### 6.946 Final Project

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## Exercise 5.32: Hierarchical Jacobi coordinates

## (a) Canonical heliocentric coordinates

The canonical heliocentric transformation singles out the center of mass of the system. The other coordinates are computed with respect to this coordinate. Specifically, the relationships between the elements of $\left(x_{0}^{\prime}, \ldots, x_{n-1}^{\prime}\right)$ and $\left(x_{0}, \ldots, x_{n-1}\right)$ are

$$
\begin{array}{r}
x_{0}^{\prime}=X=\frac{\sum_{i=0}^{i=n-1} m_{i} x_{i}}{\sum_{i=0}^{i=n-1} m_{i}} \\
x_{i}^{\prime}=x_{i}-x_{0}, \text { for } i>0 \tag{1}
\end{array}
$$

We want to construct an $F_{2}$-type generating function that relates the relationship between the transformed and original coordinates. Using $x^{\prime}=\partial_{2} F_{2}\left(t ; x ; p^{\prime}\right)$, we have

$$
\left(\begin{array}{c}
x_{0}^{\prime} \\
x_{1}^{\prime} \\
\vdots \\
x_{n-1}^{\prime}
\end{array}\right)=\left(\begin{array}{c}
X \\
x_{1}-x_{0} \\
\vdots \\
x_{n-1}-x_{0}
\end{array}\right)=\left(\begin{array}{c}
\frac{d}{d p_{0}^{\prime}} F_{2}\left(t ; q ; p^{\prime}\right) \\
\frac{d}{d p_{1}^{\prime}} F_{2}\left(t ; q ; p^{\prime}\right) \\
\vdots \\
\frac{d}{d p_{n-1}^{\prime}} F_{2}\left(t ; q ; p^{\prime}\right)
\end{array}\right)
$$

A simultaneous solution to these $n$ differential equations, assuming no crossterms depending purely on the $p^{\prime}$ (that is, we set all the integration constants to zero), is

$$
F_{2}\left(t ; q ; p^{\prime}\right)=p_{0}^{\prime} X+\sum_{i=1}^{i=n-1} p_{i}^{\prime}\left(x_{i}-x_{0}\right)
$$

From this, we can calculate the relationship between the original and transformed momenta. For an $F_{2}$-type generating function, these are given by $p=\partial_{1} F_{2}\left(t ; x ; p^{\prime}\right)$.

$$
\left(\begin{array}{c}
p_{0} \\
p_{1} \\
\vdots \\
p_{n-1}
\end{array}\right)=\left(\begin{array}{c}
\frac{d}{d x_{0}} F_{2}\left(t ; q ; p^{\prime}\right) \\
\frac{d}{d x_{1}} F_{2}\left(t ; q ; p^{\prime}\right) \\
\vdots \\
\frac{d}{d x_{n-1}} F_{2}\left(t ; q ; p^{\prime}\right)
\end{array}\right)=\left(\begin{array}{c}
m_{0} p_{0}^{\prime} \frac{1}{M}-\sum_{i=1}^{i=n-1} p_{i}^{\prime} \\
m_{1} p_{0}^{\prime} \frac{1}{M}+p_{1}^{\prime} \\
\vdots \\
m_{n-1} p_{0}^{\prime} \frac{1}{M}+p_{n-1}^{\prime}
\end{array}\right)
$$

Where we have used the fact that $\frac{d}{d x_{i}}\left(\frac{\sum_{i=0}^{i=n-1} m_{i} x_{i}}{M}\right)=\frac{m_{i}}{M}$, for $M=\sum_{i=0}^{i=n-1} m_{i}$. We have determined how the momenta transform.

Let's determine the forms of $T$ and $V$ in this new set of coordinates, starting with the potential energy. We want to find the form of $\left(x_{i}-x_{j}\right)$, which are the arguments taken by the potential
function $f$, in the new coordinate system. We note that, if $i \neq 0, x_{i}-x_{j}=\left(x_{i}^{\prime}+x_{0}\right)-\left(x_{j}^{\prime}+x_{0}\right)=$ $x_{i}^{\prime}-x_{j}^{\prime}$ for all pairs $i<j$. When $i=0<j$, we have $x_{0}-x_{j}=\left(x_{0}-x_{j}^{\prime}-x_{0}\right)=x_{j}^{\prime}$.

