Online Quantum Field Theory Course

Exercises 1

The harmonic oscillator in the operator formalism

(a) Consider the simple harmonic oscillator in 1 dimension with the Hamiltonian

\[ H = \frac{p^2}{2m} + \frac{m\omega^2}{2}x^2. \]  

(1)

Derive the eigenvectors and eigenvalues of the Hamiltonian, making use exclusively from the Heisenberg algebra

\[ [x, p]_\hbar = i\hbar. \]  

(2)

Note that we set here and in the following \( \hbar = 1 \).

**Hint:** Use the annihilation and creation operators

\[ a = \sqrt{\frac{m\omega}{2}}x + \frac{i}{\sqrt{2\omega m}}p \]  

and \( a\dagger \) to show that

\[ H = \left( a\dagger a + \frac{1}{2} \right)\omega \]  

(4)

and that the operator \( N = a\dagger a \) has the eigenvalues \( \{0, 1, 2, \ldots\} \) and that the corresponding eigenvectors \( |n\rangle \) are given recursively by \( a|0\rangle = 0 \) and \( |n + 1\rangle = 1/\sqrt{n + 1}a\dagger |n\rangle \), where we have normalised the vectors to 1.

(b) From the results of exercise (a) calculate the ground state and the first two excited energy eigenstates. For that use the known representation of quantum mechanics in position representation:

\[ x\psi(x) = x\psi(x), \quad p\psi(x) = \frac{i}{1} \frac{d}{dx} \psi(x). \]  

(5)

**Hint:** Use \( a\psi_0(x) = 0 \) to find the ground state wave function

\[ \psi_0(x) = \mathcal{N} \exp \left( -\frac{m\omega}{2}x^2 \right) \]  

(6)

and apply to it the recursion relation \( |n + 1\rangle = 1/\sqrt{n + 1}a\dagger |n\rangle \).

(c)∗ The propagator of the harmonic oscillator (operator formalism)\(^1\)

Use the Heisenberg picture, where the full time dependence is at the selfadjoint operators, which represent observables. With the Hamiltonian (1) solve the operator equations of motion in the Heisenberg picture:

\[ \dot{x} = \frac{1}{i} [x, H], \quad \dot{p} = \frac{1}{i} [p, H] \]  

(7)

\(^1\)Exercises with an asterisk are a little bit more difficult.
with the initial conditions
\[ x(t = 0) = x_0, \quad p(t = 0) = p_0, \] (8)

Now the generalised eigenvectors of the position operator is defined by
\[ x(t) \langle x,t \rangle = x \langle x,t \rangle. \] (9)

Show that then the propagator is given by
\[ U(x,t;x_0,0) = \langle x,t | x_0,0 \rangle. \] (10)

**Hint:** In the Heisenberg picture the state kets are time independent, and the wave function’s\(^2\) time dependence is completely given by the time dependence of the (generalised) eigenvectors: \( \psi(t,x) = \langle x,t | \psi \rangle \). In this definition of the wave function insert a unit operator \(1 = \sum dx_0 |x_0,0 \rangle \langle x_0,0|\).

To find the explicit expression for \( U \) can be found by using the representation in terms of the generalised basis \( |x_0,0 \rangle \), by solving the eigenvalue equation (9), using the identities
\[ x_0 \langle x_0,0 | \psi \rangle = x_0 \langle x_0,0 | \Psi \rangle, \quad p_0 \langle x_0,0 | \psi \rangle = \frac{1}{i} \frac{d}{dx_0} \langle x_0,0 | \Psi \rangle, \] (11)

where the solutions of the equations of motion (8-9) have to be used to express \( x(t) \) in terms of \( x_0 \) and \( p_0 \).

To find the normalisation of \( U \), use the fact that the time evolution has to be unitary at each \( t \), i.e.,
\[ \int dx_0 U(x,t;x_0,0)U^*(x',t;x_0,0) = \int dx_0 \langle x,t | x_0,0 \rangle \langle x_0,0 | x',t \rangle = \langle x,t | x',t \rangle = \delta(x-x'). \] (12)

To determine finally the phase of \( U \) use the fact that
\[ U(x,t = 0;x_0,0) = \langle x,0 | x_0,0 \rangle = \delta(x-x_0). \] (13)

**Hint:** For the last step, calculate
\[ f(t,x) = \int dx_0 U(x,t;x_0,0) \exp(-ax_0^2) \] (14)

and take the limit \( \lim_{t \to 0^+} f(t,x) \overset{!}{=} \exp(-ax^2) \) to determine \( U \)’s phase.

