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This problem set is not reviewed by a tutor. This is just what I have turned in.

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[disclaimer]

physics606 – Advanced Quantum Theory

Problem Set 4

Martin Ueding
mu@martin-ueding.de

Lino Lemmer
l2@uni-bonn.de

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problem number	achieved points	possible points
1		9
2		5
3		8
Total		22

In order to make this document a bit more self-sufficient, we summarize the problem statements in front of our solutions. That will hopefully allow for better presentation of the results.

1 Propagator of the harmonic oscillator

Problem statement

Let L be the Lagrangian of the harmonic oscillator in one dimension:

$$L = \frac{1}{2} m [\dot{x}^2 - \omega^2 x^2].$$

1.1 Classical action

Problem statement

Show that the classical action $S_{\mathrm{cl}}(x, x', t)$ has the given form.

The action is defined as:

$$S = \int_0^t \mathrm{d}t' \, L\left(x(t'), \dot{x}(t'), t'\right).$$

We use the hint that is given on the problem set and express the trajectory as a linear combination of basis trajectories:

$$x(t') = a\cos(\omega t') + b\sin(\omega t').$$

The boundary conditions are a little strange. In the wording, it says that the particle goes from point x_0 at $t = 0$ to the point x at time t. Then the action is written with dependency on x and x'. We will use $x(0) =: x_0$ and $x(t) =: x_1$ here. This already is the boundary condition, so a and b are:

$$a = x_0, \quad b = \frac{x_1 - x_0\cos(\omega t)}{\sin(\omega t)}.$$

This can now be inserted into the Lagrangian function:

$$\begin{aligned} S_{\text{cl}}(x_0, x_1, t) &= \int_0^t \mathrm{d}t'\, L\left(x(t'), \dot{x}(t'), t'\right) \\ &= \frac{m}{2}\int_0^t \mathrm{d}t' \left[\left[-a\omega\sin(\omega t') + b\omega\cos(\omega t')\right]^2 - \omega^2\left[a\cos(\omega t') + b\sin(\omega t')\right]^2\right] \end{aligned}$$

We expand all the squares and regroup the terms again. Currently, all arguments for sine and cosine are $\omega t'$, so we will omit them for a more compact view of the expression. When the arguments change in the next steps, we will show them explicitly. Functional arguments will always be denoted with round parentheses and never with square brackets.

$$= \frac{m}{2}\int_0^t \mathrm{d}t' \left[[a^2 - b^2][\sin^2 - \cos^2] - 4ab\cos\sin\right]$$

Now we perform the integration. The indefinite integral to $\sin^2 - \cos^2$ is given by

$$-\frac{\sin(2\omega t')}{2\omega} = -\frac{2\cos\sin}{2\omega}.$$

The integral of $\cos\sin$ is given by

$$-\frac{\cos^2}{2\omega}.$$

The use those and insert into the previous equation.

$$= -\frac{m\omega^2}{2}\left[[a^2 - b^2]\frac{\cos\sin}{\omega} - 2ab\frac{\cos^2}{\omega}\right]_0^t$$

Now we evaluate at $t' = t$ and $t' = 0$. Since all the arguments change from $\omega t'$ to ωt, we redefine the omission and still omit all the arguments.

$$= -\frac{m\omega^2}{2}\left[[a^2 - b^2]\frac{\cos\sin}{\omega} - 2ab\frac{\cos^2 - 1}{\omega}\right]$$

Now we insert a and b explicitly.

$$= -\frac{m\omega^2}{2}\left[\left[x_0^2 - \left[\frac{x_1 - x_0\cos}{\sin}\right]^2\right]\frac{\cos\sin}{\omega} - 2x_0\frac{x_1 - x_0\cos}{\sin}\frac{\cos^2 - 1}{\omega}\right]$$

We get rid of the minus in front and cancel one ω.

$$= \frac{m\omega}{2}\left[\left[-x_0^2 + \left[\frac{x_1 - x_0\cos}{\sin}\right]^2\right]\cos\sin + 2x_0\frac{x_1 - x_0\cos}{\sin}[\cos^2 - 1]\right]$$

The sine in the first denominator is squared out. Then the first summand will be brought up to a fraction with the denominator $\sin^2$. One sine is pulled out front, the other cancels the sine behind the bracket. The sine in the second term is pulled out as well.

$$= \frac{m\omega}{2\sin}\left[\left[-x_0^2\sin^2 + [x_1 - x_0\cos]^2\right]\cos + 2x_0[x_1 - x_0\cos][\cos^2 - 1]\right]$$

We swap summands, and replace the very last bracket with a sine squared.

