UNIVERSITY OF CAMBRIDGE

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

19 January 2023, 10.00-12.00

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 4 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
linear graph paper	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.

V8.4

A

1 This question concerns the spin-1/2 chain with Hamiltonian

$$H_{\text{spin}} = J_1 \sum_{j=1}^{N} \mathbf{s}_j \cdot \mathbf{s}_{j+1} + J_2 \sum_{j=1}^{N} \mathbf{s}_j \cdot \mathbf{s}_{j+2},$$

with periodic boundary conditions $\mathbf{s}_{j+N} = \mathbf{s}_j$ and $\mathbf{s}_j = (s_j^x, s_j^y, s_j^z)$. The couplings J_1 and J_2 are related to each other by $J_2 = J_1/2 > 0$.

(a) Explain *without* detailed derivation how the Hamiltonian H_{spin} arises as an effective Hamiltonian for the extended fermion Hubbard model $H_{\text{H}} = H_t + U \sum_j N_{j,\uparrow} N_{j,\downarrow}$ describing N spin-1/2 fermions (one per site) with

$$H_t \equiv -t_1 \sum_{j,s} \left[a^\dagger_{j,s} a_{j+1,s} + a^\dagger_{j+1,s} a_{j,s} \right] - t_2 \sum_{j,s} \left[a^\dagger_{j,s} a_{j+2,s} + a^\dagger_{j+2,s} a_{j,s} \right]$$

in the limit $U \gg t_{1,2}$. State the relation between t_1 and t_2 required to give $J_2 = J_1/2$. [6]

(b) H_{spin} can be written in the form

$$H_{\text{spin}} = \frac{J_2}{2} \sum_{j=1}^{N} \left[\left(\mathbf{s}_j + \mathbf{s}_{j+1} + \mathbf{s}_{j+2} \right)^2 - \frac{9}{4} \right].$$

A spin singlet formed by the spins on sites j and k is denoted by $|S\rangle_{j,k} \equiv \frac{1}{\sqrt{2}} \left[|\uparrow\rangle_j |\downarrow\rangle_k - |\downarrow\rangle_j |\uparrow\rangle_k \right] =$ and satisfies $\left(\mathbf{s}_j + \mathbf{s}_k\right) |S\rangle_{j,k} = 0$. Show that for N even the states

$$|\psi_+\rangle = |S\rangle_{2,3} |S\rangle_{4,5} |S\rangle_{6,7} \cdots |S\rangle_{N,1} =$$

$$|\psi_-\rangle = |S\rangle_{1,2} |S\rangle_{3,4} |S\rangle_{5,6} \cdots |S\rangle_{N-1,N} =$$

are both ground states of H_{spin}, and find their energy. [4]

(c) For N odd consider the states

$|2j-1\rangle \equiv$ $\quad j = 1, \ldots (N+1)/2$

$|2j\rangle \equiv$ $\quad j = 1, \ldots (N-1)/2,$

where the dot denotes an 'unpaired' spin. Show that

$$\langle 2j|H|2k\rangle = \langle 2j-1|H|2k-1\rangle = \begin{cases} -\frac{3NJ_2}{4} \langle 2j|2k\rangle, & j \neq k \\ -\frac{3(N-1)J_2}{4}, & j = k \end{cases}$$

and as $N \to \infty$

$$\langle 2j-1|2k-1\rangle = \langle 2j|2k\rangle = \left(-\frac{1}{2}\right)^{|j-k|}$$
$$\langle 2j-1|2k\rangle = \langle 2j-1|H|2k\rangle = 0.$$

[10]

(d) Use the variational state

$$|\eta\rangle = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{i\eta j} \, |j\rangle$$

to evaluate the expectation value of the energy in the large N limit. [10]

[*For large N:*

$$\langle\eta|\eta\rangle \longrightarrow \left(\sum_{j=-\infty}^{\infty} \left(-\frac{1}{2}\right)^{|j|} e^{2ij\eta} \right) = \frac{3}{5 + 4\cos 2\eta}.$$
]

