# Chem221a : Solution Set 1

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September 5, 2007

## Problem 1

We're trying to show that $\sum_i p_i \dot{q}_i = 2T$ when we're given $T$ as a function of the $q_i$ and the $\dot{q}_i$. So we'll use one of Hamilton's equations to get the conjugate momenta $p_i$. This will be independent of potential (if the potential depends only on the coordinates):

$$p_i = \frac{\partial H}{\partial \dot{q}_i} = \frac{\partial}{\partial \dot{q}_i}\left(T(q,\dot{q}) + V(q)\right) \tag{1}$$

$$= \frac{\partial T(q,\dot{q})}{\partial \dot{q}_i} \tag{2}$$

So out first goal will be to calculate the partial derivative of $T$ with repect to $\dot{q}_i$. We're given

$$T = \sum_{i,j} T_{ij}(q)\dot{q}_i\dot{q}_j \tag{3}$$

Now we can either assume that the $T_{ij}(q)$ are symmetric ($T_{ij} = T_{ji}$), or we can construct a set $T'_{ij}(q) = \frac{1}{2}(T_{ij}(q) + T_{ji}(q))$ which is symmetric. The $T'_{ij}$ can be replace the $T_{ij}$ in the problem exactly.[1] I will use the notation $T_{ij}$ to simplify, but the arguments actually apply to the symmetrized $T'_{ij}$.

Before continuing with this problem, it might be helpful to this of this as a matrix operation.

$$T = {}^t\mathbf{q}\,\hat{T}\,\mathbf{q} \tag{4}$$

[1] To show this, we just plug it in:

$$\sum_{ij} T'_{ij}\dot{q}_i\dot{q}_j = \frac{1}{2}\sum_{ij}(T_{ij}+T_{ji})\dot{q}_i\dot{q}_j = \frac{1}{2}\left(\sum_{ij} T_{ij}\dot{q}_i\dot{q}_j + \sum_{ij} T_{ji}\dot{q}_i\dot{q}_j\right)$$

Now we note that the sum in the second term is over all possibilities for both $i$ and $j$, which index the same possibilities. So the order of the index can be inverted without loss of generality (in the matrix illustration, we're summing over all elements of the matrix — whether we go by row or by column doesn't matter). Thus we continue with:

$$\frac{1}{2}\left(\sum_{ij} T_{ij}\dot{q}_i\dot{q}_j + \sum_{ij} T_{ij}\dot{q}_i\dot{q}_j\right) = \frac{1}{2}(T+T) = T \quad \square$$

where we can write the matrix $\hat{T}$ as:

$$\hat{T} = \begin{pmatrix} T_{11}(q) & T_{12}(q) & T_{13}(q) & \cdots \\ T_{21}(q) & T_{22}(q) & T_{23}(q) & \cdots \\ T_{31}(q) & T_{32}(q) & T_{33}(q) & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{5}$$

The sum over $i$ and $j$ results in adding over all elements of the matrix (multiplied by the appropriate $\dot{q}_i$ and $\dot{q}_j$). With that visual in mind, we're going to split the equation into three parts: first we'll write a part that corresponds to the diagonal elements of the matrix, where $i = j$. Then we'll write another part which corresponds to the upper triangular part of the matrix, where $i < j$. Finally, we'll write a term corresponding to the lower triangular part of the matrix, where $i > j$.

This separation gives us:

$$\begin{aligned} T &= \sum_{i,j} T_{ij}(q)\dot{q}_i\dot{q}_j && (6)\\ &= \sum_i T_{ii}(q)\dot{q}_i^2 + \sum_{i\neq j} T_{ij}(q)\dot{q}_i\dot{q}_j && (7)\\ &= \sum_i T_{ii}(q)\dot{q}_i^2 + \sum_{i<j} T_{ij}(q)\dot{q}_i\dot{q}_j + \sum_{i>j} T_{ij}(q)\dot{q}_i\dot{q}_j && (8) \end{aligned}$$