$$\begin{aligned}
&= \frac{m\omega}{2\sin}\left[\left[[x_1 - x_0\cos]^2 - x_0^2\sin^2\right]\cos + 2x_0[x_1 - x_0\cos]\sin^2\right] \\
&= \frac{m\omega}{2\sin}\left[\left[x_1^2 - 2x_0x_1\cos + x_0^2\cos^2 - x_0^2\sin^2\right]\cos + [2x_0x_1 - 2x_0^2\cos]\sin^2\right] \\
&= \frac{m\omega}{2\sin}\left[x_1^2\cos - 2x_0x_1\cos^2 + x_0^2\cos^3 - x_0^2\cos\sin^2 + 2x_0x_1\sin^2 - 2x_0^2\cos\sin^2\right] \\
&= \frac{m\omega}{2\sin}\left[x_0^2[\cos^3 - 2\cos\sin^2 - \cos\sin^2] + x_1^2\cos + 2x_0x_1[\sin^2 - \cos^2]\right] \\
&= \frac{m\omega}{2\sin}\left[x_0^2\cos[\cos^2 - 3\sin^2] + x_1^2\cos + 2x_0x_1[\sin^2 - \cos^2]\right]
\end{aligned}$$

This does not quite work out.

1.2 Separation

Problem statement

Show that the quantum mechanical propagator can be split up into a product of a time-only factor and the classical action:

$$U(x_0, x_1, t) := \int_{x_0}^{x_1} \mathscr{D}x \, \exp\left(\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}t' \, L\left(x(t'), \dot{x}(t')\right)\right) = F(t)\exp\left(\frac{\mathrm{i}}{\hbar}S_{\mathrm{cl}}\right).$$

We begin with the definition:

$$U(x_0, x_1, t) = \int_{x_0}^{x_1} \mathscr{D}x \, \exp\left(\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}t' \, L\left(x(t'), \dot{x}(t')\right)\right).$$

It is suggested to write $x(t') = x_{\text{sc}}(t') + y(t)$ where $y(0) = y(t) = 0$ is fulfilled.

$$= \int_0^0 \mathscr{D}y \, \exp\left(\frac{\mathrm{i}}{\hbar} \int_0^t \mathrm{d}t' \, L\left(x_{\text{sc}}(t') + y(t'), \dot{x}_{\text{sc}}(t') + \dot{y}(t')\right)\right).$$

This looks a bit like the variational calculus approach that one can take to derive the Euler Lagrange equations. To obtain terms that are linear in y and $\dot{y}$, we do an expansion of L around $y \equiv 0$. All instances of L are meant to be evaluated like

$$L\left(x_{\text{sc}}(t'), \dot{x}_{\text{sc}}(t')\right).$$

This gives:

$$= \int_0^0 \mathscr{D}y \, \exp\left(\frac{\mathrm{i}}{\hbar} \int_0^t \mathrm{d}t' \left[L + \frac{\partial L}{\partial x} y + \frac{\partial L}{\partial \dot{x}} \dot{y} + \mathscr{O}(y^2) + \mathscr{O}(\dot{y}^2)\right]\right).$$

Since the first part, the L, does not depend on the non-classical component of x any more, we can pull in front of the $\mathscr{D}y$ integral. The time integration of the Lagrangian over the classical path just gives the classical action.

$$= \exp\left(\frac{\mathrm{i}}{\hbar} S_{\text{cl}}\right) \int_0^0 \mathscr{D}y \, \exp\left(\frac{\mathrm{i}}{\hbar} \int_0^t \mathrm{d}t' \left[\frac{\partial L}{\partial x} y + \frac{\partial L}{\partial \dot{x}} \dot{y} + \mathscr{O}(y^2) + \mathscr{O}(\dot{y}^2)\right]\right).$$

The term linear in $\dot{y}$ will now be partially integrated. The total time derivative is contained in the bracket and does not act on the y outside of the bracket. Looking at the interesting part, we have

$$\int_0^t \mathrm{d}t' \left[\frac{\partial L}{\partial x} y + \frac{\partial L}{\partial \dot{x}} \dot{y}\right] = \int_0^t \mathrm{d}t' \left[\left[\frac{\partial L}{\partial x} - \frac{\mathrm{d}}{\mathrm{d}t'} \frac{\partial L}{\partial \dot{x}}\right] y\right] + \left[\frac{\partial L}{\partial \dot{x}} y\right]_0^t.$$

