Prof. Dr. Viatcheslav Mukhanov Winter term 2019/2020

# Exercises on Quantum Mechanics II (TM1/TV)

## Problem set 6, discussed November 25 - November 29, 2019

## Exercise 37

Consider the transition amplitude for a free particle in the path integral representation,

$$K(x_f, x_i; T) = \int\limits_{\begin{cases} x(T)=x_f \\ x(0)=x_i \end{cases}} \mathcal{D}x \, \exp\left(\frac{i}{\hbar} S[x(t)]\right) \tag{1}$$

Why does $\mathcal{D}x = \mathcal{D}y$ hold for a transformation of $x(t)$ according to $x(t) = x_{class.}(t) + y(t)$, where $y(t)$ is arbitrary?

**Solution** The integration measure is defined as

$$\mathcal{D}x = \lim_{N\to\infty} \frac{1}{\sqrt{2\pi i\hbar m^{-1}\triangle t_0}} \prod_{k=1}^{N} \frac{dx_k}{\sqrt{2\pi i\hbar m^{-1}\triangle t_k}} \tag{2}$$

We can regard the multiple integrations $dx_k$ as a multidimensional integral. Upon a change of variables $x_i \to x_{class,i} + y_i$, where $x_{class,i}$ is a constant, the integration measure changes by a factor according to the determinant of the Jacobian matrix.

$$\mathcal{D}x = \mathcal{D}y \, \det J \ , \qquad J_{ij} = \frac{\partial x_i}{\partial y_j} \tag{3}$$

But for our transformation, the Jacobian is just the identity, so the determinant is 1 and the measure does not change.

## Exercise 38 (Central Tutorial)

In the lecture it was shown that, by using the transformation from Exercise 37, the transition amplitude for a free particle can be approximated as

$$K(x_f, x_i; T) = F(T) \, \exp\left(\frac{i}{\hbar} S[x_{class}]\right) \ , \tag{4}$$

where $F(T)$ is an undetermined function of $T = t_f - t_i$. Check by direct calculation that

$$F(T) = \int_{y(t_i)=0}^{y(t_f)=0} \mathcal{D}y \, \exp\left(\frac{i}{\hbar}\frac{m}{2}\int_0^T \dot{y}^2\right) = \left(\frac{m}{2\pi i\hbar T}\right)^{\frac{1}{2}} \tag{5}$$

*Hint*: The following integral might be useful:

$$\int dx \, \exp\left[-\frac{ax^2}{2} + ibx\right] = \sqrt{\frac{2\pi}{a}} \, \exp\left[-\frac{b^2}{2a}\right] \tag{6}$$

**Solution** For the propagator we have

$$K(x_f, x_i; T) = \int_{x_i}^{x_f} \mathcal{D}x \, \exp\left[\frac{i}{\hbar}\int_0^T dt \frac{m\dot{x}^2}{2}\right] \tag{7}$$

and the total propagator is then calculated by the integrals over the intermediate points. As we showed in Exercise 38, the integration measure does not change, so we can concentrate on the integrand. Our transformation is $x_i \to x_{class,i} + y_i$ so we get

$$K(x_f, x_i; T) = \int_{y_i}^{y_f} \mathcal{D}y \, \exp\left[\frac{i}{\hbar}\int_0^T dt \frac{m}{2}(\dot{x}_{class} + \dot{y})^2\right] \tag{8}$$

Evaluating the integral gives

$$\int_0^T dt \frac{m}{2}(\dot{x}_{class} + \dot{y})^2 = \int_0^T dt \, \frac{m}{2}\dot{x}_{class}^2 + \int_0^T dt \, m\dot{x}_{class}\dot{y} + \int_0^T dt \, \frac{m}{2}\dot{y}^2 = S[x_{class}] + S[y] \tag{9}$$

where we did a partial integration on the second term and used the fact that $x_{class}$ satisfies the classical equations of motion, i.e. $\ddot{x}_{class} = 0$ and that $y(0) = y(T) = 0$. This gives the function $F(T)$ as

$$F(T) = \int_{y(t_i)=0}^{y(t_f)=0} \mathcal{D}y \, \exp\left(\frac{i}{\hbar}\frac{m}{2}\int_0^T \dot{y}^2\right) \tag{10}$$

