Quantum Mechanics 3 - Class Exercise 5

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Question 1

For the Lagrangian

$$L = a(t)\dot{x}^2 + b(t)x\dot{x} + c(t)x^2 + d(t)\dot{x} + e(t)x + f(t), \tag{1}$$

Show that the path integral can be written as

$$G(x_b, t_b; x_a, t_a) = \mathrm{e}^{iS_{\mathrm{cl}}(x_b,t_b;x_a,t_a)/\hbar} \int_{y(t_a)=0}^{y(t_b)=0} \mathcal{D}y(t) \exp\left[\frac{i}{\hbar}\int_{t_a}^{t_b} \left\{a(t)\dot{y}^2 + b(t)\dot{y}y + c(t)y^2\right\} dt\right], \tag{2}$$

where S_{cl} is the action over the classical path, and $y(t)$ are the trajectories with zero fluctuations at the end points.

Solution

The classical trajectory $x_{\mathrm{cl}}(t)$ is an extremum of the action, and it satisfies

$$\delta S_{\mathrm{cl}} = \int_{t_a}^{t_b} \delta L_{\mathrm{cl}} dt = \int_{t_a}^{t_b} \left[\left.\frac{\partial L}{\partial x}\right|_{x_{\mathrm{cl}}} \delta x + \left.\frac{\partial L}{\partial \dot{x}}\right|_{x_{\mathrm{cl}}} \delta\dot{x}\right] dt = 0, \tag{3}$$

where $\delta x(t)$ is any function for which $\delta x(t_a) = \delta x(t_b) = 0$. Thus, $\delta L_{\mathrm{cl}} = 0$ for the classical path. For the Lagrangian in Eq. (1) we have

$$\delta L_{\mathrm{cl}} = 2a\dot{x}_{\mathrm{cl}}\delta\dot{x} + b\dot{x}_{\mathrm{cl}}\delta x + bx_{\mathrm{cl}}\delta\dot{x} + 2cx_{\mathrm{cl}}\delta x + d\delta\dot{x} + e\delta x = 0. \tag{4}$$

Let us work with new coordinates, $y(t) = x(t) - x_{\mathrm{cl}}(t)$. With these coordinates the Lagrangian is

$$\begin{aligned} L &= a\dot{x}_{\mathrm{cl}}^2 + bx_{\mathrm{cl}}\dot{x}_{\mathrm{cl}} + cx_{\mathrm{cl}}^2 + d\dot{x}_{\mathrm{cl}} + ex_{\mathrm{cl}} + f \\ &+ 2a\dot{x}_{\mathrm{cl}}\dot{y} + b\dot{x}_{\mathrm{cl}}y + bx_{\mathrm{cl}}\dot{y} + 2cx_{\mathrm{cl}}y + d\dot{y} + ey \\ &+ a\dot{y}^2 + b\dot{y}y + cy^2. \end{aligned}$$

The first line is just the Lagrangian of the classical path L_{cl}. The second line vanishes due to Eq. (4) (with $\delta x = y$). Thus

$$L = L_{\mathrm{cl}} + a\dot{y}^2 + b\dot{y}y + cy^2. \tag{5}$$

And the action can be decomposed into

$$S = S_{\mathrm{cl}} + \int_{t_a}^{t_b} \left\{a\dot{y}^2 + b\dot{y}y + cy^2\right\} dt. \tag{6}$$

Finally, consider the propagator

$$G\left(x_b, t_b; x_a, t_a\right) = \int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}x\left(t\right) \mathrm{e}^{iS/\hbar}. \tag{7}$$

We can change the integration variable to $y\left(t\right)$ instead of $x\left(t\right)$. The integral measure in this case is $\mathcal{D}x\left(t\right) = \mathcal{D}y\left(t\right)$ (the transformation's Jacobian is simply one because all we do is to shift the path by a fixed classical path). In addition, by construction $y\left(t_a\right) = y\left(t_b\right) = 0$. Therefore:

$$G\left(x_b, t_b; x_a, t_a\right) = \mathrm{e}^{iS_{\mathrm{cl}}\left(x_b, t_b; x_a, t_a\right)/\hbar} \int_{y(t_a)=0}^{y(t_b)=0} \mathcal{D}y\left(t\right) \exp\left[\frac{i}{\hbar} \int_{t_a}^{t_b} \left\{a\left(t\right) \dot{y}^2 + b\left(t\right) \dot{y} y + c\left(t\right) y^2\right\} dt\right]. \tag{8}$$

Question 2

Find the Green function for a particle in a constant external field f where the Lagrangian is

$$L = \frac{1}{2}m\dot{x}^2 + fx. \tag{9}$$

Solution

The Lagrangian in Eq. (9) is a special case for the Lagrangian in Eq. (1) with $a(t) = m/2$ and $e(t) = f$ and all the other coefficients are zero. We can therefore exploit the result from previous problem

$$G(x_b, t_b; x_a, t_a) = \mathrm{e}^{iS_{\mathrm{cl}}/\hbar} \int_{y(t_a)=0}^{y(t_b)=0} \mathcal{D}y(t) \exp\left[\frac{i}{\hbar}\int_{t_a}^{t_b} \frac{1}{2}m\dot{y}^2 dt\right]. \tag{10}$$