The term

$$\left[\frac{\partial L}{\partial x} - \frac{\mathrm{d}}{\mathrm{d}t'} \frac{\partial L}{\partial \dot{x}}\right] y$$

is zero since the L are evaluated at the classical trajectory only. There, the Euler Lagrange equations hold. The surface term

$$\left[\frac{\partial L}{\partial \dot{x}} y\right]_0^t$$

is also zero because of the definition of y. The remainder of the integral therefore is:

$$= \exp\left(\frac{\mathrm{i}}{\hbar} S_{\text{cl}}\right) \int_0^0 \mathscr{D}y \, \exp\left(\frac{\mathrm{i}}{\hbar} \int_0^t \mathrm{d}t' \left[\mathscr{O}(y^2) + \mathscr{O}(\dot{y}^2)\right]\right).$$

The remaining integration that is denoted with $\int \mathscr{D}y$ does not depend on the starting and ending points x_0 and x_1 since it is only concerned with the finite variation y. The only free variable in there is the t, so we can write this whole thing, whatever it actually is, as an ominous $F(t)$:

$$= \exp\left(\frac{\mathrm{i}}{\hbar} S_{\mathrm{cl}}\right) F(t).$$

2 Ordinary path integral from phase space path integral

Problem statement

Given the relation

$$\lim_{N\to\infty} \prod_{k=1}^{N-1} \int \mathrm{d}x_k \prod_{k=1}^{N} \int \frac{\mathrm{d}p_k}{2\pi\hbar} \exp\left(-\frac{\mathrm{i}}{\hbar} \sum_{k=1}^{N} \left[\frac{\epsilon p_k^2}{2m} - p_k[x_k - x_{k-1}] + \epsilon V(x_{k-1})\right]\right).$$

Show that this reduces to

$$\frac{1}{B} \lim_{N\to\infty} \prod_{k=1}^{N-1} \int \frac{\mathrm{d}x_k}{B} \exp\left(\frac{\mathrm{i}}{\hbar} \sum_{k=1}^{N} \left[\frac{m}{2} \frac{[x_k - x_{k-1}]^2}{\epsilon} - \epsilon V(x_{k-1})\right]\right)$$

where

$$B = \sqrt{\frac{2\pi\hbar\mathrm{i}}{m}}.$$

It was not quite clear to us, how the multiple usages of the index k are meant. The interpretation that got us to the right result is written in our notation as

$$U(x,x',t) = \lim_{N\to\infty} \left[\prod_{k=1}^{N-1} \int \mathrm{d}x_k\right] \left[\prod_{k=1}^{N} \int \frac{\mathrm{d}p_k}{2\pi\hbar}\right] \exp\left(-\frac{\mathrm{i}}{\hbar} \sum_{k=1}^{N} \left[\frac{\epsilon p_k^2}{2m} - p_k[x_k - x_{k-1}] + \epsilon V(x_{k-1})\right]\right).$$

That way, the k of each summation or product sign are contained within a scope. The sum in the exponential function can be expanded into a product of exponential functions. The resulting product sign would be the same as the one for the $\mathrm{d}p_k$, so we join those together. The second product sign is meant to act on all the factors behind it, i.e. to the next plus or minus sign. We yield

$$= \lim_{N\to\infty} \left[\prod_{k=1}^{N-1} \int \mathrm{d}x_k\right] \prod_{k=1}^{N} \int \frac{\mathrm{d}p_k}{2\pi\hbar} \exp\left(-\frac{\mathrm{i}}{\hbar} \left[\frac{\epsilon p_k^2}{2m} - p_k[x_k - x_{k-1}] + \epsilon V(x_{k-1})\right]\right).$$

We rearrange the terms in the exponential function a bit to give the same signature the Gaussian integrals on problem set 3 have. Since the potential V term does not depend on any of the momenta, we can safely pull this in front of the integral. Now we have

$$= \lim_{N\to\infty} \left[\prod_{k=1}^{N-1} \int \mathrm{d}x_k\right] \prod_{k=1}^{N} \exp\left(-\frac{\mathrm{i}\epsilon}{\hbar} V(x_{k-1})\right) \int \frac{\mathrm{d}p_k}{2\pi\hbar} \exp\left(-\frac{\mathrm{i}\epsilon}{2m\hbar} p_k^2 + \frac{\mathrm{i}}{\hbar}[x_k - x_{k-1}] p_k\right),$$

where we identify

$$a := \frac{\mathrm{i}\epsilon}{2m\hbar}, \quad b := \frac{\mathrm{i}}{\hbar}[x_k - x_{k-1}].$$