The potential energy is therefore given by

$$
\begin{gathered}
V\left(x_{0}, \ldots, x_{n-1}\right)=\sum_{i<j} f_{i j}\left(\left|x_{i}-x_{j}\right|\right)=\sum_{i=0<j} f_{0 j}\left(\left|x_{0}-x_{j}\right|\right)+\sum_{0<i<j} f_{i j}\left(\left|x_{i}-x_{j}\right|\right) \\
=\sum_{i=0<j} f_{0 j}\left(\left|x_{j}^{\prime}\right|\right)+\sum_{0<i<j} f_{i j}\left(\left|x_{i}^{\prime}-x_{j}^{\prime}\right|\right)=V\left(x_{0}^{\prime}, \ldots, x_{n-1}^{\prime}\right)
\end{gathered}
$$

Which is in terms of the coordinates with $i>0$ only. This is to be expected, since the potential energy does not depend on the center of mass - only on the relative positions of the particles. (For example, if the potential energy $V$ were the Coulomb potential of many moving charges particles, the position of the center of mass should not enter the equation.)

The kinetic enery is

$$
\begin{gathered}
T\left(p_{0}, \ldots, p_{n-1}\right)=\sum_{i=0}^{i=n-1} \frac{p_{i}^{2}}{2 m_{i}}=\frac{p_{0}^{2}}{2 m_{0}}+\sum_{i=1}^{i=n-1} \frac{p_{i}^{2}}{2 m_{i}} \\
=\left(m_{0} p_{0}^{\prime} \frac{1}{M}-\sum_{i=1}^{i=n-1} p_{i}^{\prime}\right)^{2} \frac{1}{2 m_{0}}+\sum_{i=1}^{i=n-1} \frac{1}{2 m_{i}}\left(\frac{m_{i}}{M}\left[p_{0}^{\prime}\right]+\left[p_{i}^{\prime}\right]\right)^{2}
\end{gathered}
$$

This form produces combinations of crossproducts $p_{i}^{\prime} p_{j}^{\prime} .{ }^{1}$. That is, in the $\left\{p_{0}^{\prime}, \ldots, p_{n-1}^{\prime}\right\}$ basis, consider the quadratic form that is the momentum. The associated matrix is not diagonal. This is not ideal for a Hamiltonian; we prefer that the kinetic energy be a sum of squares of momenta.

So we consider another type of transformation.

## (b) Jacobi coordinates

This time, let the new coordinates be defined in terms of the old ones as follows:

$$
\begin{array}{r}
x_{0}^{\prime}=X_{n-i} \\
x_{i}^{\prime}=x_{i}-X_{i-1}, \text { for } i>0 \tag{2}
\end{array}
$$

Where the $X_{i}$ are the center of mass of the first $i+1$ particles, and $M_{i}$ is the sum of the mass of the first $i+1$ particles.

$$
X_{i}=\frac{1}{M_{i}} \sum_{j=0}^{j=i} m_{j} x_{j}, \quad M_{i}=\sum_{j=0}^{j=i} m_{j}
$$

That is, $X_{i}$ can be said to be the "increasingly inclusive" center of mass.
Again, we want to construct an $F_{2}$-type generating function that relates the relationship between the transformed and original coordinates. Using $x^{\prime}=\partial_{2} F_{2}\left(t ; x ; p^{\prime}\right)$, we have