To calculate this function we write the integration measure explicitly to get

$$F(T) = \lim_{N\to\infty} \int \frac{1}{\sqrt{2\pi i\hbar m^{-1}\triangle t_0}} \left(\prod_{k=1}^{N} \frac{dy_k}{\sqrt{2\pi i\hbar m^{-1}\triangle t_k}}\right) \exp\left[\frac{i}{\hbar}\frac{m}{2}\sum_{k=0}^{N}\left(\frac{(y_{k+1}-y_k)^2}{\triangle t_k}\right)\right] . \tag{11}$$

Now performing one of the integrals (for $1 \le k \le N$) gives

$$\begin{aligned}
&\int dy_k K(y_{k+1}, y_k; \triangle t_k) K(y_k, y_{k-1}; \triangle t_{k-1}) = \\
&= \int dy_k \frac{m}{2\pi i\hbar\sqrt{\triangle t_k \triangle t_{k-1}}} \exp\left[\frac{i}{\hbar}\frac{m}{2}\left(\frac{(y_{k+1}-y_k)^2}{\triangle t_k} - \frac{(y_k - y_{k-1})^2}{\triangle t_{k-1}}\right)\right] = \\
&= \frac{m}{2\pi i\hbar\sqrt{\triangle t_k \triangle t_{k-1}}} \exp\left[\frac{i}{\hbar}\frac{m}{2}\frac{1}{\triangle t_k \triangle t_{k-1}}\left(y_{k+1}^2 \triangle t_{k-1} + y_{k-1}^2 \triangle t_k\right)\right] \times \\
&\quad \times \int dy_k \, \exp\left[\frac{i}{\hbar}\frac{m}{2}\frac{1}{\triangle t_k \triangle t_{k-1}}\left(y_k^2(\triangle t_k + \triangle t_{k-1}) - 2y_k(y_{k+1}\triangle t_{k-1} + y_{k-1}\triangle t_k)\right)\right]
\end{aligned}$$

Now using the formula for the gaussian integral (6), we can evaluate the integral and get

$$\begin{aligned}
&\int dy_k K(y_{k+1}, y_k; \triangle t_k) K(y_k, y_{k-1}; \triangle t_{k-1}) = \\
&= \sqrt{\frac{m}{2\pi i\hbar(\triangle t_k + \triangle t_{k-1})}} \exp\left[\frac{i}{\hbar}\frac{m}{2}\frac{(y_{k+1}-y_{k-1})^2}{\triangle t_k + \triangle t_{k-1}}\right] = \\
&= K(y_{k+1}, y_{k-1}; \triangle t_k + \triangle t_{k-1})
\end{aligned}$$

In this manner we can integrate over all intermediate points to get

$$K(y_f, y_i; T) = \sqrt{\frac{m}{2\pi i\hbar T}} \exp\left[\frac{i}{\hbar}\frac{m}{2}\frac{(y_f - y_i)^2}{T}\right] . \tag{12}$$

But in this case $y_f = y_i = 0$, so

$$F(T) = \sqrt{\frac{m}{2\pi i\hbar T}} . \tag{13}$$

## Exercise 39 (Central Tutorial)

Consider the path integral with Hamiltonian $\hat{H} = \hat{q}\hat{p}^2\hat{q}$. Derive the measure for the Lagrangian path integral. *Hints*: 1) Follow the derivation of the path integral for $\hat{H} = \hat{p}^2 + V(\hat{q})$. The integration measure is explicitly dependent on $q(t)$. 2) The integral (6) might be useful.

**Solution** The propagator is defined as

$$K(q_f, q_i; t_f, t_0) = \langle q_f \,|\, \hat{U}(t_f, t_0) \,|\, q_0 \rangle \tag{14}$$

After introducing $N$ intermediate points and inserting identities we can write it as the product of intermediate propagators

$$K(q_f, q_i; t_f, t_0) = \int dq_N dq_{N-1}...dq_1 \left( \prod_{k=0}^{N} K(q_{k+1}, q_k; t_{k+1}, t_k) \right) \tag{15}$$

Now by expanding the operator $\hat{U}$ in the definition of the propagator, each intermediate propagator can be expressed in terms of the momenta and positions.

$$K(q_{k+1}, q_k; t_{k+1}, t_k) = \int \frac{dp_k}{2\pi\hbar} \exp\left[ \frac{i\triangle t_k}{\hbar} \left( p_k \frac{q_{k+1} - q_k}{\triangle t_k} - H(p_k, q_k) \right) \right] \tag{16}$$

Here $\hat{H}$ has to be in canonical form, i.e. all $\hat{q}$ to the right of the $\hat{p}$.

