Prof. Dr. Viatcheslav Mukhanov Winter term 2019/2020

# Exercises on Quantum Mechanics II (TM1/TV)

## Problem set 5, discussed November 18 - November 22, 2019

## Exercise 31

(i) Calculate $\hat{q}\hat{p}^2\hat{q} - \hat{p}\hat{q}^2\hat{p}$.

(ii) Write the Hamiltonian $\hat{H} = \hat{q}\hat{p}^2\hat{q}$ in canonical form, which corresponds to moving $\hat{p}$ operators to the left of $\hat{q}$.

### Solution

(i) Using the commutator $[\hat{q}, \hat{p}] = i\hbar$

$$\hat{q}\hat{p}^2\hat{q} - \hat{p}\hat{q}^2\hat{p} = [\hat{q}, \hat{p}]\,\hat{p}\hat{q} + \hat{p}\hat{q}\hat{p}\hat{q} - \hat{p}\hat{q}\,[\hat{q}, \hat{p}] - \hat{p}\hat{q}\hat{p}\hat{q} = 0.$$

(ii) Moving $\hat{p}$ to the left sequentially,

$$\begin{aligned}\hat{H} &= \hat{q}\hat{p}^2\hat{q} \\ &= [\hat{q}, \hat{p}]\,\hat{p}\hat{q} + \hat{p}\hat{q}\hat{p}\hat{q} \\ &= i\hbar\hat{p}\hat{q} + \hat{p}\,[\hat{q}, \hat{p}]\,\hat{q} + \hat{p}^2\hat{q}^2 \\ &= 2i\hbar\hat{p}\hat{q} + \hat{p}^2\hat{q}^2.\end{aligned}$$

## Exercise 32 (Central tutorial)

Consider the action

$$S = \int_{t_i}^{t_f} dt\ (p\dot{q} - H(p, q)), \tag{1}$$

and treat $q(t)$ and $p(t)$ as independent variables.

(i) Derive the Hamilton equations of motions from the variation of the action. What are the required boundary conditions on the variation $\delta q$ and $\delta p$?

(ii) Show that if the Hamiltonian is not explicitly time dependent, i.e. $H(p, q, t) = H(p, q)$, then $\frac{\mathrm{d}H}{\mathrm{d}t} = 0$.

### Solution

(i) By the variational Principle we require $\delta S = 0$,

$$\begin{aligned}\delta S &= \delta \int_{t_i}^{t_f} dt\ (p\dot{q} - H(p, q)) \\ &= \int_{t_i}^{t_f} dt\ \left(\delta p \frac{\mathrm{d}q}{\mathrm{d}t} + p\delta\frac{\mathrm{d}q}{\mathrm{d}t} - \frac{\partial H}{\partial p}\delta p - \frac{\partial H}{\partial q}\delta q\right) \\ &= \int_{t_i}^{t_f} dt\ \left[\left(\frac{\mathrm{d}q}{\mathrm{d}t} - \frac{\partial H}{\partial p}\right)\delta p + p\frac{\mathrm{d}\delta q}{\mathrm{d}t} - \frac{\partial H}{\partial q}\delta q\right] \\ &= \int_{t_i}^{t_f} dt\ \left[\left(\frac{\mathrm{d}q}{\mathrm{d}t} - \frac{\partial H}{\partial p}\right)\delta p - \left(\frac{\mathrm{d}p}{\mathrm{d}t} + \frac{\partial H}{\partial q}\right)\delta q\right] + [p\delta q]_{t_i}^{t_f}\,,\end{aligned}$$

where we used that $\delta \frac{\partial q}{\partial t} = \frac{\partial \delta q}{\partial t}$, integrated by parts in the last step and used that the variation of $q$ should satisfy the boundary conditions $\delta q(t_i) = \delta q(t_f) = 0$, to make the boundary term vanish. Enforcing the boundary conditions and the constraint $\delta S = 0$, we can read off Hamilton's equations as

$$\frac{\mathrm{d}q}{\mathrm{d}t} = \frac{\partial H}{\partial p} \quad \text{and} \quad \frac{\mathrm{d}p}{\mathrm{d}t} = -\frac{\partial H}{\partial q}. \tag{2}$$

