Université PSL M1 Quantum Engineering

Mathematical methods for quantum engineering
Exercise on Lagrangian, Hamiltonian, classical/quantum correspondence
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Take a spherical punctual pendulum of mass m, Cartesian coordinates (x, y, z) and rotating around the origin $(0, 0, 0)$ in the gravity field of acceleration g along the vertical ascending axis z. A possible choice of configuration variables is (x, y) with $z = -\sqrt{\ell^2 - x^2 - y^2}$ since we assume here that pendulum moves on the sphere of radius ℓ and remains under the equator $(z < 0)$.

1. Show that its potential energy reads $-mg\sqrt{\ell^2 - x^2 - y^2}$
2. Show that $\dot{z} = -\frac{x\dot{x}+y\dot{y}}{\sqrt{\ell^2-x^2-y^2}}$ and deduce that its kinetic energy reads

$$\frac{m}{2}\left(\dot{x}^2 + \dot{y}^2 + \frac{(x\dot{x} + y\dot{y})^2}{\ell^2 - x^2 - y^2}\right)$$

3. Deduce the Lagrangian.
4. Derive the first-order approximate dynamics around the equilibrium $(x, y) = 0$, compute the eigenvalues and discuss its stability (hint: use the quadratic approximation of the Lagrangian).
5. Take the quadratic Lagrangian of previous question, derive the corresponding quadratic Hamiltonian and give the Hamiltonian differential equation governing the dynamics.
6. From this quadratic Hamiltonian, derive the quantisation via the correspondence principle. Show that the average value $\langle\psi|\hat{x}|\psi\rangle$ (resp. $\langle\psi|\hat{y}|\psi\rangle$) of operator $\hat{x}$ (resp. $\hat{y}$) satisfies a second-order linear differential scalar equation.
7. Assume that the system is rotating around the vertical axis with rotational velocity Ω as a Foucault pendulum on the north pole.
   (a) Show that the kinetic energy reads now

$$\frac{m}{2}\left(\dot{x}^2 + \dot{y}^2 + \frac{(x\dot{x} + y\dot{y})^2}{\ell^2 - x^2 - y^2} + 2\Omega(y\dot{x} - x\dot{y}) + \Omega^2(x^2 + y^2)\right).$$

   (b) Derive the quadratic approximation of the Lagrangian around the equilibrium $(x, y) = 0$, deduce the corresponding quadratic Hamiltonian.
   (c) From this quadratic Hamiltonian, derive the quantisation via the correspondence principle. Show that the average values of $\hat{x}$, $\hat{x}$ satisfy a differential system of four scalar equations.

