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

Qu 1. 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 2. 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 $0 \leq x \leq L$. 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 $C^\dagger_\ell$, 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 3. 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 $\omega^2 = 2(1-\cos k)$.

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 4. 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

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

Qu 5. Consider a one dimensional fermion pairing model with Hamiltonian

$$H = -t \sum_{j=1}^{N} c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j + \gamma \left[c_j^\dagger c_{j+1}^\dagger + c_{j+1} c_j \right],$$

where c_j are fermionic annihilation operators at site j.

(a) Derive an expression for H in terms of a Fock space basis built from momentum eigenstates. Hint: use our general formula for basis transformations to relate the creation operators

$$c_j^\dagger = \sum_k c^\dagger(k) \, \langle k | j \rangle = \frac{1}{\sqrt{L}} \sum_k c^\dagger(k) \, e^{-ikj}.$$

(b) Under what conditions do the operators $\alpha(k)$, $\alpha^\dagger(k)$ defined by

$$\begin{pmatrix} \alpha(k) \\ \alpha^\dagger(-k) \end{pmatrix} = \begin{pmatrix} u(k) & v(k) \\ v^*(-k) & u^*(-k) \end{pmatrix} \begin{pmatrix} c(k) \\ c^\dagger(-k) \end{pmatrix}$$

fulfil canonical anticommutation relations?

(c) Now consider the special Bogoliubov transformation

$$\begin{pmatrix} c(k) \\ c^\dagger(-k) \end{pmatrix} \cdot \begin{pmatrix} \cos\theta_k & i\sin\theta_k \\ i\sin\theta_k & \cos\theta_k \end{pmatrix} \begin{pmatrix} \alpha(k) \\ \alpha^\dagger(-k) \end{pmatrix}$$

with $\theta_{-k} = -\theta_k$ to diagonalize the Hamiltonian. Show that the dispersion relation for the elementary excitations is

$$\epsilon(k) = -2t\cos(k)\sqrt{1 + \gamma^2 \tan^2(k)}.$$

(d) Give an expression for the ground state of H.

(e) Derive an integral expression for the ground state expectation value

$$\langle c_j^\dagger c_{j+1}^\dagger \rangle.$$

Qu 6. 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

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

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

$$H = E_0 + \sum_{\mathbf{k}} \Big[A_{\mathbf{k}} a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + B_{\mathbf{k}} b^\dagger_{\mathbf{k}} b_{\mathbf{k}} + C_{\mathbf{k}} (a^\dagger_{\mathbf{k}} b^\dagger_{\mathbf{k}} + b_{\mathbf{k}} a_{\mathbf{k}}) \Big]$$

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.

Qu 7.* 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**

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

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

$$c_\sigma(\mathbf{r}, t) \equiv e^{iHt} c_\sigma(\mathbf{r}) e^{-iHt}.$$

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

$$c_\sigma(\mathbf{p}, t) \equiv e^{iHt} c_\sigma(\mathbf{p}) e^{-iHt} = c_\sigma(\mathbf{p}) e^{-it\epsilon(\mathbf{p})} ,$$

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

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

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.