[^0]\[

\left($$
\begin{array}{c}
x_{0}^{\prime} \\
x_{1}^{\prime} \\
\vdots \\
x_{n-1}^{\prime}
\end{array}
$$\right)=\left($$
\begin{array}{c}
X_{n-1} \\
x_{1}-X_{0} \\
\vdots \\
x_{n-1}-X_{n-2}
\end{array}
$$\right)=\left($$
\begin{array}{c}
\frac{d}{d p_{0}^{\prime}} F_{2}\left(t ; x ; p^{\prime}\right) \\
\frac{d}{d p_{1}^{\prime}} F_{2}\left(t ; x ; p^{\prime}\right) \\
\vdots \\
\frac{d}{d p_{n-1}^{\prime}} F_{2}\left(t ; x ; p^{\prime}\right)
\end{array}
$$\right)
\]

Again, setting the integration constants to zero, a solution to these $n$ differential equations is

$$
\begin{aligned}
& F_{2}\left(t ; x ; p^{\prime}\right)=p_{0}^{\prime} X_{n-1}+\sum_{i=1}^{i=n-1} p_{i}^{\prime}\left(x_{i}-X_{i-1}\right) \\
& \quad=p_{0}^{\prime} X_{n-1}+\sum_{i=1}^{i=n-1} p_{i}^{\prime} x_{i}-\sum_{i=1}^{i=n-1} p_{i}^{\prime} X_{i-1}
\end{aligned}
$$

Since this is an $F_{2}$-type generating function, we can now obtain an expression for the relationship between the original and transformed momenta. These are given by $p=\partial_{1} F_{2}\left(t ; x ; p^{\prime}\right)$. Let's calculate a few derivatives we'll need later.

$$
\begin{gathered}
\frac{d}{d x_{j}}\left(X_{n-1}\right)=\frac{m_{j}}{M} \\
\frac{d}{d x_{j}}\left(\sum_{i=1}^{i=n-1} p_{i}^{\prime} X_{i-1}\right)=\sum_{i=j+1}^{i=n-1} p_{i}^{\prime} m_{j} \frac{1}{M_{i}}=m_{j} \sum_{i=j+1}^{i=n-1} p_{i}^{\prime} \frac{1}{M_{i}}
\end{gathered}
$$

The index of the sum on the most recent line starts at $i=j+1$ because that is the point at which $X_{i-1}$ begins to depend on $x_{j}$. Thus, the momenta, in terms of the Jacobi coordinates, are given by

$$
\left(\begin{array}{c}
p_{0} \\
p_{1} \\
\vdots \\
p_{n-1}
\end{array}\right)=\left(\begin{array}{c}
\frac{d}{d x_{0}} F_{2}\left(t ; q ; p^{\prime}\right) \\
\frac{d}{d x_{1}} F_{2}\left(t ; q ; p^{\prime}\right) \\
\vdots \\
\frac{d}{d x_{n-1}} F_{2}\left(t ; q ; p^{\prime}\right)
\end{array}\right)=\left(\begin{array}{c}
m_{0} p_{0}^{\prime} \frac{1}{M}+p_{0}^{\prime}-m_{0} \sum_{i=1}^{i=n-1} p_{i}^{\prime} \frac{1}{M_{i}} \\
m_{0} p_{1}^{\prime} \frac{1}{M}+p_{1}^{\prime}-m_{1} \sum_{i=2}^{i=n-1} p_{i}^{\prime} \frac{1}{M_{i}} \\
\vdots \\
m_{0} p_{n-1}^{\prime} \frac{1}{M}+p_{n-1}^{\prime}
\end{array}\right)
$$

Let's determine the form of the kinetic energy $T$ in the new coordinates. We see that from above that the old coordinates $\left(p_{0}, \ldots, p_{n-1}\right)$ can each be expressed as a polynomial in $\left(p_{0}^{\prime}, \ldots, p_{n-1}^{\prime}\right)$ of degree one. Thus, the kinetic energy, which is a sum of squares of the old coordinates, is a degree two polynomial in the new coordinates.

$$
T\left(p_{0}^{\prime}, \ldots, p_{n-1}^{\prime}\right)=\frac{1}{2 m_{0}}\left(p_{0}\left(p_{0}^{\prime}, \ldots, p_{n-1}^{\prime}\right)\right)^{2}+\ldots+\frac{1}{2 m_{n-1}}\left(p_{n-1}\left(p_{0}^{\prime}, \ldots, p_{n-1}^{\prime}\right)\right)^{2}
$$

