UNIVERSITY OF CAMBRIDGE

NATURAL SCIENCES TRIPOS: Part III Physics — NST3PHY
MASTER OF ADVANCED STUDY IN PHYSICS — MAPY

Wednesday 18 January 2017 12.00 to 14.00

MAJOR TOPICS
Paper 1/TQM (Theories of Quantum Matter)

Answer **two** *questions only.* $\hbar = 1$ ***throughout this paper***.

The approximate number of marks allocated to each part of a question is indicated in the right-hand margin where appropriate.

The paper contains 11 sides including this one and is accompanied by a book giving values of constants and containing mathematical formulae which you may quote without proof.

You should use a **separate Answer Book** *for each question.*

STATIONERY REQUIREMENTS	SPECIAL REQUIREMENTS
2 × 20-page answer books	Mathematical formulae handbook
Rough workpad	Approved calculator allowed

You may not start to read the questions printed on the subsequent pages of this question paper until instructed that you may do so by the Invigilator.

1 The transverse displacement of an elastic rod of length L is described by the continuum Hamiltonian

$$H = \int_0^L \left[\frac{1}{2\rho}\pi(x)^2 + \frac{\tau}{2}u'(x)^2 + \frac{B}{2}u''(x)^2 + \frac{\alpha}{6}u'(x)^3 \right] dx,$$

where ρ is the density, τ is the tension, and B is the bending modulus. The displacement $u(x)$ and momentum density $\pi(x)$ satisfy the commutation relations

$$[u(x), \pi(x')] = i\delta(x - x').$$

(a) Rewrite the quadratic part of the Hamiltonian, corresponding to the first three terms, in terms of the Fourier modes defined by

$$u(x) = \sum_{n=-\infty}^{\infty} u_n e^{iq_n x}, \quad \pi(x) = \frac{1}{L}\sum_{n=-\infty}^{\infty} \pi_n e^{-iq_n x},$$

where $q_n \equiv \frac{2\pi n}{L}$. [5]

(b) Write the quadratic Hamiltonian in terms of the oscillator variables

$$a_n = \frac{1}{\sqrt{2}}\left[(\kappa_n \rho L^2)^{1/4} u_n + \frac{i}{(\kappa_n \rho L^2)^{1/4}} \pi_{-n} \right]$$
$$a_n^\dagger = \frac{1}{\sqrt{2}}\left[(\kappa_n \rho L^2)^{1/4} u_{-n} - \frac{i}{(\kappa_n \rho L^2)^{1/4}} \pi_n \right].$$

where you should identify the coefficients κ_n. Find the spectrum of excitations of the quadratic Hamiltonian. [7]

(c) Express the cubic part of the Hamiltonian in terms of the oscillator variables. [5]

(d) In first order perturbation theory in the cubic part, the one phonon state $a_q^\dagger|0\rangle$ will acquire corrections

$$\sum_{q=q_1+q_2} c(q, q_1, q_2) a_{q_1}^\dagger a_{q_2}^\dagger |0\rangle.$$

Find the amplitudes $c(q, q_1, q_2)$. [5]

(e) Show that the contribution of these states to the normalisation of the state is infrared divergent, showing that phonons are not good quasiparticles in one dimension. [8]

Solution

(a) Inserting the Fourier expansion

$$u(x) = \sum_{n=-\infty}^{\infty} u_n e^{iq_n x}, \quad \pi(x) = \frac{1}{L} \sum_{n=-\infty}^{\infty} \pi_n e^{-iq_n x},$$

gives

$$H = \sum_{n,n'} \int_0^L dx\, e^{iq_n x + iq_{n'} x} \left[\frac{1}{2\rho L^2} \pi_n \pi_{n'} + \frac{1}{2} \left(-\tau q_n q_{n'} + B q_n^2 q_{n'}^2 \right) u_n u_{n'} \right] \tag{1}$$

$$= \sum_{n=-\infty}^{\infty} \left[\frac{1}{2\rho L} \pi_n \pi_{-n} + \frac{L}{2} \overbrace{\left(\tau q_n^2 + B q_n^4 \right)}^{\equiv \kappa_n} u_n u_{-n} \right], \tag{2}$$

where the coefficients κ_n are identified for later use.

