M.Phys Option in Theoretical Physics: C6. Problem Sheet 6

Qu 1. 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?

Qu 2. Consider a system of fermions moving freely in one dimension with coordinate x. Periodic boundary conditions are applied between $x = 0$ and $x = L$, and 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 $\psi(x)$.

Write down the anticommutation relation satisfied by $\psi^\dagger(x_1)$ and $\psi(x_2)$.

A transformation to a basis of momentum eigenstates is defined by

$$\Psi_k = \frac{1}{\sqrt{L}} \int_0^L dx\, e^{-ikx} \psi(x),$$

where $k = 2\pi n/L$ with integer n. Write down the corresponding expression for $\Psi_k^\dagger$. Starting from your expression for the anticommutator $\{\psi^\dagger(x_1), \psi(x_2)\}$, evaluate $\{\Psi_p^\dagger, \Psi_q\}$. Suggest with justification an expression for $\psi(x)$ in terms of Ψ_k.

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

(a) $|A|^2$

(b) $\langle\phi|N|\phi\rangle$

(c) $\langle\phi|N^2|\phi\rangle$.

Under what conditions is $|\phi\rangle$ an eigenstate of particle number?

Qu 3. 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. 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?

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.

Non-interacting spinless fermions move in one dimension in an infinite square-well potential, with position coordinate $0 \le x \le L$. 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 $\varphi_\ell(x)$. 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 $x \to \infty$.

Qu 4. 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) $Q_k = \dfrac{1}{\sqrt{N}} \displaystyle\sum_{s=1}^{N} q_s \mathrm{e}^{-\mathrm{i}ks}$ 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 $\omega^2 = 2(1 - \cos k)$.

With a_k defined by

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

show that

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

and hence obtain the spectrum of the elementary excitations of the system.

Qu 5. 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 classical ground state is a good first approximation in the quantum case.

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.