(ii) By the chain rule and substituting Eq. 2,

$$\begin{aligned} \frac{\mathrm{d}H}{\mathrm{d}t} &= \frac{\partial H}{\partial p}\frac{\mathrm{d}p}{\mathrm{d}t} + \frac{\partial H}{\partial q}\frac{\mathrm{d}q}{\mathrm{d}t} \\ &= -\frac{\partial H}{\partial p}\frac{\partial H}{\partial q} + \frac{\partial H}{\partial q}\frac{\partial H}{\partial p} \\ &= 0. \end{aligned}$$

# Exercise 33 (Central tutorial)

(i) Generalise the Hamiltonian equations of motion to systems with N degrees of freedom $p_i$ and $q_i$, $i = 1, \ldots, N$.

We now move to the field theory case where we have $N \to \infty$. The generalised coordinates become $q_i(t) \to \phi_{\boldsymbol{x}}(t) = \phi(t, \boldsymbol{x})$ and $p_i(t) \to \pi_{\boldsymbol{x}}(t) = \pi(t, \boldsymbol{x})$, where $\phi(t, \boldsymbol{x})$ is the scalar field and $\pi(t, \boldsymbol{x})$ is the canonical momentum.

(ii) Consider the action of a massless and free scalar field $\phi = \phi(t, \boldsymbol{x})$ in 4 dimensions,

$$S[\phi, \partial_\mu \phi] = \frac{1}{2}\int d^4x\ \partial_\mu \phi \partial^\mu \phi = \frac{1}{2}\int dt\ d^3x \left[(\partial_t \phi)^2 - (\nabla\phi)^2\right], \tag{3}$$

where the summation over a Greek index runs over all dimensions $\mu = 1, \ldots, 4$, and $\partial_0 = \partial_t$, $\partial_1 = \partial_x$, etc.. (By convention summation over Roman indices runs over spatial dimensions $i = 1, 2, 3$ only, i.e. $(\nabla\phi)^2 = -\partial_i \phi \partial^i \phi$.)

a) Use the Lagrangian density $\mathcal{L}$, where

$$S = \int dt\ L = \int d^4x\ \mathcal{L}$$

to find the canonical momenta $\pi(t, \boldsymbol{x})$.

b) Find the Hamiltonian $H(\phi, \pi)$.

c) Derive the Lagrange equation of motion.

d) Derive Hamilton's equations of motion.

### Solution

(i) The action for a system with N degrees of freedom is

$$\begin{aligned} S &= \int_{t_i}^{t_f} dt\ \sum_i (p_i \dot{q}_i - H(p_i, q_i)) \\ &= \sum_i \int_{t_i}^{t_f} dt\ (p_i \dot{q}_i - H(p_i, q_i)), \end{aligned}$$

where we assumed that we can exchange the sum and the integral. By taking the variation $\delta S = 0$, we can proceed exactly like in the derivation of Eq. 2 and find,

$$\frac{\mathrm{d}q_i}{\mathrm{d}t} = \frac{\partial H}{\partial p_i} \quad \text{and} \quad \frac{\mathrm{d}p_i}{\mathrm{d}t} = -\frac{\partial H}{\partial q_i}. \tag{4}$$

(ii) a) Simply by reading off, we find

$$\mathcal{L}(\phi, \partial_\mu\phi) = \frac{1}{2}\partial_\mu\phi\partial^\mu\phi.$$

