Quantum Mechanics - 1: HW 1 Solutions

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1 Problem 1

Harmonic oscillator dynamics in 2-d via Lagrangian and Hamiltonian formalism in Cartesian and Polar Coordinates.

1.1 Lagrangian

$$L = \frac{1}{2}m|\dot{\vec{r}}|^2 - \frac{1}{2}m\omega^2 r^2 \tag{1}$$

The equation of motion can be found by using the Euler-Lagrange equations

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} \tag{2}$$

1.1.1 Cartesian

I set $\vec{q} = \{x, y\}$. So $q_1 = x$ and $q_2 = y$. In this coordinate system the Lagrangian is

$$L = \frac{1}{2}m\left(\dot{x}^2 + \dot{y}^2\right) - \frac{1}{2}m\omega^2\left(x^2 + y^2\right) \tag{3}$$

Using the Euler-Lagrange equations (2)

$$\begin{aligned} m\ddot{x} + m\omega^2 x &= 0 \\ m\ddot{y} + m\omega^2 y &= 0 \end{aligned} \tag{4}$$

These two equations can be expressed in a compact form by invoking vector notation

$$\ddot{\vec{r}} = -\omega^2\vec{r} \tag{5}$$

1.1.2 Polar

I set $\vec{q} = \{r, \theta\}$. It is important to remember that the unit vectors in this coordinate system can change with time.

$$\begin{aligned} \frac{d}{dt}\hat{r} &= \dot{\theta}\hat{\theta} \\ \frac{d}{dt}\hat{\theta} &= -\dot{\theta}\hat{r} \end{aligned} \tag{6}$$

These should remind you of sine and cosine for obvious reasons. We will need to know $\dot{r}^2$. first we'll need to know $\frac{d}{dt}\vec{r}$

$$\frac{d}{dt}\vec{r} = \dot{r}\hat{r} + r\dot{\hat{r}} = \dot{r}\hat{r} + r\dot{\theta}\hat{\theta} \tag{7}$$

Dotting the above equation with itself

$$\left|\frac{d}{dt}\vec{r}\right| = \dot{r}^2 + r^2\dot{\theta}^2 \tag{8}$$

All together the Lagrangian is

$$L = \frac{1}{2}m\left(\dot{r}^2 + r^2\dot{\theta}^2\right) - \frac{1}{2}m\omega^2 r^2 \tag{9}$$

Using the Euler-Lagrange equations (2) like before

$$\begin{aligned} m\ddot{r} - mr\dot{\theta}^2 + m\omega^2 r = 0 \\ mr^2\ddot{\theta} + 2mr\dot{r}\dot{\theta} = 0 \end{aligned} \tag{10}$$

1.2 Hamiltonian

The Hamiltonian of a system is defined via the Lagrangian, coordinates, and conjugate momentum.

$$H = \sum p_i\dot{q}_i - L \tag{11}$$

where

$$p_i = \frac{\partial L}{\partial \dot{q}_i} \tag{12}$$

The Hamilton equations of motions are

$$\begin{aligned} \dot{q}_i &= \frac{\partial H}{\partial p_i} \\ \dot{p}_i &= -\frac{\partial H}{\partial q_i} \end{aligned} \tag{13}$$

1.2.1 Cartesian

First, I find the conjugate momenta.

$$\begin{aligned} p_x &= \frac{\partial L}{\partial \dot{x}} = m\dot{x} \\ p_y &= \frac{\partial L}{\partial \dot{y}} = m\dot{y} \end{aligned} \tag{14}$$

Now I can write H in terms of p's and q's

$$H = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{1}{2}m\omega^2\left(x^2 + y^2\right) \tag{15}$$

Using (14) the equations of motion are

$$\begin{aligned}
\dot{x} &= \frac{p_x}{m} \\
\dot{y} &= \frac{p_y}{m} \\
\dot{p}_x &= -m\omega^2 x \\
\dot{p}_y &= -m\omega^2 y
\end{aligned} \tag{16}$$

1.2.2 Polar

Like before I first need to find the conjugate momentum

$$\begin{aligned}
p_r &= \frac{\partial L}{\partial \dot{r}} = m\dot{r} \\
p_\theta &= \frac{\partial L}{\partial \dot{\theta}} = mr^2\dot{\theta}
\end{aligned} \tag{17}$$

Writing H in terms of p's and q's again

$$H = \frac{p_r^2}{2m} + \frac{p_\theta^2}{2mr^2} + \frac{m}{2}\omega^2 r^2 \tag{18}$$

Hamilton's equations of motion are

$$\begin{aligned}
\dot{r} &= \frac{p_r}{m} \\
\dot{\theta} &= \frac{p_\theta}{mr^2} \\
\dot{p}_r &= -m\omega^2 r + \frac{p_\theta}{mr^3} \\
\dot{p}_\theta &= 0
\end{aligned} \tag{19}$$

The last expression here is a statement that p_θ is a constant with time (constant of the motion). By which I mean angular momentum is conserved!