(d) How can one calculate from the propagator \( U(x,t;x_0,0) \) the thermodynamic partition sum
\[ Z(\beta) = \text{Tr} \exp(-\beta H)? \] (15)

**Hint:** Use the fact that from our Heisenberg picture calculation we know that
\[ U(x,t;x_0,0) = \langle x,t | x_0,0 \rangle = \langle \exp(itH)x,0 | x_0,0 \rangle = \langle x,0 | \exp(-itH) | x_0,0 \rangle. \] (16)

Which value have you to chose for \( t \) to get \( \exp(-\beta H) \) on the right-hand side of (16)?

Then use the definition of the trace:
\[ \text{Tr} O = \int dx \langle x,0 | O | x,0 \rangle. \] (17)

How can one express the thermodynamical partition sum as a path integral? What are the boundary conditions in this path integral?

\(^2\)Note that the wave function and thus also the propagator are independent of the picture of time evolution!
(e) Use the complete set of energy eigenvectors, determined in (a), in the trace definition to obtain the partition sum:

\[ Z = \text{Tr} \exp(-\beta H) = \sum_{n=0}^{\infty} \langle n | \exp(-\beta H) | n \rangle. \] (18)

Solutions

(a) From (2) and the definitions (3), one immediately finds the commutator between annihilation and creation operator:

\[ [a, a^\dagger]_\_ = 1, \] (19)

and from this we get, using \( N = a^\dagger a \):

\[ [N, a]_\_ = -a, \quad [N, a^\dagger]_\_ = +a^\dagger. \] (20)

Further we note that \( N \) is a positively semidefinite operator, because for all \( |\psi\rangle \in \mathcal{H} \)

\[ \langle \psi | N | \psi \rangle = \langle \psi | a^\dagger a | \psi \rangle = \langle a\psi | a\psi \rangle \geq 0. \] (21)

Especially all its eigenvalues \( n \geq 0 \).

Suppose now, we have found an eigenvector of \( N \) with eigenvalue \( \alpha \) which we call \( |\alpha\rangle \) as usual in the Dirac notation. Then from (20) we get

\[ N |\alpha\rangle = (N, a) a^\dagger |\alpha\rangle = (\alpha - 1) a^\dagger |\alpha\rangle. \] (22)

Thus \( a |\alpha\rangle \) is either an eigenvector of \( N \) with eigenvalue \( \alpha - 1 \) or 0. Since \( N \geq 0 \), there must exist an eigenvector \( |0\rangle \) with eigenvalue 0, because otherwise, we could apply \( a \) to \( |\alpha\rangle \) as often as we like and get as negative eigenvectors as we liked, in contradiction to \( N \geq 0 \). This argument also shows that all eigenvalues must be non-negative integers.

Using (20) again

\[ N a^\dagger |\alpha\rangle = ([N, a^\dagger]_\_ + a^\dagger N) |\alpha\rangle = (\alpha + 1) a^\dagger |\alpha\rangle, \] (23)

we see that with \( |\alpha\rangle \) also \( a^\dagger |\alpha\rangle \) is eigenvector of \( N \) with eigenvalue \( \alpha + 1 \). From this we conclude that the spectrum of \( N \) is \( \mathbb{N} = \{0, 1, 2, \ldots\} \). Assuming further that \( H \) is not degenerate, i.e., we have an elementary particle with no internal degrees of freedom, all eigenvectors can be found be successively applying \( a^\dagger \) to the ground state \( |0\rangle \).

Using the definition of the annihilation and creation operators (3), by multiplying out the product \( a^\dagger a \) and using the commutator (2), one finds immediately (4), yielding the eigenvalues of \( H \) to be \( E_n = (n + 1/2) \omega \).