We can switch the labels $i$ and $j$ in the last term, and then we can use the symmetry of the $T_{ij}$ matrix to obtain an expression for $T$:

$$\begin{aligned} T &= \sum_i T_{ii}(q)\dot{q}_i^2 + \sum_{i<j} T_{ij}(q)\dot{q}_i\dot{q}_j + \sum_{i<j} T_{ji}(q)\dot{q}_i\dot{q}_j && (9)\\ &= \sum_i T_{ii}(q)\dot{q}_i^2 + \sum_{i<j} T_{ij}(q)\dot{q}_i\dot{q}_j + \sum_{i<j} T_{ij}(q)\dot{q}_i\dot{q}_j && (10)\\ &= \sum_i T_{ii}(q)\dot{q}_i^2 + 2\sum_{i<j} T_{ij}(q)\dot{q}_i\dot{q}_j && (11) \end{aligned}$$

Now that we have this expression, we'll take the derivative of it.

$$\begin{aligned} p_k &= \frac{\partial T}{\partial \dot{q}_k} && (12)\\ &= 2T_{kk}(q)\dot{q}_k + 2\left(\sum_{i<k} T_{ik}(q)\dot{q}_i + \sum_{k<j} T_{kj}(q)\dot{q}_j\right) && (13)\\ &= 2T_{kk}(q)\dot{q}_k + 2\sum_{j\neq k} T_{kj}(q)\dot{q}_j && (14)\\ &= 2\sum_j T_{kj}(q)\dot{q}_j && (15) \end{aligned}$$

From here, the rest of the proof is just a matter of plug-and-chug:

$$\sum_i p_i \dot{q}_i = \sum_i 2 \sum_j T_{ij}(q) \dot{q}_j \dot{q}_i \tag{16}$$

$$= 2 \sum_{i,j} T_{ij}(q) \dot{q}_i \dot{q}_j \tag{17}$$

$$= 2T \quad \square \tag{18}$$

# Problem 2

(a) **Shankar 2.3.1**: This problem is simply a matter using equations (2.3.1), (2.3.3), and (2.3.4) to replace terms in equation (2.3.5). The result gives us equation (2.3.6).

If we take the time derivatives of equations (2.3.3) and (2.3.4), we obtain

$$\dot{\mathbf{r}}_1 = \dot{\mathbf{r}}_{\text{CM}} + \frac{m_2}{m_1 + m_2} \dot{\mathbf{r}} \tag{19}$$

$$\dot{\mathbf{r}}_2 = \dot{\mathbf{r}}_{\text{CM}} - \frac{m_1}{m_1 + m_2} \dot{\mathbf{r}} \tag{20}$$

Taking these, along with equation (2.3.1) (which defines $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$), and plugging them into equation (2.3.5), we obtain:

$$\mathcal{L} = \frac{1}{2} m_1 \left|\dot{\mathbf{r}}_1\right|^2 + \frac{1}{2} m_2 \left|\dot{\mathbf{r}}_2\right|^2 - V(\mathbf{r}_1 - \mathbf{r}_2) \tag{21}$$

$$= \frac{1}{2} m_1 \left|\dot{\mathbf{r}}_{\text{CM}} + \frac{m_2}{m_1 + m_2} \dot{\mathbf{r}}\right|^2 + \frac{1}{2} m_2 \left|\dot{\mathbf{r}}_{\text{CM}} - \frac{m_1}{m_1 + m_2} \dot{\mathbf{r}}\right|^2 - V(\mathbf{r}) \tag{22}$$

Since $|\mathbf{a}|^2 = \mathbf{a} \cdot \mathbf{a}$, and the dot product is independent of the coordinate system, we represent the dot product by Cartesian coordinates (using superscripts to denote each component):

$$\mathcal{L} = \frac{1}{2} m_1 \sum_{i \in \{x,y,z\}} \left( \left(\dot{r}_{\text{CM}}^{(i)}\right)^2 + \frac{2m_2}{m_1 + m_2} \dot{r}_{\text{CM}}^{(i)} \dot{r}^{(i)} + \left(\frac{m_2}{m_1 + m_2}\right)^2 \left(\dot{r}^{(i)}\right)^2 \right) \tag{23}$$

$$+ \frac{1}{2} m_2 \sum_{i \in \{x,y,z\}} \left( \left(\dot{r}_{\text{CM}}^{(i)}\right)^2 - \frac{2m_1}{m_1 + m_2} \dot{r}_{\text{CM}}^{(i)} \dot{r}^{(i)} + \left(\frac{m_1}{m_1 + m_2}\right)^2 \left(\dot{r}^{(i)}\right)^2 \right) - V(\mathbf{r})$$