Solution 1

(a) I am looking for a summary that includes the following

1. At $t = 0$ the ground states have one particle at every site and degeneracy 2^N arising from the spin. ✓✓
2. Finding an effective Hamiltonian that lifts the degeneracy requires second order degenerate perturbation theory.✓✓
3. The Heisenberg couplings are $J \propto t^2/U$ so the necessary relation is $t_2 = t_1/\sqrt{2}$.✓✓

(b) In the given states, two of any three consecutive spins are in a singlet, so $\left(\mathbf{s}_j + \mathbf{s}_{j+1} + \mathbf{s}_{j+2}\right)^2 = 3/4$ ✓. This gives the ground state energy as $-3NJ_2/4$ ✓. This is a ground state because each term in the Hamiltonian has the smallest possible value.✓✓

(c) $H = \sum_i h_i$ with $h_i \propto \left[(\mathbf{s}_{i-1} + \mathbf{s}_i + \mathbf{s}_{i+1})^2 - 9/4\right]$. When $j \neq k$, *either* $|2j\rangle$ *or* $|2k\rangle$ are eigenstates of h_i with eigenvalue $-3J_2/4$ as found before, and therefore $\langle 2j|H|2k\rangle = -\frac{3NJ_2}{4}\langle 2j|2k\rangle$.✓✓

When $j = k$ this argument fails for h_j, so we have to compute its expectation directly. $\langle 2j|h_j|2j\rangle = 0$ follows from isotropy since h_j only involves dot products between the three spins, and $\mathbf{s}_j$ and $\mathbf{s}_{j+1}$ are locked in singlets to the left and right respectively. One can also do the explicit calculation. ✓✓✓

Together with the same argument for $|2j - 1\rangle$ this gives:

$$\langle 2j|H|2k\rangle = \langle 2j-1|H|2k-1\rangle = \begin{cases} -\frac{3NJ_2}{4}\langle 2j|2k\rangle\,, & j \neq k \\ -\frac{3(N-1)J_2}{4}, & j = k \end{cases}$$

For the inner products we start from

$$\langle 2j|2j+2\rangle = \langle \pm_{2j-1}|\,\langle S_{2j,2j+1}|S_{2j-1,2j}\rangle\,|\pm_{2j+1}\rangle = -\frac{1}{2}.✓$$

Increasing the distance between the unpaired spins by two sites gives rise to another factor of $-1/2$. Thus

$$\langle 2j-1|2k-1\rangle = \langle 2j|2k\rangle = \left(-\frac{1}{2}\right)^{|j-k|} ✓$$

Strictly this is true for $|j-k| \ll N$ to to avoid the possibility of returning to the starting point. In fact, you have to move along $2N$ sites to return to $|2j\rangle$, as moving along $N-1$ sites turns $|2j\rangle$ to $|2j-1\rangle$, giving $\langle 2j|2j-1\rangle = (-1/2)^{(N-1)/2}$. Thus the ‘even’ and ‘odd’ states are orthogonal for $N \to \infty$✓✓

$$\langle 2j-1|2k\rangle = 0.$$

$\langle 2j-1|H|2k\rangle = 0$ for the same reason.✓

(d) The results of the previous part can be used to show that the evaluation of $\langle\eta|H_{\rm spin}|\eta\rangle$ is *almost* the same as calculating the norm:

$$\begin{aligned}\langle\eta|H|\eta\rangle &= \frac{1}{N}\sum_{j,k} e^{i\eta(k-j)}\langle j|H|k\rangle \checkmark\checkmark \\ &= -\frac{3NJ_2}{4}\mathcal{N}(\eta)+\frac{3NJ_2}{4}\checkmark\checkmark\checkmark\end{aligned}$$

where $\mathcal{N}(\eta)$ is the squared norm given in the hint, with the second term arising from things being different for $j=k\checkmark$. The energy is then

$$\frac{\langle\eta|H|\eta\rangle}{\langle\eta|\eta\rangle}=\frac{3NJ_2}{4}\left(\frac{1}{\mathcal{N}(\eta)}-1\right)\equiv -\frac{3NJ_2}{4}+\omega(\eta).\checkmark\checkmark$$

