Advanced Quantum Mechanics

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SS 2023

Exercise sheet 7 **Due: Sunday May 21 at 24:00**

1 Transformations of creation and annihilation operators

Suppose that we have a collection of annihilation operators $a_1, \ldots, a_K$ (corresponding to orthogonal single-particle states) and imagine that we create a new collection of operators $b_1, \ldots, b_K$ via $b_l = \sum_{k=1}^{K} Q_{l,k} a_k$ for $l = 1, \ldots, K$, where Q is a complex K times K matrix $Q \in \mathbb{C}^{K \times K}$.

a) Assume that $a_1, \ldots, a_K$ satisfy the bosonic commutation relations, i.e., $[a_k, a_{k'}] = 0$, $[a_k^\dagger, a_{k'}^\dagger] = 0$ and $[a_k, a_{k'}^\dagger] = \delta_{k,k'} \hat{1}$. *Find the necessary and sufficient conditions on Q for $b_1, \ldots, b_K$ to satisfy the bosonic commutation relations.*

(3 points)

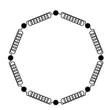
Remark: A change of (orthonormal) basis among the single-particle states (to which the annihilation operators are associated) causes a transformation of this type. It may also correspond to an active physical evolution.

b) In a) we investigated transformations that only mix the collection of annihilation operators within themselves (and in parallel mix the creation operators). However, one can consider an even more general type of transformation that combines both annihilation and creation operators. For the sake of simplicity we here only consider the transformation of a single pair $a, a^\dagger$ into a new pair $b, b^\dagger$. Let $a, a^\dagger$ be a bosonic annihilation and creation operator, and let $A, B \in \mathbb{C}$. *Find the necessary and sufficient conditions on A and B such that $b = Aa + Ba^\dagger$ and $b^\dagger = A^* a^\dagger + B^* a$, are bosonic annihilation and creation operators.*

(2 points)

Remark: This type of mappings is often called Bogoliubov transformations, and can be used to diagonalise certain types of many-body Hamiltonians.

2 Diagonalizing a Harmonic chain



In the lecture we consider the Hamiltonian of a harmonic chain (see section 2.3.1 'Phonons' in the lecture notes), which means that we have a chain of N particles that interact harmonically only with its nearest neighbors

$$H = \sum_{r=1}^{N} \left(\frac{P_r^2}{2m} + \frac{\kappa}{2} (X_r - X_{r+1})^2 \right),$$

where X_r are the deviations from equilibrium, and we assume periodic boundary conditions $X_{N+1} = X_1$. Here, X_r and P_r are the standard position and momentum operators and thus satisfy the canonical commutation relations

$$[X_r, X_{r'}] = 0, \quad [P_r, P_{r'}] = 0, \quad [X_r, P_{r'}] = i\hbar \hat{1} \delta_{r,r'}.$$

In the lecture it is claimed that we can rewrite H as

$$H = \frac{1}{2m} \sum_k \pi_k \pi_{-k} + 2\kappa \sum_k \sin^2(ka/2) \phi_k \phi_{-k}, \tag{1}$$

where

$$\phi_k = \sqrt{\frac{1}{N}} \sum_{r=1}^{N} e^{-ikra} X_r, \quad \pi_k = \sqrt{\frac{1}{N}} \sum_{r=1}^{N} e^{ikra} P_r.$$

We can also express X_r and P_r in terms of ϕ_k and π_k as

$$X_r = \sqrt{\frac{1}{N}} \sum_k e^{ikra} \phi_k, \quad P_r = \sqrt{\frac{1}{N}} \sum_k e^{-ikra} \pi_k.$$

As you might have noticed, I have avoided to say anything about what values that k spans. For the calculations it suffices to assume that

$$\frac{1}{N} \sum_{r=1}^{N} e^{i(k-k')ra} = \delta_{k,k'} \tag{2}$$

(and consequently $\frac{1}{N}\sum_{r=1}^{N} e^{i(k+k')ra} = \delta_{k,-k'}$). Moreover, if you are summing over k in expressions involving ϕ_k or π_k, then you can substitute k with $-k$. If you want to know what is behind this, then take a look at the gold star exercise.

a) *Show that the operators ϕ_k and π_k also satisfy the canonical commutation relations, i.e., that*

$$[\phi_k, \phi_{k'}] = 0, \quad [\pi_k, \pi_{k'}] = 0, \quad [\phi_k, \pi_{k'}] = i\hbar\hat{1}\delta_{k,k'}.$$

(2 points)

b) *Confirm that*

$$\phi_k^\dagger = \phi_{-k}, \quad \pi_k^\dagger = \pi_{-k}.$$

Hence, contrary to X_r and P_r, the operators ϕ_k and π_k are not Hermitian.

(1 point)

c) *Show that*

$$\sum_{r=1}^{N} P_r^2 = \sum_k \pi_k \pi_{-k}.$$

(1 point)

d) *Show that*

$$\sum_{r=1}^{N} (X_r - X_{r+1})^2 = 2\sum_{r=1}^{N} X_r^2 - 2\sum_{r=1}^{N} X_r X_{r+1}.$$

(1 point)

e) *Show that*

$$\sum_{r=1}^{N} X_r^2 = \sum_k \phi_k \phi_{-k}, \qquad \sum_{r=1}^{N} X_r X_{r+1} = \sum_k e^{-ika} \phi_k \phi_{-k} = \sum_k \cos(ka) \phi_k \phi_{-k}.$$

(2 points)

f) *Put together everything to show* (1).