$$= \sum_{i \in \{x,y,z\}} \left( \frac{1}{2}(m_1 + m_2) \left(\dot{r}_{\text{CM}}^{(i)}\right)^2 + \frac{1}{2} \left( \frac{m_1 m_2^2}{(m_1 + m_2)^2} + \frac{m_2 m_1^2}{(m_1 + m_2)^2} \left(\dot{r}^{(i)}\right)^2 \right) \right) - V(\mathbf{r}) \tag{24}$$

$$= \frac{1}{2}(m_1 + m_2) \sum_{i \in \{x,y,z\}} \left(\dot{r}_{\text{CM}}^{(i)}\right)^2 + \frac{1}{2} m_1 m_2 \frac{m_1 + m_2}{(m_1 + m_2)^2} \sum_{i \in \{x,y,z\}} \left(\dot{r}^{(i)}\right)^2 - V(\mathbf{r}) \tag{25}$$

$$= \frac{1}{2}(m_1 + m_2) \left|\dot{\mathbf{r}}_{\text{CM}}\right|^2 + \frac{1}{2} \frac{m_1 m_2}{m_1 + m_2} \left|\dot{\mathbf{r}}\right|^2 - V(\mathbf{r}) \quad \square \tag{26}$$

(b) **Shankar 2.5.4**: Using the Lagrangian obtained at the end of the first part of this problem, we're now supposed to find the Hamiltonian. We begin by finding the conjugate momenta in terms of the velocities:

$$p^{(i)} = \frac{\partial \mathcal{L}}{\partial r^{(i)}} = \frac{m_1 m_2}{m_1 + m_2} \dot{r}^{(i)} \tag{27}$$

$$p_{\text{CM}}^{(i)} = \frac{\partial \mathcal{L}}{\partial r^{(i)}} = (m_1 + m_2) \dot{r}_{\text{CM}}^{(i)} \tag{28}$$

Now we invert those to give us the velocities in terms of the conjugate momenta:

$$\dot{r}^{(i)} = \frac{m_1 + m_2}{m_1 m_2} p^{(i)} \tag{29}$$

$$\dot{r}_{\text{CM}}^{(i)} = \frac{1}{m_1 + m_2} p_{\text{CM}}^{(i)} \tag{30}$$

From here, it's a small step to get the values of $|\mathbf{r}|^2$ and $|\mathbf{r}_{\text{CM}}|^2$:

$$|\mathbf{r}|^2 = \left( \frac{m_1 + m_2}{m_1 m_2} \right)^2 |\mathbf{p}|^2 \tag{31}$$

$$|\mathbf{r}_{\text{CM}}|^2 = \left( \frac{1}{m_1 + m_2} \right)^2 |\mathbf{p}_{\text{CM}}|^2 \tag{32}$$

At this point, we do the Legendre transform to change the Lagrangian into a Hamiltonian, and use equations (29) and (30) to express the velocities in terms of the momenta. We can either do the Legendre transform explicitly (actually calculating the sum $\sum_i p_i \dot{q}_i$) or, as will be shown below, we can use the results of the first problem on this problem set:

$$\begin{aligned} \mathcal{H}(\mathbf{p}, \mathbf{p}_{\text{CM}}, \mathbf{r}, \mathbf{r}_{\text{CM}}) &= \sum_i p_i \dot{r}_i - \mathcal{L} & (33) \\ &= 2T - (T - V) & (34) \\ &= T + V & (35) \\ &= \frac{1}{2}(m_1 + m_2) |\dot{\mathbf{r}}_{\text{CM}}|^2 + \frac{1}{2} \frac{m_1 m_2}{m_1 + m_2} |\dot{\mathbf{r}}|^2 + V(\mathbf{r}) & (36) \end{aligned}$$

where the kinetic energy $T$ is identified from the Lagrangian as

$$T = \frac{1}{2}(m_1 + m_2) |\dot{\mathbf{r}}_{\text{CM}}|^2 + \frac{1}{2} \frac{m_1 m_2}{m_1 + m_2} |\dot{\mathbf{r}}|^2 \tag{37}$$