The excess energy $\omega(\eta)$ (we can't say 'relative to the ground state' but we can compare with the value of the N even ground state energy evaluated for N odd) is

$$\omega(\eta)=\frac{3NJ_2}{4\mathcal{N}(\eta)}=J_2\left(\frac{5}{4}+\cos 2\eta\right).\checkmark\checkmark$$

Note that if we had introduced an alternating sign into the definition of the states, we'd end up with a more conventional looking dispersion of the form $\frac{5}{4}-\cos 2\eta$, which is how it appears in B. Sriram Shastry and Bill Sutherland, Phys. Rev. Lett. 47, 964 (1981). More detailed variational calculations can be found in W J Caspers et al 1984 J. Phys. A: Math. Gen. 17 2687.

Relation to course

The mapping from Hubbard to spin chain is a very small variation on the case discussed in the course. The rest of the problem is new material. The excited state resembles the excited state of the Heisenberg chain (a localized departure from the ground state) discussed in lectures.

2 This question concerns a quantity called the *superfluid density* n_s. If an N-body wavefunction in one dimension obeys the generalised periodic boundary conditions:

$$\Psi_\Theta(x_1, \dots x_j + L, \dots, x_N) = \exp(i\Theta)\Psi_\Theta(x_1, \dots x_j, \dots, x_N), \text{ for all } j,$$

n_s is defined in terms of $E_0(\Theta)$, the ground state energy as a function of Θ, as:

$$n_s = mL \frac{d^2 E_0}{d\Theta^2}\bigg|_{\Theta=0}$$

(a) In the Gross–Pitaevskii approximation a uniform Bose gas of density n in the absence of an external potential is described by a condensate wavefunction $\varphi(x)$ of constant magnitude $|\varphi(x)| = \sqrt{n}$. Show that $n_s = n$. [6]

(b) For $\Theta \neq 0$ the Bogoliubov Hamiltonian is

$$H_{\text{pair}} = N\epsilon(k_0) + \frac{U_0}{2L}N(N-1) + \sum_{n\neq 0}\left(\left[\epsilon(k_n) - \epsilon(k_0) + U_0 n_0\right] a_n^\dagger a_n + \frac{U_0 n_0}{2}\left[a_n^\dagger a_{-n}^\dagger + a_n a_{-n}\right]\right),$$

where $k_n = \frac{2\pi n}{L} + \frac{\Theta}{L}$, $\epsilon(k) = \frac{k^2}{2m}$, and $a_n^\dagger$ creates a boson with wavevector k_n. Show that $n_s = n$ in the Bogoliubov approximation. [10]

(c) If the ground state wavefunction $\Psi_0(x_1, \dots x_j, \dots, x_N)$ is known for $\Theta = 0$, a possible variational wavefunction for $\Theta \neq 0$ is

$$\Psi_\Theta(x_1, \dots x_j, \dots, x_N) = \Psi_0(x_1, \dots x_j, \dots, x_N)\exp\left(i\sum_{j=1}^N \theta(x_j)\right),$$

where $\theta(x)$ is a variational function satisfying $\theta(x+L) = \theta(x) + \Theta$. Assuming Ψ_0 is real, show that the kinetic energy has an additive $\theta(x)$-dependent contribution given by

$$\frac{1}{2m}\int_0^L dx\, \rho(x)(\partial_x\theta)^2,$$

where $\rho(x)$ is the expected density

$$\rho(x) \equiv N\int_0^L dx_2 \cdots dx_N |\Psi_0(x, x_2, \dots x_N)|^2.$$

[6]

(d) Find the optimal $\theta(x)$ and the corresponding n_s, expressing your answer in terms of $\rho(x)$, which in general is not constant. [8]

Solution 2

(a) The condensate wavefunction that satisfies the boundary condition is

$$\varphi(x) = \sqrt{n}e^{i\Theta x/L}.\checkmark\checkmark$$

The only Θ dependence of the energy is in the kinetic energy, which is

$$E_K = \frac{1}{2m}\int dx|\partial_x\varphi|^2 = \frac{nL}{2m}\left(\frac{\Theta}{L}\right)^2.\checkmark\checkmark$$