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*Aside*: The above paragraphs are properly explained in the lecture, following pages 132-136 in CSQFT V. Mukhanov's book. Now the required computation begins.

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For our Hamiltonian $\hat{H} = \hat{q}\hat{p}^2\hat{q} = \hat{p}^2\hat{q}^2 + 2i\hbar\hat{p}\hat{q}$, as checked in Exercise 31. Then the propagator is

$$K(q_{k+1}, q_k; t_{k+1}, t_k) = \int \frac{dp_k}{2\pi\hbar} \exp\left[ \frac{i\triangle t_k}{\hbar} \left( p_k \frac{q_{k+1} - q_k}{\triangle t_k} - p_k^2 q_k^2 - 2i\hbar p_k q_k \right) \right] \tag{17}$$

The gaussian integral can be evaluated using (6). In our case this yields the result

$$K(q_{k+1}, q_k; t_{k+1}, t_k) = \frac{1}{2q_k\sqrt{i\pi\hbar\triangle t_k}} \exp\left[ -\frac{\hbar}{4iq_k^2\triangle t_k} \left( \frac{q_{k+1} - q_k}{\hbar} - 2iq_k\triangle t_k \right)^2 \right] . \tag{18}$$

As we have $N$ such terms we get a sum in the exponent.

$$K(q_f, q_0; t_f, t_0) = \int \left[ \prod_{k=1}^{N} dq_k \frac{1}{2q_k\sqrt{i\pi\hbar\triangle t_k}} \right] \frac{1}{2q_0\sqrt{i\pi\hbar\triangle t_0}} \exp\left[ -\sum_{k=0}^{N} \frac{\hbar}{4iq_k^2\triangle t_k} \left( \frac{q_{k+1} - q_k}{\hbar} - 2iq_k\triangle t_k \right)^2 \right] \tag{19}$$

In the limit $N \to \infty$ we can replace $q_{k+1} - q_k = \dot{q}\triangle t_k$ and the sum by an integral over $t$.

$$K(q_f, q_0; t_f, t_0) = \lim_{N\to\infty} \int \left[ \prod_{k=1}^{N} dq_k \frac{1}{2q_k\sqrt{i\pi\hbar\triangle t_k}} \right] \frac{1}{2q_0\sqrt{i\pi\hbar\triangle t_0}} \exp\left[ \frac{i}{\hbar} \int dt \frac{1}{4q^2} \left( \dot{q} - 2i\hbar q \right)^2 \right] \tag{20}$$

Partial integration with $\frac{d}{dt}\ln q = \frac{\dot{q}}{q}$ gives us a total factor of $\frac{q_f}{q_0}$ and we obtain

$$K(q_f, q_0; t_f, t_0) = \lim_{N\to\infty} \int \left[ \prod_{k=1}^{N} dq_k \frac{1}{2q_k\sqrt{i\pi\hbar\triangle t_k}} \right] \frac{1}{2q_0\sqrt{i\pi\hbar\triangle t_0}} \frac{q_f}{q_0} \exp\left[ \frac{i}{\hbar} \int dt \left( \frac{\dot{q}^2}{4q^2} - \hbar^2 \right) \right] . \tag{21}$$

We can rewrite this using the integration measure

$$\mathcal{D}q \equiv \lim_{N\to\infty} \frac{1}{2q_0\sqrt{i\pi\hbar\triangle t_0}} \frac{q_f}{q_0} \prod_{k=1}^{N} dq_k \frac{1}{2q_k\sqrt{i\pi\hbar\triangle t_k}} \tag{22}$$

which is explicitly dependent on $q$ (compare with (2)).

## Exercise 40

Show that for analytic operators $\hat{A}(\hat{p},\hat{q})$ the following holds:

$$\frac{d\hat{A}}{dt} = -\frac{i}{\hbar}[\hat{A},\hat{H}] \tag{23}$$

Remark: Generally we have $\frac{d\hat{A}}{dt} \neq \frac{\partial\hat{A}}{\partial\hat{q}}\dot{\hat{q}} + \frac{\partial\hat{A}}{\partial\hat{p}}\dot{\hat{p}}$.