(b) With the above identification we have

$$H = \sum_{n=-\infty}^{\infty} \left[\frac{1}{2\rho L} \pi_n \pi_{-n} + \frac{L}{2} \kappa_n u_n u_{-n} \right], \tag{3}$$

Writing

$$u_n = \frac{1}{\sqrt{2} (\kappa_n \rho L^2)^{1/4}} \left(a_n + a_{-n}^\dagger \right) \tag{4}$$

$$\pi_n = -i \frac{(\kappa_n \rho L^2)^{1/4}}{\sqrt{2}} \left(a_n - a_{-n}^\dagger \right) \tag{5}$$

$$H = \frac{1}{4} \sqrt{\frac{\kappa_n}{\rho}} \sum_n \left[-\left(a_n - a_{-n}^\dagger \right) \left(a_{-n} - a_n^\dagger \right) + \left(a_n + a_{-n}^\dagger \right) \left(a_{-n} + a_n^\dagger \right) \right] \tag{6}$$

$$= \sum_{n=-\infty}^{\infty} E(k_n) \left[a_n^\dagger a_n + a_n a_n^\dagger \right], \tag{7}$$

where $E(k) = \sqrt{\frac{\kappa_n}{\rho}} = \sqrt{\frac{\tau q^2 + B q^4}{\rho}}$

(c) Using

$$u_n = \frac{1}{\sqrt{2} (\kappa_n \rho L^2)^{1/4}} \left[a_n + a_{-n}^\dagger \right].$$

We have

$$
\begin{aligned}
H_3 &= \frac{\alpha}{6}\int dx u'^3 = -i\frac{\alpha}{6}\int_0^L dx \sum_{n_1,n_2,n_3} e^{i(q_{n_1}+q_{n_2}+q_{n_3})x} q_{n_1}q_{n_2}q_{n_3}u_{n_1}u_{n_2}u_{n_3} \\
&= \frac{\alpha L}{6}\sum_{q_1+q_2+q_3=0} -i(q_1q_2q_3)u_{q_1}u_{q_2}u_{q_3} \\
&= -i\frac{\alpha}{12\sqrt{2L}\rho^{3/4}}\sum_{q_1+q_2+q_3=0}\frac{q_1q_2q_3}{(\kappa_{q_1}\kappa_{q_3}\kappa_{q_2})^{1/4}}\left[a_{q_1}+a^\dagger_{-q_1}\right]\left[a_{q_2}+a^\dagger_{-q_2}\right]\left[a_{q_3}+a^\dagger_{-q_3}\right]
\end{aligned}
$$

(d) The relevant part of the perturbation is that with one annihilation and two creation operators (three equivalent terms)

$$
H_3 \to -i\frac{\alpha}{4\sqrt{2L}\rho^{3/4}}\sum_{q_1+q_2=q}\frac{q_1q_2q}{(\kappa_{q_1}\kappa_{q_3}\kappa_{q_2})^{1/4}}a^\dagger_{q_1}a^\dagger_{q_2}a_q
$$

Is ordering important? *No*, the order would only matter when one of q_1 or q_2 vanishes, but then there is no contribution.

Thus

$$
H_3a^\dagger_q|0\rangle = -i\frac{\alpha\sqrt{L}}{4\sqrt{2}\rho^{3/4}}\sum_{q_1+q_2=q}\frac{q_1q_2q}{(\kappa_{q_1}\kappa_{q_3}\kappa_{q_2})^{1/4}}a^\dagger_{q_1}a^\dagger_{q_2}|0\rangle
$$

Standard expression for first order perturbation theory gives the amplitudes

$$
\begin{aligned}
c(q,q_1,q_2) &= \frac{\langle q_1,q_2|H_3|q\rangle}{E(q)-E(q_1)-E(q_2)} \qquad (8)\\
&= -i\frac{\alpha}{4\sqrt{2L}\rho^{3/4}}\frac{q_1q_2q}{(\kappa_{q_1}\kappa_{q_3}\kappa_{q_2})^{1/4}}\frac{1}{E(q)-E(q_1)-E(q_2)} \qquad (9)
\end{aligned}
$$

where

$$
|\boldsymbol{q}\rangle = a^\dagger_{\boldsymbol{q}}|0\rangle, \qquad |\boldsymbol{q}_1,\boldsymbol{q}_2\rangle = a^\dagger_{\boldsymbol{q}_1}a^\dagger_{\boldsymbol{q}_2}|0\rangle \qquad (10)
$$

(e) Sum square modulus of these contributions

$$
\sum_{q_1+q_2=q}2|c(q,q_1,q_2)|^2 = \sum_{q_1+q_2=q}\frac{\alpha^2}{16L\rho^{3/2}}\frac{(q_1q_2q)^2}{(\kappa_{q_1}\kappa_{q_3}\kappa_{q_2})^{1/2}}\frac{1}{(E(q)-E(q_1)-E(q_2))^2}.
$$

The factor of two arises because of the two ways to pair the up the boson pairs in the amplitude and its conjugate.