Mathematical methods for quantum engineering
Solution of the exercise on Lagrangian, Hamiltonian, classical/quantum correspondence
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1. Simply use the gravitational potential $mgz = -mg\sqrt{\ell^2 - x^2 - y^2}$.
2. Inject $\dot{z} = -\frac{x\dot{x}+y\dot{y}}{\sqrt{\ell^2-x^2-y^2}}$ in the kinetic energy $\frac{m}{2}(\dot{x}^2 + \dot{y}^2 + \dot{z}^2)$.
3. The Lagrangian $L(x, y, \dot{x}, \dot{y})$ of this mechanical system is the difference between the kinetic energy and the potential energy
$$L(x, y, \dot{x}, \dot{y}) = \frac{m}{2}\left(\dot{x}^2 + \dot{y}^2 + \frac{(x\dot{x} + y\dot{y})^2}{\ell^2 - x^2 - y^2}\right) + mg\sqrt{\ell^2 - x^2 - y^2}.$$
4. Around the equilibrium $(x, y) = 0$ the quadratic approximation of the Lagrangian reads:
$$L(x, y, \dot{x}, \dot{y}) \approx \frac{m}{2}\left(\dot{x}^2 + \dot{y}^2\right) + mg\ell - m\frac{g}{2\ell}(x^2 + y^2) \triangleq L_2(x, y, \dot{x}, \dot{y})$$
since $\frac{(x\dot{x}+y\dot{y})^2}{\ell^2-x^2-y^2}$ is of order 4 and
$$\sqrt{\ell^2 - x^2 - y^2} = \ell\sqrt{1 - (x^2 + y^2)/\ell^2} = \ell\big(1 - (x^2 + y^2)/(2\ell^2) + O((x^2 + y^2)^2)\big).$$
The Lagrange differential equations $\frac{d}{dt}\left(\frac{\partial L_2}{\partial \dot{x}}\right) = \frac{\partial L_2}{\partial x}$ and $\frac{d}{dt}\left(\frac{\partial L_2}{\partial \dot{y}}\right) = \frac{\partial L_2}{\partial y}$ read
$$\frac{d^2}{dt^2}x = -\frac{g}{\ell}x, \quad \frac{d^2}{dt^2}y = -\frac{g}{\ell}y.$$
These second-order differential scalar equations are identical for x and y. For x, it corresponds to two first-order differential scalar equation of state $(x, \dot{x}) = (x, v_x)$
$$\frac{d}{dt}x = v_x \frac{d}{dt}\dot{v}_x = -\frac{g}{\ell}x$$
whose spectrum is $\pm i\sqrt{g/\ell}$ on the imaginary axis. The linear approximation of the dynamics around equilibrium $x = 0$ is stable but not exponentially stable.
5. By definition $p_x = \frac{\partial L_2}{\partial \dot{x}}$ and $p_y = \frac{\partial L_2}{\partial \dot{y}}$, the conjugate variable of x and of y read
$$p_x = m\dot{x}, \quad p_y = m\dot{y}.$$
Thus the quadratic Hamiltonian H_2 is derived from the quadratic Lagrangian L_2 via the following formula (Legendre transform)
$$H_2 \triangleq \frac{\partial L_2}{\partial \dot{x}}\dot{x} + \frac{\partial L_2}{\partial \dot{y}}\dot{y} - L_2 = p_x\dot{x} + p_y\dot{y} - L_2$$
where $\dot{x}$ and $\dot{y}$ are replaced by p_x/m and p_y/m. This gives
$$H_2(x, y, p_x, p_y) = \frac{1}{2m}\left(p_x^2 + p_y^2\right) - mg\ell + m\frac{g}{2\ell}(x^2 + y^2).$$

The Hamiltonian formulation of the dynamics reads

$$\begin{aligned}
\frac{d}{dt}x &= \frac{\partial H_2}{\partial p_x} = p_x/m \\
\frac{d}{dt}y &= \frac{\partial H_2}{\partial p_y} = p_y/m \\
\frac{d}{dt}p_x &= -\frac{\partial H_2}{\partial x} = -mgx/\ell \\
\frac{d}{dt}p_y &= -\frac{\partial H_2}{\partial y} = -mgy/\ell
\end{aligned}$$

6. To the classical Hamiltonian H_2 corresponds the quantum Hamiltonian operator

$$\hat{H}_2 = \frac{1}{2m}\left(\hat{p}_x^2 + \hat{p}_y^2\right) - mg\ell + m\frac{g}{2\ell}(\hat{x}^2 + \hat{y}^2)$$

where $\hat{x}$, $\hat{y}$, $\hat{p}_x$ and $\hat{p}_y$ are operators with the following commutations rules

$$[\hat{x},\hat{y}] = [\hat{x},\hat{p}_y] = [\hat{y},\hat{p}_x] = [\hat{p}_x,\hat{p}_y] = 0, \quad [\hat{x},\hat{p}_x] = i\hbar, \quad [\hat{y},\hat{p}_y] = i\hbar.$$

From the Schrödinger equation governing the wave function $|\psi\rangle$, $i\hbar\frac{d}{dt}|\psi\rangle = \hat{H}_2|\psi\rangle$, one has for any operator $\hat{W}$:

$$\frac{d}{dt}\langle\psi|\hat{W}|\psi\rangle = i\langle\psi|[\hat{H}_2,\hat{W}]|\psi\rangle/\hbar.$$

Since $[\hat{x},\hat{H}_2] = i\hbar\hat{p}_x/m$, $[\hat{p}_x, H_2] = -i\hbar mg\hat{x}/\ell$, we have

$$\frac{d}{dt}\langle\psi|\hat{x}|\psi\rangle = \langle\psi|\hat{p}_x|\psi\rangle/m, \quad \frac{d}{dt}\langle\psi|\hat{p}_x|\psi\rangle = -mg\langle\psi|\hat{x}|\psi\rangle/\ell.$$

We recover the classical first-order differential equations where x and p_x are replaced by the average values $\langle\psi|\hat{x}|\psi\rangle$ and $\langle\psi|\hat{p}_x|\psi\rangle$ of $\hat{x}$ and $\hat{p}_x$. Average values of $\hat{y}$ and $\hat{p}_y$ are governed by similar differential equations.