Using the results from problem set 3, we get

$$= \lim_{N\to\infty} \left[\prod_{k=1}^{N-1} \int \mathrm{d}x_k\right] \prod_{k=1}^{N} \sqrt{\frac{m}{2\pi\mathrm{i}\epsilon\hbar}} \exp\left(-\frac{\mathrm{i}\epsilon}{\hbar} V(x_{k-1})\right) \exp\left(\frac{\mathrm{i}m}{2\epsilon\hbar}[x_k - x_{k-1}]^2\right).$$

We pull the square root in front of the product sign, adding the power N. Then we collapse the two exponential functions into a single one. To match the form given on the problem set we factor out $\mathrm{i}/\hbar$. Then we incorporate the product sign into the exponential function in the form of a summation sign. With these modifications, we obtain

$$= \lim_{N\to\infty} \left[\prod_{k=1}^{N-1} \int \mathrm{d}x_k\right] \sqrt{\frac{m}{2\pi\mathrm{i}\epsilon\hbar}}^N \exp\left(\frac{\mathrm{i}}{\hbar}\sum_{k=1}^{N}\left(\frac{m}{2}\frac{[x_k - x_{k-1}]^2}{\epsilon} - \epsilon V(x_{k-1})\right)\right).$$

The product sign that is left only goes up to $N-1$, so that it only contains the power $N-1$. Therefore, we need to split up the square root into two parts.

$$= \lim_{N\to\infty} \sqrt{\frac{m}{2\pi\mathrm{i}\epsilon\hbar}} \left[\prod_{k=1}^{N-1} \sqrt{\frac{m}{2\pi\mathrm{i}\epsilon\hbar}} \int \mathrm{d}x_k\right] \exp\left(\frac{\mathrm{i}}{\hbar}\sum_{k=1}^{N}\left[\frac{m}{2}\frac{[x_k - x_{k-1}]^2}{\epsilon} - \epsilon V(x_{k-1})\right]\right).$$

The definition of B on the problem set does not have the ϵ we have. We cannot pull it in front of the limit since ϵ depends on N. Other than that, we got the result from the problem set.

$$= \lim_{N\to\infty} \frac{1}{B\sqrt{\epsilon}} \left[\prod_{k=1}^{N-1} \int \frac{\mathrm{d}x_k}{B\sqrt{\epsilon}}\right] \exp\left(\frac{\mathrm{i}}{\hbar}\sum_{k=1}^{N}\left[\frac{m}{2}\frac{[x_k - x_{k-1}]^2}{\epsilon} - \epsilon V(x_{k-1})\right]\right).$$

3 Path integral with vector potential

Problem statement

Show that

$$\psi(x,\epsilon) = \int_{\mathbb{R}} \mathrm{d}\eta\, \psi(x+\eta,0) \exp\left(\frac{\mathrm{i}}{\hbar}\left[\frac{m\eta^2}{2\epsilon} + q\epsilon\frac{\eta}{\epsilon}A(x+\alpha\eta,0)\right]\right)$$

is equivalent to

$$\psi(x,\epsilon) = \psi(x,0) - \mathrm{i}\frac{\epsilon}{\hbar}\hat{H}\psi(x,0).$$

The expansions are:

$$\psi(x+\eta,0) = \psi(x,0) + \psi'(x,0)\eta + \frac{1}{2}\psi''(x,0)\eta^2 + \mathcal{O}(\eta^3)$$
$$A(x+\eta,0) = A(x,0) + A'(x,0)\alpha\eta + \frac{1}{2}A''(x,0)[\alpha\eta]^2 + \mathcal{O}(\eta^3)$$

We start with the given expression,

$$\psi(x,\epsilon) = \int_{\mathbb{R}} \mathrm{d}\eta\, \psi(x+\eta,0) \exp\left(\frac{\mathrm{i}}{\hbar}\left[\frac{m\eta^2}{2\epsilon} + q\epsilon\frac{\eta}{\epsilon}A(x+\alpha\eta,0)\right]\right).$$

We insert the expansion of ψ and A.

$$\approx \int_{\mathbb{R}} \mathrm{d}\eta \left[\psi(x,0) + \psi'(x,0)\eta + \frac{1}{2}\psi''(x,0)\eta^2\right]$$
$$\cdot \exp\left(\frac{\mathrm{i}}{\hbar}\left[\frac{m\eta^2}{2\epsilon} + q\epsilon\frac{\eta}{\epsilon}\left[A(x,0) + A'(x,0)\alpha\eta + \frac{1}{2}A''(x,0)[\alpha\eta]^2\right]\right]\right)$$

Since all the function arguments are $(x,0)$, we drop them.