When one of the momenta (say q_2) approaches zero, the dependence of the whole sum is $\sim q_2^{-1}$, indicating a logarithmic divergence when replaced by an integral.

2 The Bose–Hubbard model on the square lattice has the Hamiltonian

$$H_{\mathrm{BH}} = -t \sum_{\langle j\,k\rangle} \left[a_j^\dagger a_k + a_k^\dagger a_j\right] + \frac{U}{2} \sum_j \mathsf{N}_j(\mathsf{N}_j - 1),$$

where $\langle j\,k\rangle$ denotes a pair of nearest neighbour sites, t is the hopping matrix element, and U is the interaction constant. $\left[a_j, a_k^\dagger\right] = \delta_{jk}$, and $\mathsf{N}_j = a_j^\dagger a_j$.

(a) Find the phase boundaries of the Mott ground states on a t/U, μ/U diagram (μ is chemical potential)) at small t/U. [6]

(b) Use perturbation theory to find how the Mott ground states are altered to first order in t/U. [6]

(c) Consider now the extended model that includes an interaction between nearest neighbours

$$H_{\mathrm{NNBH}} = \sum_{\langle j\,k\rangle} \left[-t\left(a_j^\dagger a_k + a_k^\dagger a_j\right) + V\mathsf{N}_j\mathsf{N}_k\right] + \frac{U}{2} \sum_j \mathsf{N}_j(\mathsf{N}_j - 1).$$

At $t = 0$, show that for $V > 0$ the Mott states are now separated by 'checkerboard' states where the occupancy is N and $N + 1$ on a A and B sublattices respectively (or vice versa). Find the values of μ where the checkerboard states are preferred over the Mott states. [4]

(d) When $t = 0$, one particle added to the checkerboard state gives a degenerate multiplet of ground states with the extra particle residing at one of the A sublattice sites with occupancy $N + 1$. The remaining A sublattice sites have occupancy N, and the B sublattice has occupancy $N + 1$.

By considering the hopping terms of the Hamiltonian as a perturbation, show that the upper boundary of the checkerboard state in the t/U, μ/U diagram at $t \ll U, V$ is given by the curve

$$\mu = -\frac{4t^2(N+1)(N+2)}{U - 4V} + UN + 4V(N+1).$$

[8]

(e) Find the lower boundary by considering states with one particle removed from the B sublattice. [6]

Solution

(a) This is bookwork. See `http://tqm.courses.phy.cam.ac.uk/docs/lectures/Lattice/#the-effect-of-hopping`

Let's now consider a Mott state of filling $\nu = N$ with one extra particle added at site i

$$|i, +\rangle \equiv \frac{a_i^\dagger}{\sqrt{N+1}} \bigotimes_j |N\rangle_j.$$

These matrix elements are

$$\langle j|H_t|k\rangle = -t(N+1),$$

between adjacent sites. Thus within the ground state multiplet H_t corresponds to a tight binding model, with ground state energy $-2td(N+1)$ in d-dimensions.

Removing a particle from the Mott state

$$|i, -\rangle \equiv \sqrt{N} a_i \bigotimes_j |N\rangle_j.$$

Within these states, H_t takes the form

$$H_t|_- = -tN \sum_{\langle jk\rangle} \left[|j, -\rangle\langle k, -| + \text{h.c.}\right],$$

with a ground state $-2tdN$

At $t = 0$ the energies of the Mott states with filling $\nu = N$ are

$$\frac{\mathcal{E}_\mu^{(N)}}{N_{\text{sites}}} = \frac{U}{2} N(N-1) - \mu N.$$

$\mathcal{E}_\mu^{(N)}$ and $\mathcal{E}_\mu^{(N+1)}$ become degenerate when $\mu = UN$ for $t = 0$. Compare with energy of one extra particle on top of the N Mott state.