7. (a) Since the Cartesian coordinates of the mass m in the inertial frame are

$$\left(\cos(\Omega t)x + \sin(\Omega t)y, -\sin(\Omega t)x + \cos(\Omega t)y, \sqrt{\ell^2 - x^2 - y^2}\right)$$

the kinetic energy reads

$$\frac{m}{2}\left(\left(\frac{d}{dt}(\cos(\Omega t)x + \sin(\Omega t)y)\right)^2 + \left(\frac{d}{dt}(-\sin(\Omega t)x + \cos(\Omega t)y)\right)^2 + \left(\frac{d}{dt}\sqrt{\ell^2 - x^2 - y^2}\right)^2\right).$$

Standard computations give then

$$\frac{m}{2}\left(\dot{x}^2 + \dot{y}^2 + \frac{(x\dot{x} + y\dot{y})^2}{\ell^2 - x^2 - y^2} + 2\Omega(y\dot{x} - x\dot{y}) + \Omega^2(x^2 + y^2)\right).$$

(b) The quadratic Lagrangian around the equilibrium $(x,y)=0$ is

$$L_2(x,y,\dot{x},\dot{y}) \triangleq \frac{m}{2}\left(\dot{x}^2+\dot{y}^2+2\Omega(y\dot{x}-x\dot{y})+\Omega^2(x^2+y^2)\right)+mg\ell-m\frac{g}{2\ell}(x^2+y^2)$$

With $p_x=m(\dot{x}+\Omega y)$ and $p_y=m(\dot{y}-\Omega x)$, one has

$$\begin{aligned} H_2 \triangleq \frac{\partial L_2}{\partial \dot{x}}\dot{x}+\frac{\partial L_2}{\partial \dot{y}}\dot{y}-L_2 &= \frac{m}{2}\left(\dot{x}^2+\dot{y}^2-\Omega^2(x^2+y^2)\right)-mg\ell+m\frac{g}{2\ell}(x^2+y^2) \\ &= \frac{1}{2m}\left(\dot{p}_x^2+\dot{p}_y^2\right)+\Omega(xp_y-yp_x)-mg\ell+m\frac{g}{2\ell}(x^2+y^2). \end{aligned}$$

Thus the dynamical model is given by the following system of four scalar differential equation of first-order:

$$\begin{aligned} \frac{d}{dt}x &= \frac{\partial H_2}{\partial p_x} = p_x/m-\Omega y \\ \frac{d}{dt}y &= \frac{\partial H_2}{\partial p_y} = p_y/m+\Omega x \\ \frac{d}{dt}p_x &= -\frac{\partial H_2}{\partial x} = -mgx/\ell-\Omega p_y \\ \frac{d}{dt}p_y &= -\frac{\partial H_2}{\partial y} = -mgy/\ell+\Omega p_x \end{aligned}$$

(c) To the classical Hamiltonian H_2 corresponds the quantum Hamiltionian operator

$$\hat{H}_2=\frac{1}{2m}\left(\hat{p}_x^2+\hat{p}_y^2\right)+\Omega(\hat{x}\hat{p}_y-\hat{y}\hat{p}_x)-mg\ell+m\frac{g}{2\ell}(\hat{x}^2+\hat{y}^2)$$

where $\hat{x}$, $\hat{y}$, $\hat{p}_x$ and $\hat{p}_y$ are operators as in question 6. Notice that $\hat{x}\hat{p}_y=\hat{p}_y\hat{x}$ and $\hat{y}\hat{p}_x=\hat{p}_x\hat{y}$, thus $\hat{H}_2$ is Hermitian.
We recover the differential system made of four first-order scalar equations where x, p_x, y and p_y are replaced by the average values of $\hat{x}$, $\hat{p}_x$, $\hat{y}$ and $\hat{p}_y$ respectively.