In order to calculate the path integral, recall the Green's function you saw in class for a free particle:

$$G_{\mathrm{free}}(x_b, t_b; x_a, t_a) = \int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}x(t) \exp\left[\frac{i}{\hbar}\int_{t_a}^{t_b} \frac{1}{2}m\dot{x}^2 dt\right] = \sqrt{\frac{m}{2\pi i\hbar(t_b - t_a)}} \exp\left[\frac{im(x_b - x_a)^2}{2\pi\hbar(t_b - t_a)}\right]. \tag{11}$$

The path integral in Eq. (12) is exactly like the one in Eq. (11), but with boundary conditions of $y(t_a) = y(t_b) = 0$. Thus

$$G(x_b, t_b; x_a, t_a) = \mathrm{e}^{iS_{\mathrm{cl}}/\hbar}\sqrt{\frac{m}{2\pi i\hbar(t_b - t_a)}}. \tag{12}$$

All that has remained is to compute S_{cl}. First, the equation of motion for the Lagrangian in Eq. (9) is $m\ddot{x} = f$. This has the general solution

$$x_{\mathrm{cl}}(t) = \frac{f}{2m}t^2 + c_1 t + c_0. \tag{13}$$

The Lagrangian of the classical path is

$$L_{\mathrm{cl}} = \frac{1}{2}m\dot{x}_{\mathrm{cl}}^2 + fx_{\mathrm{cl}} = \frac{f^2}{m}t^2 + 2fc_1 t + \frac{1}{2}mc_1^2 + fc_0, \tag{14}$$

and the classical action is

$$S_{\mathrm{cl}} = \int_{t_a}^{t_b} L_{\mathrm{cl}} dt = \frac{f^2\left(t_b^3 - t_a^3\right)}{3m} + fc_1\left(t_b^2 - t_b^2\right) + \left(\frac{1}{2}mc_1^2 + fc_0\right)(t_b - t_b). \tag{15}$$

Finally, we need to find the coefficients c_0 and c_1 by accounting for the boundary conditions. It's easy to do so using matrix notation:

$$\begin{bmatrix} 1 & t_a \\ 1 & t_b \end{bmatrix}\begin{bmatrix} c_0 \\ c_1 \end{bmatrix} = \begin{bmatrix} x_a - \frac{f}{2m}t_a^2 \\ x_b - \frac{f}{2m}t_b^2 \end{bmatrix} \tag{16}$$

And upon inverting the matrix, we get:

$$\begin{bmatrix} c_0 \\ c_1 \end{bmatrix} = \frac{1}{t_b - t_a}\begin{bmatrix} t_b & -t_a \\ -1 & 1 \end{bmatrix}\begin{bmatrix} x_a - \frac{f}{2m}t_a^2 \\ x_b - \frac{f}{2m}t_b^2 \end{bmatrix} = \frac{1}{t_b - t_a}\begin{bmatrix} x_a t_b - x_b t_a + \frac{f}{2m}t_a t_b(t_b - t_a) \\ x_b - x_a + \frac{f}{2m}\left(t_b^2 - t_a^2\right) \end{bmatrix} \tag{17}$$

Question 3

Use the propagator $G(x,t;y,0)$ for the harmonic oscillator,

$$G(x,t;y,0) = \sqrt{\frac{m\omega}{2\pi i\hbar \sin(\omega t)}} \exp\left\{\frac{im\omega}{2\hbar \sin(\omega t)}\left[\left(x^2+y^2\right)\cos(\omega t) - 2xy\right]\right\}, \tag{18}$$

1. to obtain the energies of the harmonic oscillator.
2. to obtain the wave-function of the ground state.

Solution to 1

As you saw in class, we can extract the energy levels from the propagator via the identity

$$\mathrm{Tr}\left(\mathrm{e}^{-i\hat{H}t/\hbar}\right) = \int_{-\infty}^{\infty} dx G(x,t;x,0) = \sum_{n=0}^{\infty} \mathrm{e}^{-iE_n t/\hbar}. \tag{19}$$

Notice that for $x = y$ the Green function is a Gaussian

$$G(x,t;x,0) = A\exp\left(-\alpha x^2\right), \tag{20}$$

with a parameter

$$\alpha = -\frac{im\omega}{2\hbar\sin(\omega t)}\left[2\cos(\omega t) - 2\right] = \frac{2im\omega}{\hbar \sin(\omega t)}\sin^2\left(\frac{\omega t}{2}\right), \tag{21}$$