Now we plug in the values of $|\mathbf{r}|^2$ and $|\mathbf{r}_{\text{CM}}|^2$ from above:

$$\begin{aligned} \mathcal{H} &= \frac{1}{2}(m_1 + m_2) \left( \frac{1}{m_1 + m_2} \right)^2 |\mathbf{p}_{\text{CM}}|^2 + \frac{1}{2} \frac{m_1 m_2}{m_1 + m_2} \left( \frac{m_1 + m_2}{m_1 m_2} \right)^2 |\mathbf{p}|^2 + V(\mathbf{r}) & (38) \\ &= \frac{1}{2} \frac{1}{m_1 + m_2} |\mathbf{p}_{\text{CM}}|^2 + \frac{1}{2} \frac{m_1 + m_2}{m_1 m_2} |\mathbf{p}|^2 + V(\mathbf{r}) & (39) \end{aligned}$$

When we take $M = m_1 + m_2$ and $\mu = \frac{m_1 m_2}{m_1 + m_2}$ (the reduced mass), as given in the problem, we obtain the desired result.

$$\mathcal{H}(\mathbf{p}, \mathbf{p}_{\text{CM}}, \mathbf{r}, \mathbf{r}_{\text{CM}}) = \frac{|\mathbf{p}_{\text{CM}}|^2}{2M} + \frac{|\mathbf{p}|^2}{2\mu} + V(\mathbf{r}) \tag{40}$$

## Problem 3

This problem is all about using the techniques of classical mechanics in spherical coordinates on an arbitrary potential. Once you have the kinetic energy in spherical coordinates (part (a)) the rest is just applying the same rules we'd use in Cartesian coordinates.

(a) The Lagrangian is always $L = T - V$, and we're given that $V = V(r, \theta, \phi)$. Now we need the kinetic energy term, $T$. Getting it is a little tedious, but pretty straightforward. We know $T$ in Cartesian coordinates:

$$T = \frac{1}{2}m\left(\dot{x}^2 + \dot{y}^2 + \dot{z}^2\right) \tag{41}$$

We also know what $x$, $y$, and $z$ are in terms of the polar coordinates $r$, $\phi$, and $\theta$:

$$x = r\cos(\phi)\sin(\theta) \tag{42}$$
$$y = r\sin(\phi)\sin(\theta) \tag{43}$$
$$z = r\cos(\theta) \tag{44}$$

(where I have used the physicist's convention for the spherical coordinates — mathematicians swap $\theta$ and $\phi$).

But we have $T$ as a function of the velocities, not the coordinates. Remembering that the coordinates themselves are functions of time, we use the product rule and the chain rule to take the time-derivatives of the coordinate definitions given above:

$$\dot{x} = \dot{r}\cos(\phi)\sin(\theta) + r(-\sin(\phi)\dot{\phi})\sin(\theta) + r\cos(\phi)(\cos(\theta)\dot{\theta}) \tag{45}$$
$$\dot{y} = \dot{r}\sin(\phi)\sin(\theta) + r(\cos(\phi)\dot{\phi})\sin(\theta) + r\sin(\phi)(\cos(\theta)\dot{\theta}) \tag{46}$$
$$\dot{z} = \dot{r}\cos(\theta) + r(-\sin(\theta)\dot{\theta}) \tag{47}$$

Now it's just a lot of simplification. Expand the squares, collect terms, and the only trig identity you need is $\sin^2(x) + \cos^2(x) = 1$.

$$T = \frac{1}{2}m\left(\dot{x}^2 + \dot{y}^2 + \dot{z}^2\right) \tag{48}$$

$$\begin{aligned} &= \frac{1}{2}m\Bigg(\left(\dot{r}\cos(\phi)\sin(\theta) - r\sin(\phi)\sin(\theta)\dot{\phi} + r\cos(\phi)\cos(\theta)\dot{\theta}\right)^2 \\ &\qquad + \left(\dot{r}\sin(\phi)\sin(\theta) + r\cos(\phi)\sin(\theta)\dot{\phi} + r\sin(\phi)\cos(\theta)\dot{\theta}\right)^2 \\ &\qquad + \left(\dot{r}\cos(\theta) - r\sin(\theta)\dot{\theta}\right)^2\Bigg) \end{aligned} \tag{49}$$