To find the new form for $T$, we collect the coefficients of on any $p_{i}^{\prime} p_{j}^{\prime}$ term. Let's start with the $\left[p_{i}^{\prime}\right]^{2}$ terms, specifically with $\left[p_{0}^{\prime}\right]^{2}$. Referring back to (2), we see that the contribution from each $p_{i}\left(p_{0}^{\prime}, \ldots, p_{n-1}^{\prime}\right)$ is $\frac{m_{i}^{2}}{M_{n-1}^{2}}\left[p_{0}^{\prime}\right]^{2}$, and thus the $\left[p_{0}^{\prime}\right]^{2}$ term is

$$
\sum_{i=0}^{i=n-1} \frac{1}{2 m_{i}}\left(\frac{m_{i}^{2}}{M_{n-1}^{2}}\left[p_{0}^{\prime}\right]^{2}\right)=\frac{1}{2 M_{n-1}^{2}}\left[p_{0}^{\prime}\right]^{2} \sum_{i=0}^{i=n-1} m_{i}=\frac{1}{2 M_{n-1}}\left[p_{0}^{\prime}\right]^{2}
$$

Now let's find the coefficient of the $\left[p_{i}^{\prime}\right]^{2}$ term for $i \neq 0$. The coefficient in the $p_{j}^{2}$ term for $j<i$ is $\left(-\frac{m_{j}}{M_{i-1}}\right)^{2}$. The coefficient of $\left[p_{i}^{\prime}\right]^{2}$ in $p_{i}^{2}$ is $(1)^{2}$, and $p_{j}$ does not depend on $p_{i}$ for $i>j$. Thus, the $\left[p_{i}^{\prime}\right]^{2}$ term is

$$
\begin{gathered}
\frac{1}{2 m_{i}}\left[p_{i}^{\prime}\right]^{2}+\sum_{j=0}^{j=i-1} \frac{1}{2 m_{j}}\left(\frac{m_{j}}{M_{i-1}} p_{i}^{\prime}\right)^{2}=\frac{1}{2 m_{i}}\left[p_{i}^{\prime}\right]^{2}+\frac{1}{2 M_{i-1}^{2}}\left[p_{i}^{\prime}\right]^{2} \sum_{j=0}^{j=i-1} m_{j} \\
=\frac{1}{2 m_{i}}\left[p_{i}^{\prime}\right]^{2}+\frac{1}{2 M_{i-1}}\left[p_{i}^{\prime}\right]^{2}=\frac{1}{2 m_{i}^{\prime}}\left[p_{i}^{\prime}\right]^{2}
\end{gathered}
$$

Where $m_{i}^{\prime}$ is the $i^{t h}$ reduced mass defined by $\frac{1}{m_{i}^{\prime}}=\frac{1}{M_{i-1}}+\frac{1}{m_{i}}$.
Let's determine the coefficients of the cross-products $p_{i}^{\prime} p_{j}^{\prime}$ for $0 \leq i<j \leq n-1$. Consider the case when $i=0$.

Every $p_{k}$ contains a $p_{0}^{\prime}$ term, but only those up to $k=j$ contain a $p_{j}^{\prime}$ term. The product of the coefficients for $k<j$ is $2\left(\frac{m_{k}}{M_{n-1}}\right)\left(-\frac{m_{k}}{M_{j-1}}\right)$, and from $k=j$, the product is $2\left(\frac{m_{j}}{M_{n-1}}\right)$ (1). Summing these, we get the $p_{0}^{\prime} p_{j}^{\prime}$ term in the kinetic energy

$$
\begin{gathered}
\frac{1}{2 m_{j}} 2\left(\frac{m_{j}}{M_{n-1}}\right)\left[p_{0}^{\prime} p_{j}^{\prime}\right]+\sum_{k=0}^{k=j-1} \frac{1}{2 m_{k}} 2\left(-\frac{m_{k}}{M_{n-1}} \frac{m_{k}}{M_{j-1}}\right)\left[p_{0}^{\prime} p_{j}^{\prime}\right] \\
=\frac{1}{M_{n-1}}\left[p_{0}^{\prime} p_{j}^{\prime}\right]-\frac{1}{M_{n-1}}\left[p_{0}^{\prime} p_{j}^{\prime}\right] \sum_{k=0}^{k=j-1} \frac{m_{k}}{M_{j-1}}=0
\end{gathered}
$$