Hint: Apply some suitable trigonometric identity.

(2 points)

g) In the lecture it is moreover claimed that H can be further rewritten as

$$H = \sum_k \hbar\omega_k \left(a_k^\dagger a_k + \frac{1}{2}\hat{1} \right), \qquad \omega_k = 2\sqrt{\frac{\kappa}{m}} |\sin(ka/2)|, \tag{3}$$

for the annihilation and creation operators a and $a^\dagger$ defined by

$$a_k = \frac{1}{\sqrt{2}} \left(\sqrt{\frac{m\omega_k}{\hbar}} \phi_k + i\sqrt{\frac{1}{m\hbar\omega_k}} \pi_{-k} \right).$$

Confirm that

$$[a_k, a_{k'}] = 0, \quad [a_k^\dagger, a_{k'}^\dagger] = 0, \quad [a_k, a_{k'}^\dagger] = \delta_{k,k'}\hat{1}.$$

(2 points)

h) *Show that*

$$\phi_k = \sqrt{\frac{\hbar}{2m\omega_k}} (a_k + a_{-k}^\dagger), \quad \pi_k = -i\sqrt{\frac{m\hbar\omega_k}{2}} (a_{-k} - a_k^\dagger). \tag{4}$$

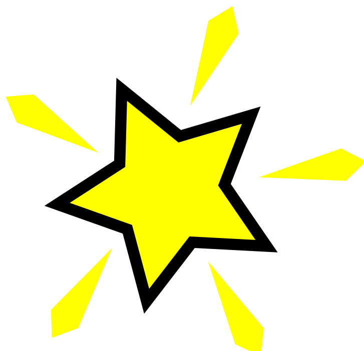
(2 points)

i) *Combine* (4) *with* (1) *to show* (3).

(2 points)

Remark: One might wonder why we refer to this exercise as a 'diagonalization'; usually this means that we find eigenvalues and eigenvectors to the given Hamiltonian. The reason is that we actually have done that, more or less, since (3) describes a collection of Harmonic oscillators, for which we know the eigenvalues and eigenvectors.

3 Gold star exercise: Some more details on exercise 2



In the previous exercise we did not go into any details concerning the index k in ϕ_k and π_k. If you take a look at the lecture notes (see section 2.3.1 'Phonons') you see that k is taken as the quasi-momentum

$$k = n\frac{2\pi}{Na}, \quad n = 1, \dots, N, \tag{5}$$

with a being the (equilibrium) distance between the particles. In this exercise, we explore the modular arithmetic associated to these notions.

In order to ease the analysis, we will here not use the quasi-momentum k, but rather the integer n in (5). In other words, instead of $\phi_k = \sqrt{\frac{1}{N}} \sum_{r=1}^N e^{-ikra} X_r$, we write

$$\phi_n = \sqrt{\frac{1}{N}} \sum_{r=1}^{N} e^{-i2\pi r \frac{n}{N}} X_r. \tag{6}$$

For what we want to focus on in this exercise, it suffices to consider X_r and ϕ_n, but the analogous results hold for P_r and π_n.

a) *Show that*

$$\phi_{n+mN} = \phi_n, \quad \forall m \in \mathbb{Z}.$$

Argue that this leads to

$$\phi_n = \phi_{n \bmod N}$$

(0 points)

b) The inverse of the mapping (6) is

$$X_r = \sqrt{\frac{1}{N}} \sum_{n=1}^{N} e^{-i2\pi r \frac{n}{N}} \phi_n.$$

Consider the following two alternative definitions

$$\tilde{X}_r = \sqrt{\frac{1}{N}} \sum_{n=0}^{N-1} e^{-i2\pi r \frac{n}{N}} \phi_n, \quad \overline{X}_r = \sqrt{\frac{1}{N}} \sum_{n=-\left\lfloor \frac{N-1}{2} \right\rfloor}^{\left\lceil \frac{N-1}{2} \right\rceil} e^{-i2\pi r \frac{n}{N}} \phi_n.$$

By comparison, one can see that X_r, $\tilde{X}_r$ and $\overline{X}_r$ differ with respect to which range of n that we sum over. *Show that*

$$X_r = \tilde{X}_r = \overline{X}_r.$$

Hint: For $\overline{X}_r$ I believe that it is easier if one separates the cases of N being even or odd.

(0 points)

Remark: These three examples of different ranges yield the same result. In fact, it would work with any N elements of $\mathbb{Z}$ that are independent with respect to mod$N$ (meaning that $x_k \bmod N \neq x_l \bmod N$ for all $k \neq l$). Each choice may have its advantages and disadvantages, and in the end it is a matter of taste. Similar considerations also apply to the index r. (Since the lecture notes uses $r = 1, \ldots, N$, I have also used it here. However, for some parts in the calculations, it would have been easier to pick $r = 0, \ldots, N-1$.)

c) In exercise 2 we claimed that for sums involving ϕ_k and π_k we can replace k with $-k$, so let us confirm this. *In other words, show that* $\sum_{n=1}^{N} f(\phi_n, \pi_n) = \sum_{n=1}^{N} f(\phi_{-n}, \pi_{-n})$, *where f is some arbitrary function.* (We assume that all that we have shown for ϕ_n also apply to π_n.)

(0 points)

d) For the sake of completeness, let us finally confirm (2), which translated from k to n reads

$$\frac{1}{N} \sum_{r=1}^{N} e^{i2\pi \frac{n-n'}{N} r} = \delta_{n,n'}.$$

(0 points)