$$
\begin{aligned}
&= \frac{1}{2}m\Big(\dot{r}^2\cos^2(\phi)\sin^2(\theta) + r^2\sin^2(\phi)\sin^2(\theta)\dot{\phi}^2 + r^2\cos^2(\phi)\cos^2(\theta)\dot{\theta}^2 \\
&\quad -2\dot{r}r\cos(\phi)\sin(\phi)\sin^2(\theta)\dot{\phi} + 2\dot{r}r\cos^2(\phi)\sin(\theta)\cos(\theta)\dot{\theta} \\
&\quad -2r^2\sin(\phi)\cos(\phi)\sin(\theta)\cos(\theta)\dot{\theta}\dot{\phi} \\
&\quad +\dot{r}^2\sin^2(\phi)\sin^2(\theta) + r^2\cos^2(\phi)\sin^2(\theta)\dot{\phi}^2 + r^2\sin^2(\phi)\cos^2(\theta)\dot{\theta}^2 \\
&\quad +2\dot{r}r\sin(\phi)\cos(\phi)\sin^2(\theta)\dot{\phi} + 2\dot{r}r\sin^2(\phi)\sin(\theta)\cos(\theta)\dot{\theta} \\
&\quad +2r^2\sin(\phi)\cos(\phi)\sin(\theta)\cos(\theta)\dot{\theta}\dot{\phi} \\
&\quad +\dot{r}^2\cos^2(\theta) + r^2\sin^2(\theta)\dot{\theta}^2 - 2\dot{r}r\cos(\theta)\sin(\theta)\dot{\theta}\Big)
\end{aligned}
\tag{50}
$$

$$
\begin{aligned}
&= \frac{1}{2}m\big(\dot{r}^2\left(\cos^2(\phi)\sin^2(\theta) + \sin^2(\phi)\sin^2(\theta) + \cos^2(\theta)\right) \\
&\quad +r^2\dot{\phi}^2\left(\sin^2(\phi)\sin^2(\theta) + \cos^2(\phi)\sin^2(\theta)\right) \\
&\quad +r^2\dot{\theta}^2\left(\cos^2(\phi)\cos^2(\theta) + \sin^2(\phi)\cos^2(\theta) + \sin^2(\theta)\right) \\
&\quad +2\dot{r}r\dot{\phi}\left(-\sin(\phi)\cos(\phi)\sin^2(\theta) + \sin(\phi)\cos(\phi)\sin^2(\theta)\right) \\
&\quad +2\dot{r}r\dot{\theta}\left(\cos^2(\phi)\sin(\theta)\cos(\theta) + \sin^2(\phi)\sin(\theta)\cos(\theta) - \cos(\theta)\sin(\theta)\right) \\
&\quad +2r^2\dot{\theta}\dot{\phi}\left(\sin(\phi)\cos(\phi)\sin(\theta)\cos(\theta) - \sin(\phi)\cos(\phi)\sin(\theta)\cos(\theta)\right)\Big)
\end{aligned}
\tag{51}
$$

$$
\begin{aligned}
&= \frac{1}{2}m\big(\dot{r}^2\left(\left(\cos^2(\phi) + \sin^2(\phi)\right)\sin^2(\theta) + \cos^2(\theta)\right) \\
&\quad +r^2\dot{\phi}^2\left(\left(\sin^2(\phi) + \cos^2(\phi)\right)\sin^2(\theta)\right) \\
&\quad +r^2\dot{\theta}^2\left(\left(\cos^2(\phi) + \sin^2(\phi)\right)\cos^2(\theta) + \sin^2(\theta)\right) \\
&\quad +2\dot{r}r\dot{\phi}(0) + 2\dot{r}r\dot{\theta}\left(\left(\cos^2(\phi) + \sin^2(\phi)\right)\sin(\theta)\cos(\theta) - \cos(\theta)\sin(\theta)\right) + 2r^2\dot{\theta}\dot{\phi}(0)\Big)
\end{aligned}
\tag{52}
$$

$$
= \frac{1}{2}m\left(\dot{r}^2 + r^2\sin^2(\theta)\dot{\phi}^2 + r^2\dot{\theta}^2\right) \tag{53}
$$

Once you have the kinetic energy, you have the Lagrangian:

$$
L = \frac{1}{2}m\left(\dot{r}^2 + r^2\sin^2(\theta)\dot{\phi}^2 + r^2\dot{\theta}^2\right) - V(r,\theta,\phi) \tag{54}
$$