$$\mathcal{E}_\mu^{(N)} + UN - \mu - 2dt(N+1).$$

Negative $t > \frac{UN-\mu}{2d(N+1)}$, giving upper phase boundary to N-Mott state

$$t = \frac{UN - \mu}{2d(N+1)}$$

Similarly, for 'hole' in the $N+1$ Mott state

$$\mathcal{E}_\mu^{(N+1)} - UN + \mu - 2dt(N+1),$$

giving lower phase boundary to $N+1$ Mott state

$$t = \frac{-UN+\mu}{2d(N+1)}$$

(b) Applying $H_t \equiv -t\sum_{\langle jk\rangle}\left[a_j^\dagger a_k + a_k^\dagger a_j\right]$ to a Mott state of filling N gives a state with an adjacent particle-hole pair. The unperturbed energy of this state is $2U$ greater than the energy of the Mott state. First order PT then gives the correction

$$\sum_{\langle jk\rangle} \frac{t\sqrt{N(N-1)}}{2U}\left(|\text{p-h on bond}\langle jk\rangle\rangle + |\text{h-p on bond}\langle jk\rangle\rangle\right)$$

(In the lectures we've taken the notation $\langle jk\rangle$ to be an *undirected* bond)

(c) The energy per site of the Mott state is now (including the chemical potential)

$$\frac{U}{2}N(N-1) + 2VN^2 - \mu N,$$

while the $(N, N+1)$ checkerboard state has an energy per site

$$\frac{U}{2}N^2 + 2VN(N+1) - \mu\left(N+\frac{1}{2}\right)$$

This means that the checkerboard exists in the range

$$4VN + UN < \mu < UN + 4V(N+1)$$

(d) An extra particle added to one of the N-occupied sites of the $(N, N+1)$ checkerboard state (say the A sublattice) has additional energy $UN + 4V(N+1)$. The states with the added particle at different A sites are not coupled by H_t. Rather, H_t will hop the particle to the B sublattice with matrix element $-t\sqrt{(N+1)(N+2)}$, where it has energy $U(N+1) + 4VN$. In the second order of degenerate perturbation theory, we therefore have the Hamiltonian

$$H_{\text{eff}} = -\frac{1}{U-4V}P_{\text{ch}}H_t H_t P_{\text{ch}} \tag{11}$$

$$= -\frac{t^2(N+1)(N+2)}{U-4V}\left(4\sum_{j\in A\text{ sublatt ice}}|j\rangle\langle j| + 2\sum_{\substack{\langle jk\rangle\\ j,k\in A\text{ sublattice}}}\left[|j\rangle\langle k| + \text{h.c.}\right]\right). \tag{12}$$

where P_{ch} denotes the projection onto the checkerboard state. The factors 4 and 2 arise from the number of ways to get back to the original site of the A sublattice or move to an adjacent site respectively.

The ground state energy of H_{eff} is $-\frac{4t^2(N+1)(N+2)}{U-4V}$. Including the chemical potential, the energy of this state with one extra particle relative to the checkerboard state is

$$-\frac{4t^2(N+1)(N+2)}{U-4V} + UN + 4V(N+1) - \mu.$$

Setting this equal to zero gives a parabola bending down from the threshold we found in the previous part

$$\mu = -\frac{4t^2(N+1)(N+2)}{U-4V} + UN + 4V(N+1).$$

(e) Similarly, introducing a hole on the B sublattice changes the energy by $-UN-4VN$, and the intermediate states have energy $U(1-N)-4V(N+1)$, giving

$$\mu = \frac{4t^2N(N+1)}{U-4V} + UN + 4VN$$

3 A model in which pairs of fermions form bosonic bound states in volume V is described by the Hamiltonian

$$H = \sum_{p,s} \xi_p a^\dagger_{p,s} a_{p,s} + \sum_q \left(\frac{\xi_p}{2} + \varepsilon_0\right) b^\dagger_q b_q + \frac{g}{\sqrt{V}} \sum_{p,q} \left[b_q a^\dagger_{q+p,\uparrow} a^\dagger_{-p,\downarrow} + a_{-p,\downarrow} a_{q+p,\uparrow} b^\dagger_q \right],$$

where $\xi_p = \frac{p^2}{2m} - \mu$, ε_0 is an energy offset, and g is the coupling between bosons and pairs. The $a_{p,s}$ operators describe fermions; the b_p operators bosons:

$$\left[b_p, b^\dagger_{p'}\right] = \delta_{p,p'},$$
$$\left\{a_{p,s}, a^\dagger_{p',s'}\right\} = \delta_{p,p'}\delta_{s,s'}$$

(a) Find the ground state energy of a system of $2N$ particles as a function of ε_0 for $g = 0$. That is, $2N = N_b + 2N_a$, but you should allow $N_{a,b}$ to vary. [5]