Assuming \( |n\rangle \) to be normalised, we obtain \( |n+1\rangle \) by application of \( a^\dagger \). With (19) we find

\[ \langle a^\dagger n | a^\dagger n \rangle = \langle n | a a^\dagger | n \rangle = \langle n | N + 1 | n \rangle = n + 1, \] (24)

where we have assumed \( |n\rangle \) to be normalised. Choosing all normalisation constants to be real, we thus have

\[ |n\rangle = \frac{1}{\sqrt{n!}} a^{\dagger n} |0\rangle, \quad a |n\rangle = \sqrt{n-1} |n-1\rangle. \] (25)

The latter equation follows hereby from the former by applying once more (19).
(b) We denote the eigenvectors in the position representation as \( \varphi_n(x) = \langle x | \varphi \rangle \). Using the definition (3) in the position representation and the fact that the vacuum is defined by \( a |0 \rangle = 0 \), we get

\[
\left[ \sqrt{\frac{m\omega}{2}} x + \frac{1}{\sqrt{2\omega m}} d_x \right] \varphi_0(x) = 0 \Rightarrow d_x \varphi_0 = -m\omega x \varphi_0.
\]

This differential equation is immediately solved by “separation of variables”:

\[
\varphi_0(x) = \mathcal{N} \exp \left( -\frac{m\omega}{2} x^2 \right).
\]

The normalisation condition

\[
1 = \langle 0 | 0 \rangle = \int dx \varphi_0(x)^* \varphi_0(x) = |\mathcal{N}|^2 \int \exp \left( -\frac{m\omega}{2} x^2 \right) = |\mathcal{N}|^2 \frac{\sqrt{\pi}}{m\omega} \Rightarrow \mathcal{N} = \left( \frac{m\omega}{\pi} \right)^{1/4}.
\]

(c) It should be emphasised that all calculations so far were independent of the picture of time evolution. For this part (c) of the exercises we now choose the Heisenberg picture where all the time dependence is shuffled to the operators, which represent observables. The state kets are time independent. This choice has the advantage that the quantum-mechanical covariant time derivative is identical with the usual mathematical time derivative of the operators.

Thus, in the case of the harmonic oscillator we find, by application of the (picture independent!) commutator rule (2):

\[
\frac{d}{dt} x = \frac{i}{\hbar} [x, H] = \frac{p}{m}, \quad \frac{d}{dt} p = \frac{i}{\hbar} [p, H] = -m\omega x.
\]

The fact that here the operator equations of motion in the Heisenberg picture look the same as the classical equations of motion for phase-space coordinates is a nice feature of the harmonic oscillator and the free particle. For more general cases this needs not to hold true!

To calculate the propagator, for convenience we choose \( t_i = 0 \). Then we have to solve the e.o.m. (29) with the initial conditions \( x(t = 0) = x_0 \) and \( p(t = 0) = p_0 \). The solutions are found as in classical mechanics:

\[
x(t) = x_0 \cos(\omega t) + \frac{p_0}{m\omega} \sin(\omega t),
\]

\[
p(t) = -m\omega x_0 \sin(\omega t) + p_0 \cos(\omega t).
\]

Now let \( |x, t\rangle \) be the eigenket of \( x(t) \) of the eigenvalue \( x \) (note that \( x \) does not depend on time).

From the formal solution of the Heisenberg-picture equations of motion

\[
O(t) = \exp(itH) O_0 \exp(-itH) \text{ follows } |x, t\rangle = \exp(itH) |x, 0\rangle.
\]

The propagator is now defined as

\[
U(x,t; x_0,0) = \langle x, t | x_0, 0 \rangle.
\]