$$= \int_{\mathbb{R}} \mathrm{d}\eta \left[\psi + \psi'\eta + \frac{1}{2}\psi''\eta^2\right] \exp\left(\frac{\mathrm{i}}{\hbar}\left[\frac{m\eta^2}{2\epsilon} + q\epsilon\frac{\eta}{\epsilon}\left[A + A'\alpha\eta + \frac{1}{2}A''[\alpha\eta]^2\right]\right]\right)$$

We rearrange the terms in the exponential function. While we do that, we drop the η^3 term that would come with A''. Then we bring it into the $\exp(-ax^2 + bx)$ form to use the solution formulas later on.

$$= \int_{\mathbb{R}} \mathrm{d}\eta \left[\psi + \psi'\eta + \frac{1}{2}\psi''\eta^2\right] \exp\left(-\left[-\frac{\mathrm{i}m}{2\epsilon\hbar} - \frac{\mathrm{i}q\alpha A'}{\hbar}\right]\eta^2 + \frac{\mathrm{i}qA}{\hbar}\eta\right)$$

We now expand the first bracket and use the linearity of the integral to get three of them.

$$= \psi \int_{\mathbb{R}} \mathrm{d}\eta \, \exp(\dots) + \psi' \int_{\mathbb{R}} \mathrm{d}\eta \, \eta \exp(\dots) + \frac{1}{2}\psi'' \int_{\mathbb{R}} \mathrm{d}\eta \, \eta^2 \exp(\dots)$$

We now explicitly define a and b to be

$$a := -\frac{\mathrm{i}m}{2\epsilon\hbar} - \frac{\mathrm{i}q\alpha A'}{\hbar}, \quad b := \frac{\mathrm{i}qA}{\hbar}.$$

Then we can use the different solutions formulas for the various integrals:

$$= \psi \exp\left(\frac{b^2}{4a}\right)\sqrt{\frac{\pi}{a}} + \psi' \exp\left(\frac{b^2}{4a}\right)\frac{b\sqrt{\pi}}{2a^{3/2}} + \psi'' \exp\left(\frac{b^2}{4a}\right)\frac{[2a+b^2]\sqrt{\pi}}{8a^{5/2}}$$

We pull out the common terms to the front.

$$= \sqrt{\pi} \exp\left(\frac{b^2}{4a}\right)\left[\psi \frac{1}{\sqrt{a}} + \psi' \frac{b}{2a^{3/2}} + \psi'' \frac{[2a+b^2]}{8a^{5/2}}\right]$$

We can compute the inverse of a:

$$a = -\frac{\mathrm{i}m + 2\mathrm{i}\epsilon q\alpha A'}{2\epsilon\hbar} \iff \frac{1}{a} = -\frac{2\epsilon\hbar}{\mathrm{i}m + 2\mathrm{i}\epsilon q\alpha A'} = \frac{2\mathrm{i}\epsilon\hbar}{m + 2\epsilon q\alpha A'}.$$

This does not have a singularity at $\epsilon = 0$ any more, which is probably a good thing.

The b^2 is

$$b^2 = -\frac{q^2A^2}{\hbar^2}$$

such that

$$\frac{b^2}{4a} = -\frac{\mathrm{i}\epsilon q^2 A^2}{2\hbar[m + 2\epsilon q\alpha A']}.$$

Since we are only interested in the first order of ϵ, we can expand the exponential function into a "$1 + x$" linear fashion. The problem is that the $\sqrt{1/a}$ terms cannot be expanded because the first derivative has a singularity at $\epsilon = 0$. So it could only be expanded in terms of $\sqrt{\epsilon}$ which does not allow use to get an expansion in terms of ϵ. To give the form of equation (6) from the problem set, we will still have to get rid of the $\sqrt{\pi}$ that we got from the Gaussian integration. This is where we do not know how to proceed.

To motivate equation (6) a bit: Starting from the Schrödinger equation

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\psi(x,t) = \hat{H}\psi(x,t),$$

we can derive the time evolution operator of a time-independent Hamiltonian operator by solving the differential equation formally:

$$\psi(x,t) = \underbrace{\exp\left(-\frac{\mathrm{i}}{\hbar}\hat{H}t\right)}_{U(t)}\psi(x,0).$$

Now we can expand this to first order around $t = 0$ and then relabel it with ϵ.

$$\psi(x,\epsilon) = \left[1 - \frac{\mathrm{i}}{\hbar}\hat{H}\epsilon\right]\psi(x,0).$$

Rearranging the terms, we yield the version on the problem set:

$$\psi(x,\epsilon) = \psi(x,0) - \mathrm{i}\frac{\epsilon}{\hbar}\hat{H}\psi(x,0).$$