(b) A BCS-like state has the form

$$|\mathrm{BCS}\rangle = \prod_p \left[\sin(\theta_p/2) a^\dagger_{p,\uparrow} a^\dagger_{-p,\downarrow} + \cos(\theta_p/2)\right] e^{-\lambda^2/2} e^{\lambda b^\dagger_0} |\mathrm{VAC}\rangle$$

where θ_p and λ are real variational parameters. Show that the expectation value of the energy is

$$\langle \mathrm{BCS}|H|\mathrm{BCS}\rangle = \sum_p \left[\xi_p(1 - \cos\theta_p) + \frac{g\lambda}{\sqrt{V}} \sin\theta_p\right] + \varepsilon_0 \lambda^2$$

[10]

(c) By minimising the energy with respect to θ_p and λ, show that

$$\frac{\varepsilon_0}{g^2} = \frac{1}{V} \sum_p \frac{1}{2E_p},$$

where you should give the form of E_p. [10]

(d) Find and equation for the total number of particles, and describe a limit in which the predictions of this model coincide with the predictions of the BCS theory. [5]

[30]

Solution

(a) The ground state corresponds to filling the Fermi sea to $\varepsilon_0/2$. The total energy is

$$N_b\varepsilon_0 + 2\frac{L}{(2\pi)^3}\int_{\boldsymbol{k}^2/2m<\varepsilon_0/2}\frac{\boldsymbol{k}^2}{2m}d\boldsymbol{k} = \varepsilon_0\left[2N - \frac{V}{3\pi^2}(m\varepsilon_0)^{3/2}\right] + \frac{V}{10m\pi^2}(m\varepsilon_0)^{5/2} \quad (13)$$

$$= 2N\varepsilon_0 - \frac{7V}{30\pi^2}m^{3/2}\varepsilon_0^{5/2} \quad (14)$$

(b) For the expectation values we can use the commutator

$$\left[a^\dagger_{\boldsymbol{p},\uparrow}a_{\boldsymbol{p},\uparrow}, a^\dagger_{\boldsymbol{p},\uparrow}a^\dagger_{-\boldsymbol{p},\downarrow}\right] = a^\dagger_{\boldsymbol{p},\uparrow}a^\dagger_{-\boldsymbol{p},\downarrow} \quad (15)$$

$$\left[a^\dagger_{-\boldsymbol{p},\downarrow}a_{-\boldsymbol{p},\downarrow}, a^\dagger_{\boldsymbol{p},\uparrow}a^\dagger_{-\boldsymbol{p},\downarrow}\right] = a^\dagger_{\boldsymbol{p},\uparrow}a^\dagger_{-\boldsymbol{p},\downarrow}. \quad (16)$$

Thus

$$\langle a^\dagger_{\boldsymbol{p},\uparrow}a_{-\boldsymbol{p},\downarrow}\rangle = \sin^2\theta_{\boldsymbol{p}}/2.$$

We also have

$$\langle b_0^\dagger b_0\rangle = \lambda^2,$$

and finally

$$\langle b_0 a^\dagger_{\boldsymbol{p},s}a^\dagger_{-\boldsymbol{p},s}\rangle = \lambda\sin\theta_{\boldsymbol{p}}\cos\theta_{\boldsymbol{p}} \quad (17)$$

(c) Minimising w.r.t. $\theta_{\boldsymbol{p}}$ gives

$$\cos\theta_{\boldsymbol{p}} = \frac{\xi_{\boldsymbol{p}}}{E_{\boldsymbol{p}}} \qquad \sin\theta_{\boldsymbol{p}} = \frac{g\lambda}{\sqrt{V}E_{\boldsymbol{p}}}$$

where $E_{\boldsymbol{p}}^2 = \xi_{\boldsymbol{p}}^2 + g^2\lambda^2/V$. On the other hand, the saddle point in λ gives

$$2\varepsilon_0\lambda + \frac{g}{\sqrt{V}}\sum_{\boldsymbol{p}}\sin\theta_{\boldsymbol{p}}.$$

Substituting in the solution for $\theta_{\boldsymbol{p}}$ gives the stated equations

(d) The equation for the total number of particles follows from the above

$$N = \lambda^2 + 2\sum_{\boldsymbol{p}}\sin^2\theta_{\boldsymbol{p}}/2.$$

Condition is $g \to \infty$ while $g^2/V\varepsilon_0$ remains finite. In this limit the λ^2 term in the number equation can be neglected, and we return to the number equation in the BCS theory.

END OF PAPER