigma(\mathbf{p}, t) \equiv e^{\frac{i}{\hbar}Ht} c_\sigma(\mathbf{p}) e^{-\frac{i}{\hbar}Ht} = c_\sigma(\mathbf{p}) e^{-\frac{i}{\hbar}t\epsilon(\mathbf{p})} ,$$

where $\epsilon(\mathbf{p}) = \mathbf{p}^2/2m - \mu$. Use this to show that

$$c_\sigma(\mathbf{r}, t) = \frac{1}{L^{3/2}} \sum_{\mathbf{p}} e^{-\frac{i}{\hbar} t\epsilon(\mathbf{p}) + i\mathbf{p}\cdot\mathbf{r}}\, c_\sigma(\mathbf{p}). \tag{2}$$

Now insert (2) into (1) and evaluate the ground state expectation value to obtain an integral representation for $G_{\sigma\tau}(t, \mathbf{r}; t', \mathbf{r}')$. Why does the Green's function only depend on $t - t'$ and $\mathbf{r} - \mathbf{r}'$? Finally, calculate $G_{\sigma\tau}(\omega, \mathbf{q})$.

Note: the imaginary part of the single-particle Green's function is (approximately) measured by angle resolved photoemission (ARPES) experiments.