Problem Sheet 2: One-Dimensional Model

Comments on these questions are always welcome. For instance if you spot any typos or feel the wording is unclear, drop me an email at `T.Evans` at the usual Imperial address.
Note: problems marked with a $*$ are the most important to do and are core parts of the course. Those without any mark are recommended. It is likely that the exam will draw heavily on material covered in these two types of question. Problems marked with a ! are harder and/or longer. Problems marked with a $\sharp$ are optional. For the exam it will be assumed that material covered in these optional $\sharp$ questions has not been seen before and such optional material is unlikely to be used in an exam.

$\sharp$1. Maths note

In the following questions on a 1+1 dimensional ring of masses connected by chains (i.e. looking at phonons in a one-dimensional crystal), we will make use the Fourier series of a periodic discrete function. This question is to remind you of some of its mathematical properties.
Consider a periodic discrete function u_n defined at the points labelled by an integer n. Let its period be N such that $u_n = u_{n+N}$. This function can be represented as a sum of linearly independent plane waves, *i.e.* Fourier series:

$$u_n = \sum_k U_k e^{ikn} \tag{1}$$

(i) What are the allowed wavevectors k which obey the periodic conditions and the condition that these plane waves are linearly independent of each other? How many of these wavevectors are there?

(ii) Show that, for any two allowed wavevectors k and q:

$$\sum_{n=0}^{N-1} e^{i(k+q)n} = N\delta_{k+q,0} \tag{2}$$

Use the result for a geometric series with a finite number of terms:
$1 + z + z^2 + \ldots + z^M = (1 - z^{M+1})/(1 - z)$.

2. Periodic Potential and Mass Gap

Consider N particles, with positions r_n and momenta p_n ($n = 0, 1, \ldots, (N-1)$) confined to lie in a ring length $L = Na$. The particles interact pairwise with the interaction energy for the n-th and m-th particles being $U(r_n - r_m) = U(r_m - r_n)$. They also each interact with an periodic external potential of the form $V(r_n) = V(r_n + a)$.
Why do we expect the classical ground state to be where the particles are stationary at $r_n = na$?
By considering **small** deviations u_n from this state, and by assuming that the pairwise interactions U are short range, explain why we can write the Hamiltonian of this system in the approximate form

$$H = \sum_{n=0}^{N-1} \left[\frac{p_n^2}{2m} + \frac{m\omega_D^2}{2}(u_{n+1} - u_n)^2 + \frac{m\Omega^2}{2}u_n^2 \right] + (\text{constants}) \tag{3}$$

where we define $u_N = u_0$. You should be able to give the constants ω_D and Ω in terms of derivatives of the potentials U and V respectively.
For a model of lattice vibrations in a physical material, why should $\Omega = 0$?

*3. Harmonic Ring: Normal modes

Background

This is an exercise in expressing the Hamiltonian in terms of its normal modes. This is a common technique so make sure you are familiar with these ideas.

The question is simple because the Hamiltonian is quadratic, the equations of motion are linear differential equations — here wave equations. In this case the normal modes are just plane waves of given wavenumber and frequency. If we expand our solutions as a sum of normal modes (legitimate *only* because we have linear equations of motion) then this just equivalent to a Fourier transform.

In the real world the Hamiltonians are more complicated and more interesting. There are non-linear effects, springs are not perfect. This means that the plane waves modes mix and are no longer exact solutions, no longer normal modes. We can not solve such systems exactly so we tend to start with the system we can solve — perfect springs with plane wave normal modes — and then we do perturbation theory in terms of the non-linearities, that is expansion in a parameter that characterises the size of the interactions between the modes.

This is a purely classical analysis yet it contains much of what you see in a full QFT approach. Be clear in your mind where we are using purely classical ideas (here) and where we add new quantum aspects (see next question).

Question

Consider a ring of an even number of N balls with mass m. Their displacements around the ring are u_n and momenta p_n where $n = 0, 1, 2, \ldots, (N-1)$. The dynamics of the balls is given by the Hamiltonian of (3) with $\Omega = 0$, namely

$$H = \sum_{n=0}^{N-1} \left[\frac{p_n^2}{2m} + \frac{m\omega_0^2}{2}(u_{n+1} - u_n)^2 \right] \tag{4}$$

The ring means we use *periodic* boundary conditions: $u_N = u_0$ and $p_N = p_0$.

(i) How can you interpret the first two terms in terms of masses connected by springs with natural frequency ω_0 lying on a ring?

(ii) Consider the Fourier decomposition

$$u_n = \frac{1}{\sqrt{N}} \sum_k U_k e^{ikna} \qquad p_n = \frac{1}{\sqrt{N}} \sum_k P_k e^{ikna} \,. \tag{5}$$

for $n = 0, \ldots, N$.

Show that a set of allowed values of k in this system are

$$k = \frac{2\pi m}{Na} \quad \text{for} \quad m = 0, \pm 1, \pm 2, \ldots, \pm N/2. \tag{6}$$

You should consider the boundary conditions, and the fact that u_n is only defined at discrete values of n rather than as a continuous function of the spatial coordinate x.