(b) To obtain the Euler-Lagrange equations of motion, we simply plug the Lagrangian from part (a) into the Euler-Lagrange formula

$$
\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}_i} = \frac{\partial L}{\partial q_i} \tag{55}
$$

where the $q_i$ are our coordinates, $r, \theta, \phi$. Using $L$ from part (a) for each case:

(i) $q_i = r$

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{r}} = \frac{\partial L}{\partial r} \tag{56}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}(m\dot{r}) = \left(mr\sin^2(\theta)\dot{\phi}^2 + mr\dot{\theta}^2\right) - \frac{\partial}{\partial r}V(r,\theta,\phi) \tag{57}$$

$$m\ddot{r} = mr\left(\sin^2(\theta)\dot{\phi}^2 + \dot{\theta}^2\right) - \frac{\partial}{\partial r}V(r,\theta,\phi) \tag{58}$$

(ii) $q_i = \theta$

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{\theta}} = \frac{\partial L}{\partial \theta} \tag{59}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(mr^2\dot{\theta}\right) = mr^2\sin(\theta)\cos(\theta)\dot{\phi}^2 - \frac{\partial}{\partial \theta}V(r,\theta,\phi) \tag{60}$$

$$2mr\dot{r}\dot{\theta} + 2mr^2\ddot{\theta} = mr^2\sin(\theta)\cos(\theta)\dot{\phi}^2 - \frac{\partial}{\partial \theta}V(r,\theta,\phi) \tag{61}$$

(iii) $q_i = \phi$

$$\frac{\partial L}{\partial \phi} = \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{\phi}} \tag{62}$$

$$-\frac{\partial}{\partial \phi}V(r,\theta,\phi) = \frac{\mathrm{d}}{\mathrm{d}t}\left(mr^2\sin^2(\theta)\dot{\phi}\right) \tag{63}$$

$$-\frac{\partial}{\partial \phi}V(r,\theta,\phi) = m\left(2r\dot{r}\sin^2(\theta)\dot{\phi} + r^2\cos(\theta)\sin(\theta)\dot{\theta}\dot{\phi} + r^2\sin^2(\theta)\ddot{\phi}\right) \tag{64}$$

(c) To determine the conjugate momenta, we simply use the standard definition from the Lagrangian formulation of classical mechanics that

$$p_i = \frac{\partial L}{\partial \dot{q}_i} \tag{65}$$

Of course, we actually already calculated these in part (b): one side of the Euler-Lagrange equation takes the time derivative of the conjugate momentum. So we'll just write out what they are:

$$p_r = m\dot{r} \tag{66}$$

$$p_\theta = mr^2\dot{\theta} \tag{67}$$

$$p_\phi = mr^2\sin^2(\theta)\dot{\phi} \tag{68}$$

Calculating the Hamiltonian is a little more work. We recall that the Hamiltonian is the

Legendre transform of the Lagrangian:

$$H(p,q) = \sum_i p_i \dot{q}_i - L(q,\dot{q}) \tag{69}$$
$$= \left((m\dot{r})\dot{r} + (mr^2\dot{\theta})\dot{\theta} + (mr^2\sin^2(\theta)\dot{\phi})\dot{\phi}\right) \tag{70}$$
$$- \left(\frac{1}{2}\left(m\dot{r}^2 + mr^2\sin^2(\theta)\dot{\phi}^2 + mr^2\dot{\theta}^2\right) - V(r,\theta,\phi)\right)$$
$$= \frac{1}{2}\left(m\dot{r}^2 + mr^2\sin^2(\theta)\dot{\phi}^2 + mr^2\dot{\theta}^2\right) + V(r,\theta,\phi) \tag{71}$$

Note that we don't actually have the Hamiltonian yet: this is the Legendre transformation of the Lagrangian as a function of $q$ and $\dot{q}$, not of $q$ and $p$. So we'll find a way to replace the $\dot{q}_i$ with the $p_i$ — fortuntately, the definitions of the $p_i$ above make that easy:

$$\dot{r} = \frac{p_r}{m} \tag{72}$$
$$\dot{\theta} = \frac{p_\theta}{mr^2} \tag{73}$$
$$\dot{\phi} = \frac{p_\phi}{mr^2\sin^2(\theta)} \tag{74}$$

Plugging these into equation (71) we get

$$H(p,q) = \frac{1}{2}\left(m\left(\frac{p_r}{m}\right)^2 + mr^2\sin^2(\theta)\left(\frac{p_\phi}{mr^2\sin^2(\theta)}\right)^2 + mr^2\left(\frac{p_\theta}{mr^2}\right)^2\right) + V(r,\theta,\phi) \tag{75}$$
$$= \frac{1}{2}\left(\frac{{p_r}^2}{m} + \frac{{p_\phi}^2}{mr^2\sin^2(\theta)} + \frac{{p_\theta}^2}{mr^2}\right) + V(r,\theta,\phi) \tag{76}$$

Now *that* is our correct Hamiltonian.