1.3 Poisson Brackets

Another way to show that p_θ is a constant of the motion is to show that its Poisson bracket with H is 0. This is the mathematical definition of a 'constant of the motion.' The Poisson bracket is defined

$$\{A,\, B\} = \frac{\partial A}{\partial q}\frac{\partial B}{\partial p} - \frac{\partial A}{\partial p}\frac{\partial B}{\partial q} \tag{20}$$

$$\{p_\theta,\, H\} = \underbrace{\frac{\partial p_\theta}{\partial \theta}}_{=0}\frac{\partial H}{\partial p_\theta} - \frac{\partial p_\theta}{\partial p_\theta}\underbrace{\frac{\partial H}{\partial \theta}}_{=0} = 0 \tag{21}$$

Now $\frac{\partial p_\theta}{\partial \theta} = 0$ and $\frac{\partial H}{\partial \theta} = 0$, so this Poisson bracket is zero and p_θ is a constant of the motion. In Quantum Mechanics Poisson brackets are replaced with commutators. Every eigenstate of an operator which commutes with Hamiltonian does not change with time.

2 Problem 2

The action is defined

$$S\left[x_{cl},\dot{x}_{cl}\right]=\int_0^T\left[\frac{1}{2}m\dot{x}_{cl}^2-\frac{1}{2}m\omega^2x_{cl}^2\right]dt \tag{22}$$

The solution to a harmonic oscillator is

$$x_{cl}(t)=x_i\cos\omega t+Bcos\omega t \tag{23}$$

Its location at time T.

$$x_f=x_i\cos\omega T+B\sin\omega T \tag{24}$$

I use expression (23) to eliminate B.

$$B=\frac{x_f-x_i\cos\omega T}{\sin\omega T} \tag{25}$$

In terms of x_i, x_f, t, and T our solution is

$$x_{cl}=x_i\cos\omega t+\frac{x_f-x_i\cos\omega T}{\sin\omega T}\sin\omega t \tag{26}$$

t can be eliminated by simply integrating.

$$\begin{aligned} S\left(x_i,x_f,T\right) &= \int_0^T\left[\frac{m}{2}\dot{x}_{cl}^2-\frac{m}{2}\omega^2x_{cl}^2\right]dt & (27)\\ &= \int_0^T\left[\frac{m}{2}\frac{d}{dt}\left(x_{cl}\dot{x}_{cl}\right)-\frac{m}{2}x_{cl}\underbrace{\left(\ddot{x}_{cl}+\omega^2x_{cl}\right)}_{=0\text{ see}(4)}\right]dt & (28)\end{aligned}$$

From the equations of motion we know $\ddot{x}_c+\omega^2x_c=0$. The integral can now be solve via fundamental theorem of calculus.

$$S=\frac{m}{2}\left(x_f\dot{x}_f-x_i\dot{x}_i\right) \tag{29}$$

where

$$\begin{aligned} \dot{x}_f &= -x_i\omega\sin\omega T+\frac{x_f-x_i\cos\omega T}{\sin\omega T}\omega\cos\omega T & (30)\\ \dot{x}_i &= \frac{x_f-x_i\cos\omega T}{\sin\omega T}\omega & (31)\end{aligned}$$

Put together we have

$$\begin{aligned} S\left(x_i,x_f,T\right) &= \frac{m\omega}{2\sin\omega T}\left[-x_ix_f\sin^2\omega T+\right.\\ &\quad \left.\left(x_f-x_i\cos\omega T\right)x_f\cos\omega T-x_i\left(x_f-x_i\cos\omega T\right)\right] & (32)\end{aligned}$$

$$\boxed{S\left(x_i,x_f,T\right)=\tfrac{m\omega}{2\sin\omega T}\left[\left(x_i^2+x_f^2\right)\cos\omega T-2x_ix_f\right]} \tag{33}$$

3 Problem 3

There is more than one way to do this problem. One approach is to generalize what I did in class for a particle's coordinate $q(t)$ using the definition of functional derivative $\delta q(t')/\delta q(t) = \delta(t-t')$ to a field $\psi(\vec{r},t)$, with $\delta\psi(\vec{r'},t')/\delta\psi(\vec{r},t) = \delta^{(3)}(\vec{r}-\vec{r})\delta(t-t')$, and similarly for $\overline{\psi(\vec{r},t)}$.

