UNIVERSITY OF CAMBRIDGE

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

Thursday 23 January 2025, 10.00-12.00

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

$\hbar = 1$ ***throughout this paper***.

Answer **two** *questions only.*

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

The paper contains 6 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
Rough workpad

SPECIAL REQUIREMENTS
Mathematical Formulae Handbook
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.

V8.5

A

1 The t-J model describes the dynamics of spin and the motion of empty sites in the large U/t limit of the Hubbard model and is described by the Hamiltonian

$$H = \overbrace{-t \sum_{\substack{\langle j,k\rangle \\ s=\uparrow,\downarrow}} \left[a^\dagger_{j,s}a_{k,s} + a^\dagger_{k,s}a_{j,s}\right]}^{\equiv H_t} + J \sum_{\langle j,k\rangle} \left[\mathbf{s}_j \cdot \mathbf{s}_k - \frac{N_j N_k}{4}\right],$$

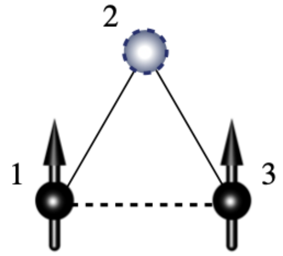
together with the constraint that there are no doubly occupied sites. Here $a^\dagger_{j,s}$, $a_{j,s}$ are canonical fermion operators and the spin operators $\mathbf{s}_j$ are

$$\mathbf{s}_j = \frac{1}{2}\sum_{s,s'} a^\dagger_{j,s}\boldsymbol{\sigma}_{ss'}a_{j,s'},$$

where $\boldsymbol{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$ are the Pauli matrices.

(a) Explain how the $\mathbf{s}_j \cdot \mathbf{s}_k$ part of the Hamiltonian arises in the large U limit of the Hubbard model. Give the dependence of the exchange coupling J on t and U, the Hubbard interaction parameter. [5]

From now on we consider three sites arranged in a triangle, with two fermions (and one empty site), and study only the tight-binding Hamiltonian H_t.



(b) A basis of $S_z = 1$ states is

$$\begin{aligned}
|A\rangle &= a^\dagger_{2,\uparrow}a^\dagger_{3,\uparrow}|\mathrm{VAC}\rangle \\
|B\rangle &= a^\dagger_{3,\uparrow}a^\dagger_{1,\uparrow}|\mathrm{VAC}\rangle \\
|C\rangle &= a^\dagger_{1,\uparrow}a^\dagger_{2,\uparrow}|\mathrm{VAC}\rangle\,.
\end{aligned}$$

Evaluate the matrix elements of H_t between these states, and show that in this basis the states

$$\begin{pmatrix}1\\-1\\0\end{pmatrix} \qquad \begin{pmatrix}0\\1\\-1\end{pmatrix} \qquad \begin{pmatrix}1\\0\\-1\end{pmatrix}$$

are eigenstates. Find their eigenvalue. [9]

(c) A basis of six $S_z = 0$ states is

$$
\begin{aligned}
|1\rangle &= a^\dagger_{2,\uparrow} a^\dagger_{3,\downarrow} |\mathrm{VAC}\rangle \\
|2\rangle &= a^\dagger_{3,\downarrow} a^\dagger_{1,\uparrow} |\mathrm{VAC}\rangle \\
|3\rangle &= a^\dagger_{1,\uparrow} a^\dagger_{2,\downarrow} |\mathrm{VAC}\rangle \\
|4\rangle &= a^\dagger_{2,\downarrow} a^\dagger_{3,\uparrow} |\mathrm{VAC}\rangle \\
|5\rangle &= a^\dagger_{3,\uparrow} a^\dagger_{1,\downarrow} |\mathrm{VAC}\rangle \\
|6\rangle &= a^\dagger_{1,\downarrow} a^\dagger_{2,\uparrow} |\mathrm{VAC}\rangle \, .
\end{aligned}
$$

Show that the matrix representation of H_t in this basis is a circulant matrix, and in this way find the eigenstates and eigenvalues for $S_z = 0$. [10]

(d) Label the states in part (c) by their total angular momentum quantum numbers S and compare with your answer to part (b). [6]

Good resource on Nagoka is Junkai Dong's notes. See also Tasaki's review.