Substituting into the definition gives $n_s = n$.✓✓

(b) Starting from

$$\begin{aligned} H_{\text{pair}} &= N\epsilon(k_0) + \frac{U_0}{2L}N(N-1) \\ &+ \sum_{n\neq 0}\left([\epsilon(k_n) - \epsilon(k_0) + U_0 n_0]\, a_n^\dagger a_n + \frac{U_0 n_0}{2}\left[a_n^\dagger a_{-n}^\dagger + a_n a_{-n}\right]\right). \end{aligned}$$

The first term gives the Gross–Pitaevskii result $n_s = n$✓. The only other place Θ appears is

$$\epsilon(k_n + \Theta/L) - \epsilon(\Theta/L) = \epsilon\left(\frac{2\pi n}{L}\right) + \frac{2\pi n\Theta}{mL^2},\checkmark\checkmark$$

which has opposite sign for $\pm n$. In order to preserve the commutation relations the Bogoliubov transformation

$$\overbrace{\begin{pmatrix} b_n \\ b_{-n}^\dagger \end{pmatrix}}^{\equiv B_n} = \Lambda \overbrace{\begin{pmatrix} a_n \\ a_{-n}^\dagger \end{pmatrix}}^{\equiv A_n}\checkmark$$

has to satisfy the property $\Lambda^\dagger\sigma_3\Lambda = \sigma_3$✓✓. The Θ dependent part of the Bogoliubov Hamiltonian has the form $\sum_n A_n^\dagger\sigma_3 A_n$ and since

$$\sum_n nA_n^\dagger\sigma_3 A_n = \sum_n nB_n^\dagger\sigma_3 B_n\checkmark$$

for any valid Λ this does not affect the form of Λ, which is therefore unchanged from $\Theta = 0$. In the ground state $\langle 0|B_n^\dagger\sigma_3 B_n|0\rangle$ is even in n by symmetry ✓ and so there is no Θ dependence in the Bogoliubov part of the ground state energy ✓. Thus $n_s = n$ in the Bogoliubov theory too.✓

I expect many attempts will try to re-do the Bogoliubov transformation including the new term and so credit will be given in proportion to how well the above facts are established by explicit calculation.

(Note that if $\epsilon(k)$ were not quadratic – on a lattice, say – the superfluid density would be changed)

(c) Substituting the given variational form into the kinetic energy we find the expectation

$$\frac{N}{2m}\int dx_1 \cdots dx_N \partial_{x_1}\Psi^* \partial_{x_1}\Psi \checkmark = \frac{N}{2m}\int dx_1 \cdots dx_N \left[\partial_{x_1}\Psi_0^* \partial_{x_1}\Psi_0 + |\Psi_0|^2 (\partial_{x_1}\theta)^2\right] . \checkmark\checkmark\checkmark$$

The second term, which contains the θ dependence, evaluates to

$$\frac{1}{2m}\int dx\, \rho(x)(\partial_x \theta)^2 . \checkmark\checkmark$$

(d) The Euler–Lagrange equation is

$$\partial_x(\rho(x)\partial_x\theta) = 0 \checkmark\checkmark$$

or $\rho\partial_x\theta = \mathrm{k}$, constant $\checkmark$. The constant is determined by the phase shift, i.e.

$$\Theta = \int \frac{k}{\rho(x)} dx . \checkmark\checkmark$$

The contribution of Θ to the kinetic energy is then

$$\frac{1}{2m}\int dx\, \rho(x)(\partial_x\theta)^2 = \frac{1}{2m}k^2 \int dx \frac{1}{\rho(x)} = \frac{\Theta^2}{2m}\left(\int dx \frac{1}{\rho(x)}\right)^{-1} . \checkmark\checkmark\checkmark$$

(You can check this reproduces $n_s = \rho$ when the density is constant. n_s vanishes any time a vanishing density causes the integral to diverge. Note that – being variational – this is an upper bound on n_s. This bound appears in Journal of Statistical Physics volume 93, pages927–941 (1998))

Relation to course

(a), (b), and (c) are all meant to be small tweaks of calculations done in the lectures. For (b) they have been taught that an odd contribution to the Bogoliubov Hamiltonian does not change its form. Part (d) will be more challenging as an explicit solution of the Euler–Lagrange equation is required.