Another approach is to simply compute the differential of S, remembering that the boundary terms vanish by definition that fields do not vary at the boundary.

$$S = \int \left(-\imath\hbar\Psi^*\partial_t\Psi + \frac{\hbar^2}{2m}\nabla\Psi^*\cdot\nabla\Psi + V\Psi^*\Psi \right) d^3r\, dt \tag{34}$$

$$\delta_{\Psi^*}S = \int \left(-\imath\hbar\partial_t\Psi \underbrace{-\frac{\hbar^2}{2m}\nabla^2\Psi}_{\text{int. by parts}} +V\Psi \right) \delta\Psi^* d^3r\, dt = 0 \tag{35}$$

$$\delta_{\Psi}S = \int \left(\underbrace{\imath\hbar\partial_t\Psi^* - \frac{\hbar^2}{2m}\nabla^2\Psi^*}_{\text{int. by parts}} +V\Psi^* \right) \delta\Psi d^3r\, dt = 0 \tag{36}$$

The above conditions are met if each integrand is $= 0$. This leads us to Schrödringer's equation, and it's conjugate

$$-\tfrac{\hbar^2}{2m}\nabla^2\Psi + V\Psi = \imath\hbar\partial_t\Psi \tag{37}$$

$$-\tfrac{\hbar^2}{2m}\nabla^2\Psi^* + V\Psi^* = -\imath\hbar\partial_t\Psi^* \tag{38}$$

4 Problem 4

Bohr-Sommerfeld quantization states

$$\oint_{orbit} \vec{p}\cdot d\vec{q} = h\, n \tag{39}$$

If the electron is just moving in a circular orbit, then it has momentum.

$$\vec{p} = m_e\omega r\hat{\phi} \tag{40}$$

I use our orbit, which is circular, for my contour, so $d\vec{q} = rd\phi\hat{\phi}$. After taking the integral I'm left with

$$2\pi m_e\omega r^2 = nh \tag{41}$$

$$\ell_\phi = n\hbar \tag{42}$$

The Hamiltonian is

$$H = \frac{\ell_\phi^2}{2m_e r^2} - \frac{Ze^2}{r} \tag{43}$$

The election will orbit so that it's energy is minimized

$$\frac{\partial E}{\partial r} = -\frac{n^2\hbar^2}{m_e r_n^3} + \frac{Ze^2}{r_n^2} \Rightarrow r_n = \frac{n^2\hbar^2}{m_e e^2 Z} \tag{44}$$

Using the above relation we can write the Energy without r_n dependence.

$$E_n = -\frac{Z^2 e^4 m_e}{2\hbar^2 n^2} = -\frac{1}{2}mc^2 Z^2\alpha^2\frac{1}{n} \tag{45}$$

$$r_n = \frac{\hbar^2 n^2}{me^2 Z} = \frac{\lambda_e n^2}{2\pi Z\alpha} \tag{46}$$

where

$$\alpha = \frac{e^2}{\hbar c} \approx \frac{1}{137} \text{ (you should memorize this number!)} \tag{47}$$

$$\lambda_e = \frac{hc}{mc^2} \tag{48}$$

5 Problem 5

5.1 harmonic oscillator

$$E_n = \frac{p_n^2}{2m} + \frac{m}{2}\omega^2 x_n^2 \tag{49}$$

Using our rough quantization rule.

$$p_n = \frac{n\hbar}{x_n} \Rightarrow E_n = \frac{n^2\hbar^2}{2mx_n^2} + \frac{m}{2}\omega^2 x_n^2 \tag{50}$$

I find x_n by minimizing the energy.

$$-\frac{n^2\hbar^2}{mx_n^3} + m\omega^2 x_n = 0 \Rightarrow$$

$$\boxed{x_n = \sqrt{\frac{\hbar n}{m\omega}} = x_0 n^{\frac{1}{2}}, \text{ where } x_0 = \sqrt{\frac{\hbar}{m\omega}}} \tag{51}$$

In terms of dimensional constants and n our energy is

$$E_n = \frac{n^2\hbar^2 m\omega}{2m\hbar n} + \frac{m}{2}\omega^2\frac{\hbar n}{m\omega}$$

$$\boxed{E_n = \hbar\omega n} \tag{52}$$

5.2 quartic oscillator

$$E_n = \frac{p_n^2}{2m} + \frac{a}{4}x^4 \tag{53}$$

$$E_n = \frac{n^2\hbar^2}{2mx_n^2} + \frac{a}{4}x_n^4 \tag{54}$$

Finding minimum energy

$$-\frac{n^2\hbar^2}{mx_n^3} + ax_n^3 = 0 \Rightarrow \boxed{x_n = \left(\frac{n^2\hbar^2}{ma}\right)^{\frac{1}{6}}} \tag{55}$$