(a) **Bookwork**. Key points

•In the $U \to \infty$ limit have degenerate states (2^N for a half filled system). ✓

•At finite U this degeneracy is lifted by (second order) degenerate perturbation theory. ✓

•$J > 0$ arises because singlets on neighbouring sites are coupled to a singlet doubly occupied site. ✓

•$J = 4t^2/U$. The numerical factor is not important, but the t^2/U is. ✓✓

(b) We find (accounting for fermionic statistics)

$$\langle 1|H_t|2\rangle = -t\,\langle \mathrm{VAC}|a_{3,\uparrow}a_{2,\uparrow}a^\dagger_{2,\uparrow}a_{1,\uparrow}a^\dagger_{3,\uparrow}a^\dagger_{1,\uparrow}|\mathrm{VAC}\rangle = t✓✓$$
$$\langle 2|H_t|3\rangle = -t\,\langle \mathrm{VAC}|a_{1,\uparrow}a_{3,\uparrow}a^\dagger_{3,\uparrow}a_{2,\uparrow}a^\dagger_{1,\uparrow}a^\dagger_{2,\uparrow}|\mathrm{VAC}\rangle = t✓✓$$
$$\langle 3|H_t|1\rangle = -t\,\langle \mathrm{VAC}|a_{2,\uparrow}a_{1,\uparrow}a^\dagger_{1,\uparrow}a_{3,\uparrow}a^\dagger_{2,\uparrow}a^\dagger_{3,\uparrow}|\mathrm{VAC}\rangle = t✓✓$$

These are all the same by cyclic permutations; the remainder are zero. Calculations of this type appear several times in the course of the material on tight-binding models. This gives a circulant matrix (these are met *by name* multiple times in the course) with eigenvalues

$$E = 2t\cos(\eta) \qquad \eta = 0, \pm 2\pi/3 \tag{1}$$
$$= 2t, -t \tag{2}$$

Substitution shows that the given states are eigenstates (only two are linearly independent) with eigenvalue $-t$.✓✓✓

(c) Now the matrix element calculation yields

$$\langle 1|H_t|2\rangle = -t\,\langle \mathrm{VAC}|a_{3,\downarrow}a_{2,\uparrow}a^\dagger_{2,\uparrow}a_{1,\uparrow}a^\dagger_{3,\downarrow}a^\dagger_{1,\uparrow}|\mathrm{VAC}\rangle = t✓$$
$$\langle 2|H_t|3\rangle = -t\,\langle \mathrm{VAC}|a_{1,\uparrow}a_{3,\downarrow}a^\dagger_{3,\downarrow}a_{2,\downarrow}a^\dagger_{1,\uparrow}a^\dagger_{2,\downarrow}|\mathrm{VAC}\rangle = t✓$$
$$\langle 3|H_t|4\rangle = -t\,\langle \mathrm{VAC}|a_{2,\downarrow}a_{1,\uparrow}a^\dagger_{1,\uparrow}a_{3,\uparrow}a^\dagger_{2,\downarrow}a^\dagger_{3,\uparrow}|\mathrm{VAC}\rangle = t✓$$
$$\langle 4|H_t|5\rangle = -t\,\langle \mathrm{VAC}|a_{3,\uparrow}a_{2,\downarrow}a^\dagger_{2,\downarrow}a_{1,\downarrow}a^\dagger_{3,\uparrow}a^\dagger_{1,\downarrow}|\mathrm{VAC}\rangle = t✓$$
$$\langle 5|H_t|6\rangle = -t\,\langle \mathrm{VAC}|a_{1,\downarrow}a_{3,\uparrow}a^\dagger_{3,\uparrow}a_{2,\uparrow}a^\dagger_{1,\downarrow}a^\dagger_{2,\uparrow}|\mathrm{VAC}\rangle = t✓$$
$$\langle 6|H_t|1\rangle = -t\,\langle \mathrm{VAC}|a_{2,\uparrow}a_{1,\downarrow}a^\dagger_{1,\downarrow}a_{3,\downarrow}a^\dagger_{2,\uparrow}a^\dagger_{3,\downarrow}|\mathrm{VAC}\rangle = t✓.$$

Again we have a circulant matrix with plane wave eigenstates for the chain $1-2-3-4-5-6-1-\cdots$ and eigenvalues

$$E = 2t\cos(\eta) \qquad \eta = 0, \pm\pi/3, \pm 2\pi/3, \pi$$
$$= 2t, t, -t, -2t✓✓✓✓$$

(d) **Note:** One can use the information given in the previous part that the matrix is circulant to deduce that the eigenstates are plane waves. The states with $\eta = 0, \pm 2\pi/3$ have the same sign for states $|1\rangle$ and $|4\rangle$, $|2\rangle$ and $|5\rangle$, $|3\rangle$ and $|6\rangle$. These are therefore spin triplet states ($S = 1$) ✓✓✓. For $\eta = \pm 2\pi/3$ (with energy $-t$) these are the $S_z = 0$ partners of $\eta = \pm 2\pi/3$ states found in part (b). The state with $\eta = 0$ is the $S_z = 0$ partner of the $\eta = 0$ state of part (b). I will be generous with marks here even if the latter identifications are not made.