Note that this is a picture-independent object since it can be uniquely determined as the time-evolution kernel of the picture-independent wave function. Expressed in the here used Heisenberg picture, this is seen immediately as follows: For any state ket (time independent!) we have:

\[
\psi(t, x) = \langle x, t | \psi \rangle = \int dx_0 \langle x, t | x_0, 0 \rangle \langle x_0, 0 | \psi \rangle = \int dx_0 U(x, t; x_0,0) \psi(0, x_0).
\]
But now back to our exercise! We use the observation
\[ U^*(x, t; x_0, 0) = \langle x_0, 0 | x, t \rangle \]  
(34)
and the fact that in the representation with respect to eigenkets of \( x_0 \), namely \( |x_0, 0\rangle \), we have (11) which is valid for any ket \( |\psi\rangle \) and thus also for \( |\psi\rangle = |x, t\rangle \). The condition that \( |x, t\rangle \) is eigenvector of \( x(t) \) with eigenvalue \( x \) thus, using (30) reads in \( |x_0, 0\rangle \)-representation:
\[ xU^*(x, t; x_0, 0) = \left[ x_0 \cos(\omega t) + \frac{1}{im\omega} \sin(\omega t) \right] U^*(x, t; x_0, 0) = xU^*(x, t; x_0, 0). \]  
(35)
This equation has to be solved with the initial condition
\[ U(x, 0; x_0, 0) = \delta(x - x_0). \]  
(36)
The general solution of (35) is (taking the conjugate complex again):
\[ U(x, t; x_0, t_0) = N(x, t) \exp \left\{ \frac{im\omega}{2\sin(\omega t)} [x_0^2 \cos(\omega t) - 2xx_0] \right\}. \]  
(37)
Here we have indicated that the integration constant depends on \( x \) and \( t \).
To find this \( N \) under the initial condition (36), as a first step we use:
\[ \delta(x - x') = \langle x, t | x', t \rangle = \int dx_0 \langle x, t | x_0, 0 \rangle \langle x_0, 0 | x', t \rangle = \int dx_0 U(x, t; x_0, 0)U^*(x', t; x_0, 0). \]  
(38)
Plugging in (37), one finds
\[ \delta(x - x') = N^*(x', t)N(x, t)2\pi\delta \left[ \frac{m\omega}{\sin(\omega t)} (x - x') \right] = |N(x, t)|^2 \frac{2\pi \sin(\omega t)}{m\omega} \delta(x - x'). \]  
(39)
So we must have
\[ N(x, t) = \sqrt{ \frac{m\omega}{2\pi \sin(\omega t)} } \exp[i\alpha(x, t)], \quad \alpha(x, t) \in \mathbb{R}. \]  
(40)
Now we have to use \( \alpha \) to ensure (36). To this end we calculate (14)
\[ \int dx_0 U(x, t; x_0, 0) \exp(-ax_0^2) = \frac{\exp[i\alpha(x, t)]}{\sqrt{A \sin(\omega t) - i \cos(\omega t)}} \times \exp \left\{ -\frac{im\omega x^2}{2\sin(\omega t)} \left[ \frac{\sin^2(\omega t) - iA \sin(\omega t) \cos(\omega t)}{\cos(\omega t) + iA \sin(\omega t)} + \cos(\omega t) \right] \right\}. \]  
(41)
Here for convenience we have set \( A = 2a/(m\omega) \). Clearly, we get the right limit for \( t \to 0^+ \) by setting
\[ \alpha = -\frac{\pi}{4} + \frac{m\omega^2x^2 \cos(\omega t)}{2\sin(\omega t)}. \]  
(42)
So, finally we arrive at the same result as with the path integral:
\[ U(x, t; x_0, 0) = \sqrt{ \frac{m\omega}{2\pi \sin(\omega t)} } \exp \left\{ \frac{im\omega}{2\sin(\omega t)} \left[ (x^2 + x_0^2) \cos(\omega t) - 2xx_0 \right] - \frac{i\pi}{4} \right\}. \]  
(43)
(d) In (16) we have to set $t = -i\beta$ to get an operator $\exp(-\beta H)$. Then using $|x,0\rangle$ as basis in the definition of the trace, we get

$$Z = \text{Tr} \exp(-\beta H) = \int \text{d}x U(x,-i\beta,x,0) = \frac{1}{2 \sinh(\beta \omega/2)} = \frac{\exp(\beta \omega/2)}{\exp(\beta \omega) - 1}. \quad (44)$$

Up to a factor $\exp(\beta E_0)$ this is the Bose-Einstein distribution. The additional factor is physically irrelevant, since it can be eliminated by a “renormalisation” of the ground-state energy.