Thus, this cross-term cancels out. Now let's consider the case when $0<i<j$. The contribution to the coefficient of $p_{i}^{\prime} p_{j}^{\prime}$ from a given $p_{k}^{2}$ only exists when $k \leq i$. If $k<i$, the coefficient in the polynomial $p_{k}^{2}$ is $2\left(-\frac{m_{k}}{M_{i-1}}\right)\left(-\frac{m_{k}}{M_{j-1}}\right)$. If $k=i$, the coefficient is $2(1)\left(-\frac{m_{i}}{M_{j-1}}\right)$. Summing these, the $p_{i}^{\prime} p_{j}^{\prime}$ term in the kinetic energy is

$$
\begin{gathered}
\frac{1}{2 m_{i}}\left(-\frac{m_{i}}{M_{j-1}}\right)\left[p_{i}^{\prime} p_{j}^{\prime}\right]+\sum_{k=0}^{k=i-1} \frac{1}{2 m_{k}}\left(\frac{m_{k}}{M_{i-1}} \frac{m_{k}}{M_{j-1}}\right)\left[p_{i}^{\prime} p_{j}^{\prime}\right] \\
=-\frac{1}{2 M_{j-1}}\left[p_{i}^{\prime} p_{j}^{\prime}\right]+\frac{1}{2 M_{j-1}}\left[p_{i}^{\prime} p_{j}^{\prime}\right] \sum_{k=0}^{k=i-1} \frac{m_{k}}{M_{i-1}}=0
\end{gathered}
$$

Again, the cross-terms cancel. The form of the kinetic energy in the $\left(p_{0}^{\prime}, \ldots, p_{n-1}^{\prime}\right)$ coordinate frame is, as we have shown,

$$
T\left(p_{0}^{\prime}, \ldots, p_{n-1}^{\prime}\right)=\frac{1}{2 M_{n-1}}\left[p_{0}^{\prime}\right]^{2}+\sum_{i=1}^{i=n-1} \frac{1}{2 m_{i}^{\prime}}\left[p_{i}^{\prime}\right]^{2}, \quad \frac{1}{m_{i}^{\prime}}=\frac{1}{M_{i-1}}+\frac{1}{m_{i}}
$$

This is a nice form which depends only on the squares of the momenta. The first term is the kinetic energy of the center of mass, and the other terms are the relative kinetic energy between the $n^{\text {th }}$ particle and the center of mass of the particles with index less than $n$.

Let's investigate the form of the potential energy $V$ in the new coordinate frame. In particular, we want to investigate the dependence of the arguments $\left(x_{i}-x_{j}\right)$, for $i<j$, that the potential function $f$ takes, in terms of the new coordinates. To construct these, we note that if we can find the forms corresponding to $\left(x_{i}-x_{i+1}\right)$ for all $i$, then we can generate any $\left(x_{i}-x_{j}\right)$ form with sums of these.