### Solution

$$\begin{aligned}
\left\langle \psi \left| \frac{d\hat{A}(p(t),q(t))}{dt} \right| \psi \right\rangle_H &= \left\langle \frac{\partial\psi(t)}{\partial t} \left| \hat{A} \right| \psi(t) \right\rangle_S + \left\langle \psi(t) \left| \hat{A} \right| \frac{\partial\psi(t)}{\partial t} \right\rangle_S \\
&= -\frac{1}{i\hbar} \langle \psi(t) \,|\, \hat{H}\hat{A} \,|\, \psi(t) \rangle_S + \frac{1}{i\hbar} \langle \psi(t) \,|\, \hat{A}\hat{H} \,|\, \psi(t) \rangle_S \\
&= -\frac{i}{\hbar} \langle \psi \,|\, [\hat{A},\hat{H}] \,|\, \psi \rangle_H
\end{aligned}$$

Therefore we have

$$\frac{d\hat{A}}{dt} = -\frac{i}{\hbar}[\hat{A},\hat{H}] \tag{24}$$

An alternative proof comes directly from the definition of the operator in Heisenberg picture

$$\hat{A}^{(H)}(t) = \hat{U}^\dagger(t)\hat{A}^{(S)}\hat{U}(t) \; . \tag{25}$$

Then

$$\begin{aligned}
\frac{d}{dt}\hat{A}^{(H)}(t) &= \frac{\partial\hat{U}^\dagger(t)}{\partial t}\hat{A}^{(S)}\hat{U}(t) + \hat{U}^\dagger(t)\hat{A}^{(S)}\frac{\partial\hat{U}(t)}{\partial t} \\
&= \frac{i}{\hbar}\hat{U}(t)^\dagger\hat{H}\hat{U}(t)\hat{U}(t)^\dagger\hat{A}^{(S)}\hat{U}(t) - \frac{i}{\hbar}\hat{U}^\dagger(t)\hat{A}^{(S)}\hat{U}(t)\hat{U}(t)^\dagger\hat{H}\hat{U}(t) \\
&= -\frac{i}{\hbar}[\hat{A}^{(H)},\hat{H}]
\end{aligned} \tag{26}$$

## Exercise 41

Consider a Hamiltonian of the form

$$\hat{H} = \hat{H}_0 + \hat{V}(t), \tag{27}$$

where $\hat{H}_0$ describes the free part of the system and $\hat{V}(t)$ describes interactions. In the interaction picture we consider the time evolution of operators according to the free part of the Hamiltonian, $\hat{U}_0(t) = \exp\left(-\frac{i}{\hbar}\hat{H}_0 t\right)$, satisfying $\frac{\partial\hat{U}_0}{\partial t} = -\frac{i}{\hbar}\hat{H}_0\hat{U}_0$.

(i) How is a state $|\,\phi(t)\rangle_I$ defined in the interaction picture?

(ii) Show that $|\,\phi(t)\rangle_I$ satisfies

$$i\hbar\frac{\partial}{\partial t}\,|\,\phi(t)\rangle_I = \hat{V}_I(t)\,|\,\phi(t)\rangle_I \,, \tag{28}$$

where $\hat{V}_I(t) = \hat{U}_0^\dagger\hat{V}(t)\hat{U}_0$.

(iii) Take $|\,\phi(t)\rangle_I = \hat{U}_V(t)\,|\,\phi_0\rangle$, and making use of your result of (ii), find the differential equation, satisfied by $\hat{U}_V$. Solve this equation iteratively and use it to express $|\,\phi(t)\rangle_I$ only in terms of $\hat{V}(t)$ and $|\,\phi_0\rangle$.

**Solution** *Notation: Subscripts $S, H, I$ refer to the Schrödinger, Heisenberg and interaction picture, respectively.*

(i) Defining

$$\hat{U}_V(t) = \hat{U}_0^\dagger \hat{U} = e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{U},$$

where $\hat{U}(t)$ satisfies $\frac{\partial \hat{U}}{\partial t} = -\frac{i}{\hbar}(\hat{H}_0 + \hat{V})\hat{U}$ the expectation value of a general operator is

$$\langle \hat{A} \rangle = \left\langle \phi_0 \,\middle|\, \hat{U}_V^\dagger \hat{U}_0^\dagger \hat{A}_S \hat{U}_0 \hat{U}_V \,\middle|\, \phi_0 \right\rangle = \left\langle \phi(t) \,\middle|\, \hat{A}_I(t) \,\middle|\, \phi(t) \right\rangle_I,$$

where $\hat{A}_I(t) = \hat{U}_0^\dagger \hat{A}_S \hat{U}_0$ and

$$|\,\phi(t)\rangle_I = \hat{U}_V\,|\,\phi_0\rangle = e^{\frac{i}{\hbar}\hat{H}_0 t}\,|\,\phi(t)\rangle_S\,. \tag{29}$$