Hence for the canonical momentum we find

$$\pi = \frac{\partial\mathcal{L}}{\partial(\partial_t\phi)} = \partial_t\phi.$$

b) By performing a Legendre transform,

$$H(\phi, \pi, \partial_i\phi) := \int d^3x \ [\pi\partial_t\phi - \mathcal{L}] = \frac{1}{2}\int \ d^3x \left[\pi^2 + (\nabla\phi)^2\right] = \int d^3x \ \mathcal{H}(\phi, \pi, \partial_i\phi)$$

c) Using the least action principle, as in Question 32,

$$\begin{aligned}
\delta S &= \int d^4x \ \delta\mathcal{L}[\phi, \partial_\mu\phi] \\
&= \int d^4x \left[\frac{\partial\mathcal{L}}{\partial\phi}\delta\phi + \frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi)}\delta(\partial_\mu\phi)\right] \\
&= \int d^4x \left[\frac{\partial\mathcal{L}}{\partial\phi}\delta\phi + \partial_\mu\left(\frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi)}\delta\phi\right) - \partial_\mu\left(\frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi)}\right)\delta\phi\right] \\
&= \int d^4x \left[\frac{\partial\mathcal{L}}{\partial\phi}\delta\phi - \partial_\mu\left(\frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi)}\right)\delta\phi\right] + \int d^4x \ \partial_\mu\left[\frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi)}\delta\phi\right],
\end{aligned}$$

where the last term is a total differential integrated over the volume of 4 dimensional spacetime, which is equal to a surface integral over the boundary of spacetime. On this boundary, we require $\delta\phi = 0$, as in the 1 dimensional case. Therefore the last term in the above result is equal to zero. Hence we find the Lagrange equation

$$\frac{\partial\mathcal{L}}{\partial\phi} = \partial_\mu\frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi)}. \tag{5}$$

Substituting the above Lagrangian, we find the Lagrange equation of motion

$$\partial_\mu\partial^\mu\phi = (\partial_t^2 - \Delta)\phi = 0. \tag{6}$$

d) We can derive the Hamilton equations in a similar fashion,

$$\begin{aligned}
\delta S &= \delta\int d^4x \left[\pi \ \partial_t\phi - \mathcal{H}(\phi, \pi, \partial_i\phi)\right] \\
&= \int d^4x \left[\delta\pi \ \partial_t\phi + \pi\delta(\partial_t\phi) - \frac{\partial\mathcal{H}}{\partial\phi}\delta\phi - \frac{\partial\mathcal{H}}{\partial\pi}\delta\pi - \frac{\partial\mathcal{H}}{\partial(\partial_i\phi)}\delta\partial_i\phi\right] \\
&= \int d^4x \left[\left(\partial_t\phi - \frac{\partial\mathcal{H}}{\partial\pi}\right)\delta\pi - \left(\partial_t\pi + \frac{\partial\mathcal{H}}{\partial\phi} - \partial_i\frac{\partial\mathcal{H}}{\partial(\partial_i\phi)}\right)\delta\phi\right] - \int d^4x \ \partial_i\left[\frac{\partial\mathcal{H}}{\partial(\partial_i\phi)}\delta\phi\right],
\end{aligned}$$

where the last term is again zero due to the same arguments as above. Therefore the Hamilton equations are

$$\partial_t\phi = \frac{\partial\mathcal{H}}{\partial\pi} \quad \text{and} \quad \partial_t\pi = -\frac{\partial\mathcal{H}}{\partial\phi} + \partial_i\frac{\partial\mathcal{H}}{\partial(\partial_i\phi)}, \tag{7}$$

giving the same result as in Eq. 6.

# Exercise 34

Prove that:

$$[\hat{p}, \hat{p}^n\hat{q}^m] = -i\hbar\frac{\partial}{\partial\hat{q}}(\hat{p}^n\hat{q}^m) \tag{8}$$

**Solution**

$$[\hat{p}, \hat{p}^n\hat{q}^m] = \hat{p}^n(\hat{p}\hat{q}^m - \hat{q}^m\hat{p}) = \hat{p}^n[\hat{p}, \hat{q}^m] \overset{ex.22}{=} -im\hbar\hat{p}^n\hat{q}^{m-1} = -i\hbar\frac{\partial}{\partial\hat{q}}(\hat{p}^n\hat{q}^m) \tag{9}$$

## Exercise 35

Does the hermiticity of $\hat{H}$ follow from the unitarity of the time evolution operator?