(d) With the Hamiltonian we just determined in part (c), we can obtain Hamilton's equations in the standard way:

$$\dot{q}_i = \frac{\partial H}{\partial p_i} \tag{77}$$
$$\dot{p}_i = -\frac{\partial H}{\partial q_i} \tag{78}$$

We'll do this first for the $\dot{q}_i$, then for the $\dot{p}_i$:

$$\dot{r} = \frac{p_r}{m} \tag{79}$$
$$\dot{\phi} = \frac{p_\theta}{mr^2\sin^2(\theta)} \tag{80}$$
$$\dot{\theta} = \frac{p_\theta}{mr^2} \tag{81}$$

$$\dot{p_r} = \frac{1}{mr^3}\left(\frac{{p_\phi}^2}{\sin^2(\theta)} + {p_\theta}^2\right) - \frac{\partial}{\partial r}V(r,\theta,\phi) \tag{82}$$

$$\dot{p_\phi} = -\frac{\partial}{\partial \phi}V(r,\theta,\phi) \tag{83}$$

$$\dot{p_\theta} = \frac{{p_\phi}^2\cos(\theta)}{mr^2\sin^3(\theta)} - \frac{\partial}{\partial \theta}V(r,\theta,\phi) \tag{84}$$

# Problem 4

Using the hint, we'll make use of the identity that a function is equal to the inverse Fourier transform of the Fourier transform of itself. That is to say,

$$f(k) = \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} \mathrm{d}x\, e^{ikx}F(x) \tag{85}$$

$$= \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} \mathrm{d}x\, e^{ikx}\frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} \mathrm{d}k\, e^{-ikx}f(k) \tag{86}$$

Plugging in $f(k) = \delta(k-k')$, we simply use the definition of the delta function to obtain

$$\delta(k-k') = \frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{d}x\, e^{ikx}\int_{\mathbb{R}} \mathrm{d}k\, e^{-ikx}\delta(k-k') \tag{87}$$

$$= \frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{d}x\, e^{ikx}e^{-ik'x} \tag{88}$$

$$2\pi\ \delta(k-k') = \int_{\mathbb{R}} \mathrm{d}x\, e^{i(k-k')x} \quad \square \tag{89}$$

In equation (87) we identify $e^{ikx} = f(k)$ from the definition of the Dirac delta function, which, when we integrate across $k = k'$, fixes the variable $k$ at the constant value $k'$. That gives us equation (88).

# Problem 5

This is just a matter of working out the Fourier transforms of these functions by plugging them into the definition given in the previous problem.

(a) **Fourier transform of a Gaussian.** We begin with a standard plug-and-chug:

$$F(\lambda) = \int_{\mathbb{R}} \mathrm{d}t\, e^{-i\lambda t}f(t) \tag{90}$$

$$= \int_{\mathbb{R}} \mathrm{d}t\, e^{-i\lambda t}e^{-t^2/\tau^2} \tag{91}$$

$$= \int_{\mathbb{R}} \mathrm{d}t\ \exp(-(t^2/\tau^2 + i\lambda t)) \tag{92}$$

As usual, I take the hard way (to show you that it isn't that hard!) I'll simplify this down to a basic Gaussian integral by completing the square and making the substitution $u = t/\tau + \lambda\tau/2$, which also gives $\mathrm{d}t = \tau \mathrm{d}u$.