You should check you know the following identities

$$\sum_{n=0}^{N-1} e^{ikna} = N\delta_{k,0} \,, \qquad \sum_k e^{ikna} = N\delta_{n,0} \,. \tag{7}$$

(iii) Show that

$$\sum_n (u_n)^2 = \sum_k U_k U_{-k} \,, \qquad \sum_n (p_n)^2 = \sum_k P_k P_{-k} \,, \qquad \sum_n (u_n - u_{n-1})^2 = \sum_k U_k U_{-k} 4(\sin(ka/2))^2 \,. \tag{8}$$

You need to recall the result for the geometric series given in equation (2).

Hence show that the Hamiltonian may be rewritten as (ignoring the $k=0$ mode)

$$H = \sum_{k \neq 0} \left[\frac{1}{2m} P_{-k} P_k + \frac{m\omega_k^2}{2} U_{-k} U_k \right] \tag{9}$$

with $\omega_k^2 = 4\omega_D^2 (\sin(ka/2))^2$.

*4. Harmonic Ring: quantisation

Background

The previous question identified the normal modes of a quadratic hamiltonian, one with linear equations of motion. There the normal modes were waves. A key part of quantisation and the QFT approach is that we can create quanta in each normal mode of a system. Thus $\hat{a}_n^\dagger$ adds one quanta to the n-th normal mode, and we say that we created one 'particle' or 'quasiparticle' of the system with properties associated with the n-th classical normal mode. This can be thought of as a postulate of QFT, much like we can start Quantum Mechanics with a series of postulates. In almost all cases the normal modes are just plane waves of given wavenumber and frequency so $\boldsymbol{k}$ is used to label our quanta. Again here we may expand our solutions as a sum of normal modes because we have linear equations of motion and so we see expressions which remind us of Fourier transforms.

Real Hamiltonians also have non-linear effects, imperfect springs. This means that the plane waves modes mix and are no longer exact solutions, no longer normal modes. In terms of particles we are saying that these particles interact. Provided these interactions are local in space, it makes sense to start from the normal modes, and to use them to represent widely separated particles, i.e. non-interacting or free particles. We can not solve the full non-linear/interacting system exactly so we do perturbation theory around the exactly solvable free/non-interacting Hamiltonian.

In this question we look only at the non-interacting part. We have a Hamiltonian which is quadratic. We can solve the QFT of this exactly. We start from the normal modes found from the purely classical analysis of the previous question. Hopefully this split into two questions about the same system makes it clear what is a purely classical idea where we are adding add new quantum aspects (putting hats on things).

Question

(i) To quantise this Hamiltonian we replace the classical variables u_n and p_n by operators $\hat{u}_n$ and $\hat{p}_n$ where $\hat{u}_n$ and $\hat{p}_n$ are Hermitian operators and

$$[\hat{u}_m, \hat{p}_n] = i\hbar\delta_{n,m}\,, \qquad [\hat{u}_m, \hat{u}_n] = [\hat{p}_m, \hat{p}_n] = 0\,. \tag{10}$$

Suppose we define $\widehat{U}_k$ and $\widehat{P}_k$ through

$$\hat{u}_n = \frac{1}{\sqrt{N}}\sum_k \widehat{U}_k e^{ikna} \qquad \hat{p}_n = \frac{1}{\sqrt{N}}\sum_k \widehat{P}_k e^{ikna}\,. \tag{11}$$

Show that the operators $\widehat{U}_k$ and $\widehat{P}_k$ satisfy (for momenta $k = 2\pi m/(Na)$ with m integer)

$$\widehat{U}_k^\dagger = \widehat{U}_{-k}\,, \qquad \widehat{P}_k^\dagger = \widehat{P}_{-k}\,, \qquad [\widehat{U}_p, \widehat{P}_q] = i\hbar\delta_{p+q,0}\,, \qquad [\widehat{U}_p, \widehat{U}_q] = [\widehat{P}_p, \widehat{P}_q] = 0\,. \tag{12}$$

(ii) We define the annihilation operators

$$\hat{a}_k = \frac{1}{\sqrt{2}}\left(\frac{l_k}{\hbar}\widehat{P}_k - \frac{i}{l_k}\widehat{U}_k\right)\,, \qquad l_k = \left(\frac{\hbar}{m\omega_k}\right)^{1/2}\,. \tag{13}$$

Check that l_k is a length scale. Hence what are the units of $\hat{a}$?

The creation operators must therefore be

$$\hat{a}_k^\dagger = \frac{1}{\sqrt{2}}\left(\frac{l_k}{\hbar}\widehat{P}_k^\dagger + \frac{i}{l_k}\widehat{U}_k^\dagger\right)\,. \tag{14}$$

Compute the commutator of $\hat{a}_p$ with the Hermitian conjugate $\hat{a}_q^\dagger$ where $\boldsymbol{p}$ and $\boldsymbol{q}$ need not be equal. Check this is the expected commutation relation.

(iii) The quantum Hamiltonian operator is (ignoring the $k = 0$ mode and any constants)

$$\widehat{H} = \sum_{k\neq 0}\left[\frac{1}{2m}\widehat{P}_{-k}\widehat{P}_k + \frac{m\omega_k^2}{2}\widehat{U}_{-k}\widehat{U}_k\right] \tag{15}$$

Show that it may be rewritten as

$$\widehat{H} = \sum_{k\neq 0}\hbar\omega_k\left(\hat{a}_k^\dagger\hat{a}_k + \frac{1}{2}\right) \tag{16}$$