#### Solution

$$\hat{U}^\dagger = (e^{-i\hat{H}t/\hbar})^\dagger = e^{i\hat{H}^\dagger t/\hbar} \overset{!}{=} e^{i\hat{H}t/\hbar} = \hat{U}^{-1} \Leftrightarrow \hat{H}^\dagger = \hat{H} \tag{10}$$

## Exercise 36

Let's consider the Hamiltonian

$$\hat{H} = \hat{H}_0 + \hat{V} \tag{11}$$

(i) Show that the equation

$$\frac{\partial \hat{\rho}_u}{\partial \beta} = -\hat{H}\hat{\rho}_u \tag{12}$$

can be written in the integral form:

$$\hat{\rho}_u(\beta) = \hat{\rho}_0(\beta) - \int_0^\beta d\beta' \hat{\rho}_0(\beta - \beta')\hat{V}\hat{\rho}_u(\beta') \qquad \text{with} \qquad \hat{\rho}_0(\beta) = e^{-\beta\hat{H}_0} \tag{13}$$

(ii) Now let $\hat{V}$ be a small perturbation, $\hat{V} \ll \hat{H}_0$. Find the first order in perturbation theory for $\rho(\boldsymbol{x}, \boldsymbol{x}'; \beta)$ with $\hat{V} = V(\hat{x})$.

#### Solution

(i) We will show this by inserting the integral form in the equation:

$$\begin{aligned}
\partial_\beta \hat{\rho}_u(\beta) &= \partial_\beta \hat{\rho}_0(\beta) - \hat{\rho}_0(0)\hat{V}\hat{\rho}_u(\beta) - \int_0^\beta d\beta' \partial_\beta(\hat{\rho}_0(\beta - \beta'))\hat{V}\hat{\rho}_u(\beta') = \\
&= -\hat{H}_0\hat{\rho}_0(\beta) - \hat{V}\hat{\rho}_u(\beta) - \int_0^\beta d\beta'(-\hat{H}_0)\hat{\rho}_0(\beta - \beta')\hat{V}\hat{\rho}_u(\beta') = \\
&= -\hat{H}_0\hat{\rho}_u(\beta) - \hat{V}\hat{\rho}_u(\beta) = -\hat{H}\hat{\rho}_u(\beta)
\end{aligned} \tag{14}$$

(ii) In order to find the first order in the perturbation theory, one can see that it is easiest to use the integral form of the starting equation. There, one can see that the higher orders in the potential come from the $\rho_u$ within the integral. In order to see what the higher terms would be, one can simply insert again the expression for $\rho_u$, and so on. (In other words, find the higher orders by iteration.) Then to the first order in $\hat{V}$, we have

$$\hat{\rho}_u(\beta) = \hat{\rho}_0(\beta) - \int_0^\beta d\beta' \hat{\rho}_0(\beta - \beta')\hat{V}\hat{\rho}_0(\beta') \tag{15}$$

Then the matrix elements are

$$\rho_u(x, x'; \beta) = \rho_0(x, x'; \beta) - \int_0^\beta d\beta' dx'' \hat{\rho}_0(x, x''; \beta - \beta')V(x'')\hat{\rho}_0(x'', x'; \beta') \tag{16}$$

## General information

The *lecture* takes place on:
  Monday at 10:00 - 12:00 c.t. in B 052 (Theresienstraße 37)
  Friday at 10:00 - 12:00 c.t. in B 052 (Theresienstraße 37)
The *central tutorial* takes place on Monday at 12:00 - 14:00 c.t. in B 139 (Theresienstraße 37)
The *webpage* for the lecture and exercises can be found at

`https://www.physik.uni-muenchen.de/lehre/vorlesungen/wise_19_20/T_M1_TV_-Quantum-Mechanics-II`