The states with $\pm\pi/3$ and $\eta = \pi$ have *opposite* signs for $|1\rangle$ and $|4\rangle$ etc., and are spin singlet states ($S = 0$). ✓✓✓

The discussion of singlet and triplet states on the lattice appears in the notes on the Fermi Hubbard model.

> For $t > 0$ the $\eta = 0$ state has the lowest energy and is a uniform superposition of singlet states

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2 A tight-binding Hamiltonian for fermions without spin has the form

$$H_t = -t \sum_j \left[a_j^\dagger a_{j+1} + a_{j+1}^\dagger a_j \right],$$

where a_j, $a_j^\dagger$ are canonical fermion operators with periodic boundary conditions $a_{j+N} = a_j$.

(a) Show that the Hamiltonian can be written in the form

$$H_t = \sum_{n=0}^{N-1} \epsilon_n N_n,$$

where you should find ϵ_n and explain how the occupation number operators N_n are related to $a_j^\dagger$, a_j. Give the eigenstates and eigenvalues of the Hamiltonian H_t. [7]

The remainder of the question concerns the Hamiltonian $H = H_t + H_{\mathrm{ph}}$, where

$$H_{\mathrm{ph}} = \sum_j \left[\frac{\omega}{2} \left(b_j^\dagger b_j + b_j b_j^\dagger \right) + \frac{g}{\sqrt{2}} N_j \left(b_j + b_j^\dagger \right) \right],$$

where b_j, $b_j^\dagger$ are canonical bosonic operators obeying $[b_j, b_k^\dagger] = \delta_{jk}$ and $N_j = a_j^\dagger a_j$ is the fermionic number operator.

(b) Show that the second term of H_{ph} (containing g) can be removed by transforming $H_{\mathrm{ph}} \longrightarrow H'_{\mathrm{ph}} \equiv U H_{\mathrm{ph}} U^\dagger$ with a unitary operator of the form

$$U = \exp\left(i\alpha \sum_j N_j p_j \right)$$

where $p_j = -\frac{i}{\sqrt{2}} \left(b_j - b_j^\dagger \right)$ [*Hint: This can be accomplished by transforming the Hamiltonian's constituent operators*]. Find α and give the transformed Hamiltonian H'_{ph}. Comment on the physical meaning of any new terms you find. [9]

(c) Show that the transformed fermion operator is

$$U a_j U^\dagger = e^{-i\alpha p_j} a_j$$

and find $H'_t \equiv U H_t U^\dagger$. [4]

(d) Assuming that $\omega \gg t$, find an effective Hamiltonian for the fermions assuming that the transformed bosons remain in their ground state. [10]

[*The formula*

$$\exp(\lambda b + \mu b^\dagger) = \exp(\lambda\mu/2) \exp(\mu b^\dagger) \exp(\lambda b)$$

may be useful.]

See Han and Kivelson (2023) for a similar calculation

(a) **Bookwork**. By writing the fermion operator in terms of the Fourier modes

$$a_j = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} \tilde{a}_n \exp(2\pi i j n/N) ✓$$

we obtain

$$H = \sum_{n=0}^{N-1} \epsilon_n \tilde{a}_n^\dagger \tilde{a}_n ✓✓$$

where $\epsilon_n = -2t\cos(2\pi n/N)$ ✓✓. A general eigenvector therefore has the form

$$|\mathbf{N}\rangle = \prod_{n=0}^{N-1} (\tilde{a}_n^\dagger)^{N_n} |\mathrm{VAC}\rangle ✓$$

where $N_n = 0, 1$ ✓. The corresponding energy is $\sum_n \epsilon_n N_n$.

(b) It's useful to write the Hamiltonian in terms of the canonical variables

$$x_j = \frac{1}{\sqrt{2}}\left(b_j + b_j^\dagger\right) \qquad p_j = -\frac{i}{\sqrt{2}}\left(b_j - b_j^\dagger\right). ✓$$

In terms of these operators the phonon Hamiltonian takes the form

$$H_{\mathrm{ph}} = \sum_j \left[\frac{\omega}{2}\left(x_j^2 + p_j^2\right) + g N_j x_j\right]. ✓$$

Transforming the coordinate operator gives

$$U x_j U^\dagger = x_j + \alpha N_j. ✓✓$$

Therefore the choice $\alpha = -\frac{g}{\omega}$ removes the second term from the Hamiltonian ✓✓, leaving

$$H'_{\mathrm{ph}} = U H_{\mathrm{ph}} U^\dagger = \sum_j \left[\frac{\omega}{2}\left(x_j^2 + p_j^2\right) - \frac{g^2}{2\omega} N_j^2\right]. ✓✓$$

The last term is an attractive interaction induced by the bosons.✓A similar contribution arises in one of the Problems on the attraction due to optical phonons, though the technique used here is different from the one suggested there.