3 Two systems of identical fermions are described by the Hamiltonian

$$H = \overbrace{\sum_k \left[\epsilon_k a^\dagger_k a_k + \epsilon_k b^\dagger_k b_k\right]}^{\equiv H_0} + \overbrace{v \sum_{k_1,k_2} \left[a^\dagger_{k_1} b_{k_2} + b^\dagger_{k_2} a_{k_1}\right]}^{\equiv H_{\mathrm{t}}}.$$

The number difference operator $\mathcal{N}$ is defined as

$$\mathcal{N} = \frac{1}{2} \sum_k \left[a^\dagger_k a_k - b^\dagger_k b_k\right].$$

(a) Show that the Heisenberg equation of motion for $\mathcal{N}(t) = e^{iHt}\mathcal{N}e^{-iHt}$ is

$$\frac{d\mathcal{N}(t)}{dt} = J(t),$$

where $a_k(t) = e^{iHt}a_k e^{-iHt}$, $b_k(t) = e^{iHt}b_k e^{-iHt}$ and

$$J(t) \equiv -iv \sum_{k_1,k_2} \left[a^\dagger_{k_1}(t)b_{k_2}(t) - b^\dagger_{k_2}(t)a_{k_1}(t)\right].$$

[6]

When $H = H_0$ the quantum noise spectrum of the operator J has the following representation in terms of the eigenstates $|n\rangle$ and eigenenergies E_n of H_0

$$S(\omega) = 2\pi \sum_{m,n} p_n |\langle n| J |m\rangle|^2 \delta(\omega - E_m + E_n),$$

where the probabilities $p_n = \exp\left[-\beta(E_n - \mu_A N_{A,n} - \mu_B N_{B,n})\right]/\mathcal{Z}$, $N_{A,n}$ and $N_{B,n}$ are the numbers of A and B fermions in state $|n\rangle$, and $\mathcal{Z}$ is the grand partition function.

(b) Show that $S(\omega)$ can be written

$$S(\omega) = 2\pi v^2 \sum_{k_1,k_2} \delta(\omega - \epsilon_{k_1} + \epsilon_{k_2}) \left[n_B(\epsilon_{k_2})(1 - n_A(\epsilon_{k_1})) + n_A(\epsilon_{k_2})(1 - n_B(\epsilon_{k_1}))\right],$$

where you should define the functions $n_{A,B}(\epsilon)$. [10]

From now on you should express sums over k in terms of the level spacing $\delta = \epsilon_{k+1} - \epsilon_k$ using

$$\sum_{k=0}^{\infty} f(\epsilon_k) \longrightarrow \frac{1}{\delta} \int_0^\infty f(\epsilon) d\epsilon.$$

(c) Evaluate $S(\omega)$ when the two systems of fermions are at equal temperatures with equal chemical potentials $\mu_A = \mu_B$, with $e^{\beta\mu_{A,B}} \gg 1$. [7]

[*If* $\epsilon_\pm = \epsilon \pm \omega/2$

$$\int_{-\infty}^{\infty} \frac{d\epsilon}{\left(e^{\beta\epsilon_+} + 1\right)\left(e^{-\beta\epsilon_-} + 1\right)} = \frac{2\omega}{e^{\beta\omega} - 1}$$
]

(d) Evaluate $S(\omega)$ at zero temperature when the chemical potentials are different (but both positive). [7]

Solution 3

(a) The equation of motion implies

$$\frac{d\mathcal{N}(t)}{dt} = i[H, \mathcal{N}(t)]\checkmark = ie^{iHt}[H, \mathcal{N}]e^{-iHt} = ie^{iHt}[H_{\mathrm{t}}, \mathcal{N}]e^{-iHt}\checkmark\checkmark \tag{1}$$