Writing energy in terms of n and constants

$$E_n = \frac{n^2\hbar^2}{2m\left(\frac{n^2\hbar^2}{ma}\right)^{\frac{1}{3}}} + \frac{a}{4}\left(\frac{n^2\hbar^2}{ma}\right)^{\frac{2}{3}} \tag{56}$$

$$\boxed{E_n = \frac{3a}{4}\left(\frac{\hbar^2 n^2}{ma}\right)^{\frac{2}{3}} = E_1 n^{\frac{4}{3}}} \tag{57}$$

5.3 H-atom with Coulomb potential

$$E_n = \frac{p_n^2}{2m} - \frac{Ze^2}{r_n} \tag{58}$$

$$E_n = \frac{n^2\hbar^2}{2mr_n^2} - \frac{Ze^2}{r_n} \tag{59}$$

Finding minimum energy

$$-\frac{n^2\hbar^2}{mr_n^3} + \frac{Ze^2}{r_n^2} = 0 \Rightarrow \boxed{r_n = \frac{\hbar^2 n^2}{me^2 Z}} \tag{60}$$

Writing energy in terms of n and constants, and simplifying

$$\boxed{E_n = -\frac{Z^2e^4m}{2\hbar^2n^2}} \tag{61}$$

5.4 e^- in the potential $\frac{1}{s}V_0\left(\frac{x}{x_1}\right)^s$

$$E_n = \frac{n^2\hbar^2}{2mx_n^2} + \frac{1}{s}V_0\left(\frac{x_n}{x_1}\right)^s \tag{62}$$

Finding the minimum energy

$$-\frac{n^2\hbar^2}{m_e x_n^3} + \frac{V_0}{x}\left(\frac{x_n}{x_1}\right)^{s-1} \Rightarrow \boxed{x_n = x_1\left(\frac{n^2\hbar^2}{m_e x_1^2 V_0}\right)^{\frac{1}{s+2}}} \tag{63}$$

Writing energy in terms of n and constants

$$\boxed{E_n = \frac{s+2}{2s} V_0 \left(\frac{n^2\hbar^2}{m_e V_0 x_1^2}\right)^{\frac{s}{s+2}}} \tag{64}$$

In the limit $s \gg 1$

$$E_n = \frac{V_0}{2} \frac{n^2\hbar^2}{m_e x_1^2 V_0} \sim n^2 \tag{65}$$

This limit is consistent with the infinite square well result.

6 Problem 6

By definition the probability density is

$$P(\vec{r},t) = |\Psi(\vec{r},t)| \tag{66}$$

$$\frac{dP}{dt} = \Psi^* (\partial_t \Psi) + (\partial_t \Psi^*) \Psi \tag{67}$$

I trade the time derivatives for space derivatives by using Schödinger's equation (36) and its complex conjugate (37).

$$\begin{aligned}
\frac{dP}{dt} &= \frac{1}{\imath\hbar} \left\{ \Psi^* \left(-\frac{\hbar^2\nabla^2}{2m} + V \right) \Psi - \left[\left(-\frac{\hbar^2\nabla^2}{2m} + V \right) \Psi^* \right] \Psi \right\} && (68) \\
&= \frac{\hbar}{2m\imath} \left\{ -\vec{\nabla} \cdot \left[\Psi^* \vec{\nabla} \Psi \right] + \vec{\nabla}\Psi^* \vec{\nabla}\Psi + \vec{\nabla} \cdot \left[\left(\vec{\nabla}\Psi^* \right) \Psi \right] - \vec{\nabla}\Psi^* \cdot \vec{\nabla}\Psi \right\} \\
&= -\vec{\nabla} \cdot \left\{ \frac{\hbar}{2m\imath} \left[\Psi^* \vec{\nabla}\Psi - \left(\vec{\nabla}\Psi^* \right) \Psi \right] \right\} && (69) \\
& && (70)
\end{aligned}$$

So we can call $\boxed{\vec{J}_p = \frac{\hbar}{2m\imath} \left[\Psi^* \vec{\nabla}\Psi - \left(\vec{\nabla}\Psi^* \right) \Psi \right]}$ (71)

the probability current, which is conserved $\boxed{\partial_t P(\vec{r},t) + \vec{\nabla} \cdot \vec{J} = 0}$ (72)