(c) The transformed fermion operator is

$$U a_j U^\dagger = e^{i\alpha N_j p_j} a_j e^{-i\alpha N_j p_j} = e^{-i\alpha p_j} a_j. ✓✓$$

Thus the transformed tight-binding model is

$$H'_t = U H_t U^\dagger = -t \sum_j \left[e^{i\alpha(p_j - p_{j+1})} a_j^\dagger a_{j+1} + e^{i\alpha(p_{j+1} - p_j)} a_{j+1}^\dagger a_j\right] ✓✓$$

(d) Using the given formula (which is used in the lecture on the elastic chain, in a more complicated setting), we just need to evaluate the exponentials in the hopping terms in the ground state of the bosons ✓✓

$$\langle 0|e^{i\alpha(p_j - p_{j+1})}|0\rangle = \left(\langle 0|e^{i\alpha p_j}|0\rangle\right)^2 = \left(e^{-\alpha^2/4}\right)^2 = e^{-\alpha^2/2} = e^{-g^2/(2\omega^2)}. ✓✓✓✓$$

This renormalizes the hopping matrix element to $\tilde{t} = te^{-g^2/(2\omega^2)}$ ✓✓and gives the final effective Hamiltonian

$$H_{\text{eff}} = -\sum_j \left(\tilde{t}\left[a_j^\dagger a_{j+1} + a_{j+1}^\dagger a_j\right] - \frac{g^2}{2\omega} N_j^2\right). ✓✓$$

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3 The elastic chain is described by the Hamiltonian

$$H = \sum_{j=1}^{N} \left[\frac{p_j^2}{2m} + \frac{k}{2}(u_j - u_{j+1})^2 \right]$$

with $u_j = u_{j+N}$. u_j and p_j are written in terms of canonically conjugate normal mode variables q_n and π_n as

$$u_j = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} q_n \exp\left(\frac{2\pi i n j}{N}\right)$$
$$p_j = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} \pi_n \exp\left(\frac{-2\pi i n j}{N}\right).$$

This question is concerned with the response of the mass at $j = 1$.

(a) Write the Hamiltonian in terms of the normal modes, find the Heisenberg equations of motion and show that a solution is given by

$$q_n(t) = q_n(0)\cos(\omega_n t) + \frac{\pi_{-n}(0)}{m\omega_n}\sin(\omega_n t)$$
$$\pi_n(t) = \pi_n(0)\cos(\omega_n t) - m\omega_n q_{-n}(0)\sin(\omega_n t).$$

Give an expression for the normal mode frequencies ω_n. [8]

(b) The *mobility* $\mu(\omega)$ is defined as the linear response of the expectation of particle 1's velocity p_1/m to a force $f_1(\omega)e^{-i\omega t}$ applied to particle 1:

$$\frac{\langle p_1 \rangle}{m} = \mu(\omega) f_1(\omega) e^{-i\omega t}.$$

Derive the relation between $\mu(\omega)$ and the response function

$$\chi_{p_1 u_1}(t) \equiv i \langle 0 | [p_1(t), u_1(0)] | 0 \rangle, \qquad t > 0.$$ [5]

(c) Evaluate $\chi_{p_1 u_1}(t)$ and show that $\mu(\omega)$ has the form

$$\mu(\omega) = \frac{1}{m\sqrt{\Omega^2 - \omega^2}},$$

where you should give an expression for Ω. [8]

(d) Explain how $\mu(\omega)$ describes energy dissipation for $|\omega| < \Omega$ and $|\omega| > \Omega$. [3]

(e) Find the mobility for the classical version of the model when the mass at $j = 1$ is acted on by an external force. Compare with your answer to (c). [6]

(a) **Bookwork**. Writing the Hamiltonian in terms of the normal modes gives

$$H = \sum_{|n|\leq(N-1)/2}\left[\frac{1}{2m}\pi_n\pi_{-n} + k(1-\cos\eta_n)q_nq_{-n}\right].\checkmark\checkmark$$