To write the thermodynamical partition sum as path integral we note that we have to calculate $U(x,-i\beta;x,0)$. This describes the time evolution along the imaginary time axis (from $t_i = 0$ to $t_f = -i\beta$). The boundary condition is given by the fact that we have to look for propagator for the same position in the “initial” and the “final” state. This yields to a path integral which is for a formal “motion” of the particle along the imaginary time axis from 0 to $-i\beta$ with boundary conditions

$$x(-i\beta) = x(0) = x. \quad (45)$$

Finally, one has to integrate over $x$. Usually, one defines the thermal path integral including this final integration, i.e.,

$$Z(\beta) = \int D'x \exp\{iS_E[x]\}, \quad (46)$$

where $S_E$ stands for the Euclidean version of the action in the Lagrange formalism. Here, we have assumed that the momentum integration yields from the Hamilton version of the path integral to the Lagrangian version. The integration measure has to be chosen as described in my QFT script. Here, the factors can be important, contrary to the case of the generating functional in vacuum QFT since here these factors may depend on $\beta$. We will come back to this problem at a later point in our discussion.

(e) Once knowing the energy-eigenvalues, the partition sum (44) is much easier found by using the energy-eigenkets to calculate the trace:

$$\text{Tr} \exp(-\beta H) = \sum_{n=0}^{\infty} \langle n | \exp(-\beta H) | n \rangle = \exp(-\beta \omega/2) \sum_{n=0}^{\infty} \exp(-n\beta \omega) = \frac{\exp(-\beta \omega/2)}{1 - \exp(-\beta \omega)}. \quad (47)$$

Appendix: Alternative solution for (c)

During our discussion of (c), a nice alternative solution came from Tom. It has the advantage that we can get the complete $x,x_0$-dependence of the propagator before we find the overall constant factor.

The trick is to use the time-translation invariance of the problem in the following way:

$$U(x,t;x_0,0) = \langle x,t|x_0,0 \rangle = \langle x_0,0|x,t \rangle^* = \langle x_0,-t|x,0 \rangle^* = U^*(x_0,-t;x,0). \quad (48)$$

To prove this formally, we note

$$\langle x_0,0|x,t \rangle = \langle x_0,0|\exp(+iHt)|x,0 \rangle = \langle \exp(-iHt)x_0,0|x,0 \rangle = \langle x_0,-t|x,0 \rangle := U(x_0,-t;x,0). \quad (49)$$

Now we use this with (37):

$$\mathcal{N}(x,t) \exp \left\{ \frac{im\omega}{2 \sin(\omega t)} \left[ x_0^2 \cos(\omega t) - 2xx_0 \right] \right\} = \mathcal{N}^*(x_0,-t) \exp \left\{ + \frac{im\omega}{2 \sin(\omega t)} \left[ x^2 \cos(\omega t) - 2xx_0 \right] \right\} \quad (50)$$
or
\[ N(x, t) \exp \left[ -\frac{im\omega}{2\sin(\omega t)} x^2 \cos(\omega t) \right] = N^*(x_0, -t) \exp \left[ -\frac{im\omega}{2\sin(\omega t)} x_0^2 \cos(\omega t) \right] := N'(t). \] (51)
Since the right-hand side of this equation does not depend on \( x \), the same must hold true for (51). Thus the propagator must be of the structure
\[ U(x, t; x_0, 0) = N'(t) \exp \left\{ \frac{im\omega}{2\sin(\omega t)} [(x_0^2 + x^2) \cos(\omega t) - 2xx_0] \right\}. \] (52)
As before (38) yields
\[ N'(t) = \sqrt{\frac{m\omega}{2\pi \sin(\omega t)}} \exp[i\alpha'(t)], \quad \alpha'(t) \in \mathbb{R}. \] (53)
Now we can directly take the limit of the analogue to (41), yielding
\[ \lim_{t \to 0^+} \int dx U(x, t; x_0, 0) \exp(-ax_0^2) = \exp(-ax^2 + i\pi/4 + i\alpha'(t)) \Rightarrow \alpha'(t) = -\frac{\pi}{4}. \] (54)
So, of course, we finally obtain the same result as before, i.e., (43).