$$F(\lambda) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \mathrm{d}t \, \exp(-(t^2/\tau^2 + i\lambda t - \lambda^2\tau^2/4)) \exp(-\lambda^2\tau^2/4) \tag{93}$$

$$= \frac{1}{\sqrt{2\pi}} \exp(-\lambda^2\tau^2/4) \int_{\mathbb{R}} \mathrm{d}t \, \exp(-(t/\tau + i\lambda\tau/2)^2) \tag{94}$$

$$= \frac{1}{\sqrt{2\pi}} \exp(-\lambda^2\tau^2/4) \int_{\mathbb{R}} \mathrm{d}u \, \tau \, \exp(-u^2) \tag{95}$$

$$= \frac{1}{\sqrt{2\pi}} \tau \sqrt{\pi} \exp(-\lambda^2\tau^2/4) \tag{96}$$

$$= \frac{\tau}{\sqrt{2}} \exp(-\lambda^2\tau^2/4) \tag{97}$$

This function is clearly a Gaussian in $\lambda$.

(b) **Fourier transform of an Exponential.** Again, we just plug-and-chug:

$$F(\lambda) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \mathrm{d}t \, e^{-i\lambda t} e^{-|t|/\tau} \tag{98}$$

$$= \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \mathrm{d}t \, \exp(-|t|/\tau - i\lambda t) \tag{99}$$

$$= \frac{1}{\sqrt{2\pi}} \left( \int_{-\infty}^{0} \mathrm{d}t \, \exp(t/\tau - i\lambda t) + \int_{0}^{\infty} \mathrm{d}t \, \exp(-t/\tau - i\lambda t) \right) \tag{100}$$

$$= \frac{1}{\sqrt{2\pi}} \left( \int_{-\infty}^{0} \mathrm{d}t \, \exp((1/\tau - i\lambda)t) + \int_{0}^{\infty} \mathrm{d}t \, \exp((-1/\tau - i\lambda)t) \right) \tag{101}$$

$$= \frac{1}{\sqrt{2\pi}} \left( \left( \frac{1}{1/\tau - i\lambda} e^{(1/\tau - i\lambda)t} \right) \Bigg|_{-\infty}^{0} + \left( \frac{-1}{1/\tau + i\lambda} e^{-(1/\tau + i\lambda)t} \right) \Bigg|_{0}^{\infty} \right) \tag{102}$$

$$= \frac{1}{\sqrt{2\pi}} \left( \left( \frac{1}{1/\tau - i\lambda} - 0 \right) + \left( 0 - \frac{-1}{1/\tau + i\lambda} \right) \right) \tag{103}$$

$$= \frac{1}{\sqrt{2\pi}} \left( \frac{1}{1/\tau - i\lambda} + \frac{1}{1/\tau + i\lambda} \right) \tag{104}$$

Although I won't use this fact in any special way, I thought I should pause here to point out that we've brought this down to the sum of complex conjugates. This means that it the result will be a real function — in fact, it will be twice the real component of either term. But I'll solve this using the good old method of removing complex quantities from the denominator:

$$F(\lambda) = \frac{1}{\sqrt{2\pi}} \left( \frac{1}{1/\tau - i\lambda} \left( \frac{1/\tau + i\lambda}{1/\tau + i\lambda} \right) + \frac{1}{1/\tau + i\lambda} \left( \frac{1/\tau - i\lambda}{1/\tau - i\lambda} \right) \right) \tag{105}$$

$$= \frac{1}{\sqrt{2\pi}} \left( \frac{1/\tau + i\lambda}{1/\tau^2 + \lambda^2} + \frac{1/\tau - i\lambda}{1/\tau^2 + \lambda^2} \right) \tag{106}$$

$$= \frac{1}{\sqrt{2\pi}} \frac{2/\tau}{1/\tau^2 + \lambda^2} \tag{107}$$

Now we have something that looks quite conveniently like a Lorentzian. We'll massage it into the form $N\left(\frac{1}{1+a\lambda^2}\right)$ in order to identify $N$ and $a$.

$$F(\lambda) = \frac{2}{\tau\sqrt{2\pi}}\frac{1}{1/\tau^2(1+\tau^2\lambda^2)} \tag{108}$$

$$= \frac{2\tau^2}{\tau\sqrt{2\pi}}\frac{1}{1+\tau^2\lambda^2} \tag{109}$$

$$= \tau\sqrt{\frac{2}{\pi}}\frac{1}{1+\tau^2\lambda^2} \tag{110}$$

Here we can easily identify $N = \tau\sqrt{\frac{2}{\pi}}$ and $a = \tau^2$.