Not exactly bookwork The Heisenberg equations of motion are

$$\begin{aligned}\dot{q}_n &= i\,[H,q_n] = \frac{\pi_{-n}}{m}\checkmark\\ \dot{\pi}_n &= i\,[H,\pi_n] = -m\omega_n^2 q_{-n}.\checkmark\end{aligned}$$

Here $\omega_n = \Omega|\sin(\eta_n/2)|$ ✓, where $\eta_n = 2\pi n/N$, and $\Omega = 2\sqrt{\frac{k}{m}}$ is the maximum frequency ✓. Verify that these are solved by the given expressions. ✓✓

(b) Introducing a perturbing potential $-f_1(t)x_1$ ✓allows us to use the Kubo formula (covered in the notes) for the response function of p_1 to the coordinate x_1

$$\langle p_1(t)\rangle = \int^t dt'\chi_{p_1x_1}(t-t')f_1(t').\checkmark\checkmark$$

Taking the Fourier transform shows

$$\mu(\omega) = \frac{\chi_{p_1x_1}(\omega)}{m}\checkmark\checkmark$$

(c) Using the given solution we evaluate the response function

$$\begin{aligned}\chi_{p_1u_1}(t) &= i\,[p_1(t),u_1(0)]\\ &= \frac{i}{N}\sum_{n,n'}[\pi_n(t),q_{n'}(0)]\,e^{i(n'-n)}\checkmark\checkmark\\ &= \frac{1}{N}\sum_n \cos(\omega_n t)\checkmark\checkmark\\ &\longrightarrow \int_{-\pi}^{\pi}\frac{d\eta}{2\pi}\cos(\omega(\eta)t)\checkmark.\end{aligned}$$

Taking the Fourier transform

$$\chi_{p_1u_1}(\omega) = \frac{1}{2}\int_{-\pi}^{\pi}d\eta\,[\delta(\omega-\omega(\eta))+\delta(\omega+\omega(\eta))] = \frac{1}{\sqrt{\Omega^2-\omega^2}}\checkmark\checkmark$$

where as before $\Omega = 2\sqrt{\frac{k}{m}}$ ✓. Strictly this is the real part of $\chi(\omega)$, but we can recognize it as an analytic function for complex ω.

(d) The rate of energy dissipation is $\frac{1}{2}\mathrm{Re}\mu(\omega)|f(\omega)|^2$ ✓. μ is real for $|\omega| < \Omega$ where energy can be dissipated to infinity by waves ✓, and imaginary when $|\omega| > \Omega$ where this is not possible ✓. The connection between response functions and dissipation is explained. I am looking for answers to recognize that the behaviour is related to finite bandwidth of the phonons.

(e) The classical equations of motion are

$$m\ddot{u}_j + k(2u_j - u_{j-1} - u_{j+1}) = \delta_{j,1} f_1(t).\checkmark$$

Substituting the mode expansion

$$u_j(t) = \frac{1}{\sqrt{N}} \sum_n q_n(t) e^{i\eta_n j},$$

with $\eta_n = 2\pi n/N$, we multiply by $e^{-i\eta_n j}$ and sum over j to find the frequency response

$$\begin{aligned}
-m\omega^2 q_n(\omega) + 2k(1 - \cos\eta_n) q_n &= e^{-i\eta_n} \frac{f_1(\omega)}{\sqrt{N}}, \\
q_n(\omega) &= \frac{e^{-i\eta_n} f_1(\omega)}{\sqrt{N} m(\omega(\eta_n)^2 - \omega^2)} \checkmark \\
u_1(\omega) &= \frac{e^{-i\eta_n} f_1(\omega)}{N} \sum_n \frac{1}{m(\omega(\eta_n)^2 - \omega^2)} \checkmark.
\end{aligned}$$

The velocity response is

$$\begin{aligned}
v_1(\omega) &= \frac{f_1(\omega)}{N} \sum_n \frac{-i\omega}{m(\omega(\eta_n)^2 - \omega^2)}.\checkmark \\
&= -i \frac{f_1(\omega)}{2mN} \sum_n \left[\frac{1}{\omega(\eta_n) - \omega} - \frac{1}{\omega(\eta_n) + \omega} \right] \\
&= -i \frac{f_1(\omega)}{2m} \int_{-\pi}^{\pi} \frac{d\eta}{2\pi} \left[\frac{1}{\omega(\eta) - \omega} - \frac{1}{\omega(\eta) + \omega} \right] \checkmark
\end{aligned}$$

Using the prescription $\omega \to \omega - i\delta$ and the formula

$$\frac{1}{x + i0} = \mathcal{P}\frac{1}{x} - i\pi\delta(x)$$

gives back the same expression for $\mu(\omega)$. ✓

END OF PAPER