Therefore:

$$\begin{aligned}
\sum_{n=0}^{\infty} \mathrm{e}^{-iE_n t/\hbar} &= \int_{-\infty}^{\infty} dx G(x,t;x,0) = A\int_{-\infty}^{\infty} dx \exp\left(-\alpha x^2\right) = A\sqrt{\frac{\pi}{\alpha}} \\
&= \sqrt{\frac{m\omega}{2\pi i\hbar\sin(\omega t)}}\sqrt{\frac{\pi\hbar\sin(\omega t)}{2im\omega\sin^2\left(\frac{\omega t}{2}\right)}} = \frac{1}{2i\sin\left(\frac{\omega t}{2}\right)} \qquad (22) \\
&= \frac{1}{\mathrm{e}^{i\omega t/2} - \mathrm{e}^{-i\omega t/2}} = \mathrm{e}^{-i\omega t/2}\frac{1}{1-\mathrm{e}^{-i\omega t}} = \mathrm{e}^{-i\omega t/2}\sum_{n=0}^{\infty}\mathrm{e}^{-in\omega t}. \qquad (23)
\end{aligned}$$

By comparing the LHS with the RHS we find the energy levels of the harmonic oscillator:

$$\boxed{E_n = \hbar\omega\left(n + \frac{1}{2}\right)}. \tag{24}$$

Solution to 2

Let us write the propagator in the following way:

$$G(x,t;y,0) = \langle x|\mathrm{e}^{-i\hat{H}t/\hbar}|y\rangle = \sum_n\sum_{n'}\langle x|n\rangle\langle n|\mathrm{e}^{-i\hat{H}t/\hbar}|n'\rangle\langle n'|y\rangle = \sum_n \psi_n^*(y)\,\psi_n(x)\,\mathrm{e}^{-iE_n t/\hbar} \tag{25}$$

Now take $t = -i\beta\hbar$ and take the limit $\beta \to \infty$:

$$\lim_{\beta\to\infty} G(x,-i\beta\hbar;y,0) = \lim_{\beta\to\infty}\sum_n \psi_n^*(y)\,\psi_n(x)\,\mathrm{e}^{-\beta E_n} = \lim_{\beta\to\infty}\psi_0^*(y)\,\psi_0(x)\,\mathrm{e}^{-\beta E_0}. \tag{26}$$

Thus

$$
\begin{aligned}
\psi_0(x)\,\psi_0^*(y) &= \lim_{\beta\to\infty} \mathrm{e}^{\beta E_0} G(x,-i\beta\hbar;y,0)\\
&= \lim_{\beta\to\infty} \mathrm{e}^{\beta\hbar\omega/2}\sqrt{\frac{m\omega}{2\pi i\hbar\sin(-i\omega\beta\hbar)}}\exp\left\{\frac{im\omega}{2\hbar\sin(-i\omega\beta\hbar)}\left[\left(x^2+y^2\right)\cos(-i\omega\beta\hbar)-2xy\right]\right\}\\
&= \lim_{\beta\to\infty} \mathrm{e}^{\beta\hbar\omega/2}\sqrt{\frac{m\omega}{2\pi\hbar\sinh(\omega\beta\hbar)}}\exp\left\{-\frac{m\omega}{2\hbar\sinh(\omega\beta\hbar)}\left[\left(x^2+y^2\right)\cosh(\omega\beta\hbar)-2xy\right]\right\}\\
&= \lim_{\beta\to\infty} \mathrm{e}^{\beta\hbar\omega/2}\sqrt{\frac{m\omega}{\pi\hbar}}\mathrm{e}^{-\beta\hbar\omega/2}\exp\left\{-\frac{m\omega}{2\hbar}\left(x^2+y^2\right)\coth(\omega\beta\hbar)\right\}\\
&= \sqrt{\frac{m\omega}{\pi\hbar}}\exp\left\{-\frac{m\omega}{2\hbar}\left(x^2+y^2\right)\right\}, \qquad (27)
\end{aligned}
$$

where we have used the following identities:

$$\sin(ix) = i\sinh(x) \qquad \cos(ix) = \cosh(x) \qquad (28)$$

$$\sinh(x) = \frac{\mathrm{e}^x - \mathrm{e}^{-x}}{2} \underset{x\to\infty}{\rightarrow} \frac{1}{2}\mathrm{e}^x \qquad (29)$$

$$\coth(x) = \frac{\cosh(x)}{\sinh(x)} = \frac{\mathrm{e}^x - \mathrm{e}^{-x}}{\mathrm{e}^x + \mathrm{e}^{-x}} \underset{x\to\infty}{\rightarrow} 1. \qquad (30)$$

Thus, it is easy to extract from the wave-function of the ground state from Eq. (27):

$$\boxed{\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega}{2\hbar}x^2\right)}. \qquad (31)$$

Note: Does this ring any bell? Where have you seen that in the limit of $\beta\to\infty$ the system find itself in the ground state? What is the physical meaning of β?