(ii) By substituting Eq. 29,

$$\begin{aligned}
i\hbar\frac{\partial}{\partial t}\,|\,\phi(t)\rangle_I &= i\hbar\frac{\partial}{\partial t}\hat{U}_0^\dagger \hat{U}\,|\,\phi_0\rangle = i\hbar\frac{\partial}{\partial t}\left(e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{U}\right)|\,\phi_0\rangle \\
&= -\hat{U}_0^\dagger \hat{H}_0 \hat{U}\,|\,\phi_0\rangle + \hat{U}_0^\dagger(\hat{H}_0 + \hat{V}(t))\hat{U}\,|\,\phi_0\rangle \\
&= \hat{U}_0^\dagger \hat{V}(t)\hat{U}_0\;\hat{U}_0^\dagger \hat{U}\,|\,\phi_0\rangle \\
&= \hat{V}_I(t)\,|\,\phi(t)\rangle_I\,.
\end{aligned}$$

(iii) From the above calculation we also see

$$\frac{\partial}{\partial t}\hat{U}_V = -\frac{i}{\hbar}\hat{V}_I(t)\hat{U}_V.$$

Solving this expression iteratively, we find

$$\begin{aligned}
\hat{U}_V(t) &= \mathbb{1} - \frac{i}{\hbar}\int_0^t dt\;\hat{V}(t_1)\hat{U}_V(t_1) \\
&= \mathbb{1} + \frac{i}{\hbar}\int_0^t dt\;\hat{V}(t_1) + \left(-\frac{i}{\hbar}\right)^2\int_0^t dt_1\int_0^{t_1} dt_2\;\hat{V}(t_1)\hat{V}(t_2) + \ldots
\end{aligned}$$

Therefore we have

$$\begin{aligned}
|\,\phi(t)\rangle_I &= \hat{U}_V(t)\,|\,\phi_0\rangle \\
&= \left[\sum_{n=0}^{\infty}\left(-\frac{i}{\hbar}\right)^n\int_0^t dt_1\int_0^{t_1} dt_2\cdots\int_0^{t_{n-1}} dt_n\;\hat{V}(t_1)\hat{V}(t_2)\ldots\hat{V}(t_n)\right]|\,\phi_0\rangle\,.
\end{aligned}$$

# Exercise 42

Evaluate directly the matrix elements of the evolution operator

$$\mathcal{K}(x_f, x_i; t_f, t_i) = \langle x_f\,|\,e^{-\frac{i}{\hbar}\hat{H}(t_f - t_i)}\,|\,x_i\rangle$$

where $\hat{H} = \frac{\hat{p}^2}{2m}$ is the Hamiltonian of the free particle. How would the result change in $d$ space dimensions?

**Solution** We insert one decomposition of the identity between $\langle x_f\,|$ and the evolution operator,

$$\mathcal{K}(x_f, x_i; t_f, t_i) = \int dp\,\langle x_f\,|\,p\rangle\,e^{-\frac{i}{\hbar}\frac{p^2}{2m}(t_f - t_i)}\,\langle p\,|\,x_i\rangle \tag{30}$$

$$= \int dp\frac{1}{\sqrt{2\pi\hbar}}e^{\frac{i}{\hbar}px_f}\,e^{-\frac{i}{\hbar}\frac{p^2}{2m}(t_f - t_i)}\frac{1}{\sqrt{2\pi\hbar}}e^{-\frac{i}{\hbar}px_i} \tag{31}$$

This is of the form of the Gaussian integral (6) with

$$a = \frac{i(t_f - t_i)}{\hbar m}, \quad b = \frac{x_f - x_i}{\hbar} \tag{32}$$

so we can write it as

$$\mathcal{K}(x_f, x_i; t_f, t_i) = \sqrt{\frac{m}{2\pi i\hbar(t_f - t_i)}} \exp\left[\frac{im(x_f - x_i)^2}{2\hbar(t_f - t_i)}\right]. \tag{33}$$

In $d$ space dimensions all the Gaussian integrals would just factorize so we would find a $d$th power of the result, i.e.

$$\mathcal{K}(\vec{x}_f, \vec{x}_i; t_f, t_i) = \left(\frac{m}{2\pi i\hbar(t_f - t_i)}\right)^{\frac{d}{2}} \exp\left[\frac{im(\vec{x}_f - \vec{x}_i)^2}{2\hbar(t_f - t_i)}\right]. \tag{34}$$