(because H_0 conserves the number difference). Computing the commutator gives

$$[H_{\mathrm{t}}, \mathcal{N}] = v\sum_{k_1,k_2}\left[b^\dagger_{k_1}a_{k_2} - a^\dagger_{k_2}b_{k_1}\right],\checkmark\checkmark \tag{2}$$

which leads to the stated result. ✓

(b) We need the matrix elements $\langle m|J|n\rangle$. The form of J means that $|m\rangle$ can be obtained from $|n\rangle$ by the removal of one particle at k_1 from A and addition of one particle at k_2 to B, or vice versa✓✓. In the first case we have the matrix element $iv\sqrt{N_{A,k_1}(1-N_{B,k_2})}$ ✓ and the energy changes by $E_m - E_n = \epsilon(k_2) - \epsilon(k_1)$ ✓ and in the second the matrix element is $-iv\sqrt{N_{B,k_2}(1-N_{A,k_1})}$ ✓ and the energy change is $E_m - E_n = \epsilon(k_1) - \epsilon(k_2)$ ✓. This gives

$$S(\omega) = 2\pi v^2 \sum_{n,k_1,k_2} p_n\delta(\omega - \epsilon_{k_1} + \epsilon_{k_2})\left[N_{B,k_2}(1-N_{A,k_1}) + N_{A,k_2}(1-N_{B,k_1})\right].\checkmark\checkmark$$

The sum over n now computes the expectations $\langle N_{A/B,k}\rangle \equiv n_{A,B}(\epsilon_k)$, with the probability distribution factoring over the different k values and A and B subsystems, giving the Fermi-Dirac distribution

$$n_{A,B}(\epsilon_k) = \frac{1}{e^{\beta(\epsilon_k - \mu_{A,B})}+1}.\checkmark\checkmark$$

(c) Replacing sums by integrals gives

$$\begin{aligned}
S(\omega) &= \frac{2\pi v^2}{\delta^2}\int_0^\infty d\epsilon_1 d\epsilon_2 \delta(\omega - \epsilon_1 + \epsilon_2)\left[n_B(\epsilon_2)(1-n_A(\epsilon_1)) + n_A(\epsilon_2)(1-n_B(\epsilon_1))\right]\checkmark\checkmark \\
&= \frac{2\pi v^2}{\delta^2}\int_0^\infty d\epsilon_1 \left[n_B(\epsilon_1-\omega)(1-n_A(\epsilon_1)) + n_A(\epsilon_1-\omega)(1-n_B(\epsilon_1))\right]\checkmark\checkmark \\
&= \frac{8\pi v^2}{\delta^2}\frac{\omega}{1-e^{-\beta\omega}}\checkmark\checkmark.
\end{aligned}$$

By using the given integral we are implicitly using the condition $e^{\beta\mu_{A,B}} \gg 1$ to extend the domain of integration to $-\infty$. $S(0) = \frac{8\pi v^2}{\delta^2}k_{\mathrm{B}}T$ is Johnson noise.✓

(d) You can either work with the step functions that appear at zero temperature, or keep the temperature finite and take $T = 0$ at the end. In the latter case we get

$$\begin{aligned}
S(\omega) &= \frac{2\pi v^2}{\delta^2}\int d\epsilon_1 \left[n_B(\epsilon_1-\omega)(1-n_A(\epsilon_1)) + n_A(\epsilon_1-\omega)(1-n_B(\epsilon_1))\right]\checkmark\checkmark \\
&= \frac{4\pi v^2}{\delta^2}\left[\frac{\omega+\mu_B-\mu_A}{1-e^{-\beta(\omega+\mu_B-\mu_A)}} + \frac{\omega+\mu_A-\mu_B}{1-e^{-\beta(\omega+\mu_A-\mu_B)}}\right].\checkmark\checkmark
\end{aligned}$$

Now taking $T = 0$ gives ✓

$$S(\omega) = \frac{4\pi v^2}{\delta^2} \left[|\omega + \mu_B - \mu_A| + |\omega + \mu_A - \mu_B| \right] . ✓✓$$

The noise is piecewise linear, vanishing for $\omega < -|\mu_A - \mu_B|$ and with the gradient doubling at $\omega = |\mu_A - \mu_B|$.

Relation to course

The spectral representation of $S(\omega)$ is a core part of the lectures on response and correlation, and evaluating the matrix elements of bilinears appears at several stages in the course. The calculations in (c) and (d) are similar to (but easier than) the calculation of the dynamic structure factor for free fermions that appears on one of the problem sheets.

END OF PAPER