Let's begin. By the definition of $x_{1}^{\prime}$, we have $x_{0}-x_{1}=x_{1}^{\prime}$. Now consider the definition of any $x_{i}^{\prime}$ and $x_{i+1}^{\prime}$, below, for $0<i<n-1$.

$$
\begin{gathered}
M_{i-1} x_{i}^{\prime}=M_{i-1} x_{i}-m_{0} x_{0}-\ldots-m_{i-1} x_{i-1} \\
M_{i} x_{i+1}^{\prime}=M_{i} x_{i+1}-m_{0} x_{0}-\ldots-m_{i} x_{i}
\end{gathered}
$$

Taking the difference, we have

$$
\begin{gathered}
M_{i} x_{i+1}^{\prime}-M_{i-1} x_{i}^{\prime}=M_{i} x_{i+1}-M_{i-1} x_{i}-m_{i} x_{i} \\
x_{i+1}^{\prime}-\frac{M_{i-1}}{M_{i}} x_{i}^{\prime}=x_{i+1}-x_{i}
\end{gathered}
$$

We note that $x_{0}^{\prime}$ never enters the equations, except as an intermediary that is later cancelled. Thus, we can write any of the arguments $\left(x_{i}-x_{j}\right)$ to $f$ (and thus derive the potential energy $V$ ) as a linear combination of $x_{1}^{\prime}, \ldots, x_{n-1}^{\prime}$ terms alone. Again, this makes sense, because the potential energy depends only on the relative positions of the bodies.

Let's generalize this practice of computing partial centers of mass while preserving the form of the kinetic energy.

## (c) Hierarchical Jacobi coordinates

We introduce the linking transformation $\mathcal{L}_{j k}$, with $j \neq k$, that leaves the position, momentum and mass of all elements for which $j, k \neq i$ the same, and transforms the mass, momentum and position of the $k^{\text {th }}$ and $j^{\text {th }}$ particles as follows:

$$
\begin{array}{r}
x_{j}^{\prime}=x_{k}-x_{j}, \quad m_{j}^{\prime}=\left(\frac{1}{m_{j}}+\frac{1}{m_{k}}\right)^{-1}=\frac{m_{j} m_{k}}{m_{j}+m_{k}} \\
x_{k}^{\prime}=\frac{m_{j} x_{j}+m_{k} x_{k}}{m_{j}+m_{k}}, \quad m_{k}^{\prime}=m_{j}+m_{k} \tag{3}
\end{array}
$$

Let's consider what the transformed momenta must look like. We find that we can derive these from the definitions in (3) above.

$$
\begin{gathered}
p_{k}^{\prime}=m_{k}^{\prime} x_{k}^{\prime}=\left(m_{k}+m_{k}\right) \frac{m_{j} x_{j}+m_{k} x_{k}}{m_{j}+m_{k}}=m_{j} x_{j}+m_{k} x_{k}=p_{j}+p_{k} \\
p_{j}^{\prime}=m_{j}^{\prime} x_{j}^{\prime}=\frac{m_{j} m_{k}}{m_{j}+m_{k}}\left(x_{k}-x_{j}\right)=\frac{m_{j} p_{k}-m_{k} p_{j}}{m_{j}+m_{k}}
\end{gathered}
$$

Next, we want to show that this form of transformation preserves the sum of squares form of the kinetic energy. Showing that a similar form of the kinetic energy leads to the original one is straightforward. The terms of the energy that depend on $\left[p_{i}^{\prime}\right]^{2}=p_{i}^{2}$ for $k, j \neq i$ are the same. So we only consider the $p_{j}^{\prime}$ and $p_{k}^{\prime}$ terms.

$$
\begin{aligned}
& \frac{1}{2 m_{j}^{\prime}}\left[p_{j}^{\prime}\right]^{2}+\frac{1}{2 m_{k}^{\prime}}\left[p_{k}^{\prime}\right]^{2}=\frac{1}{2 m_{j}^{\prime}}\left(\frac{m_{j} p_{k}-m_{k} p_{j}}{m_{j}+m_{k}}\right)^{2}+\frac{1}{2 m_{k}^{\prime}}\left(p_{j}+p_{k}\right)^{2} \\
& =\frac{1}{2 m_{j}^{\prime}}\left(\frac{m_{j}^{2} p_{k}^{2}-2 m_{j} m_{k} p_{j} p_{k}+m_{k}^{2} p_{j}^{2}}{M^{2}}\right)+\frac{1}{2 M}\left(p_{j}^{2}+2 p_{j} p_{k}+p_{k}^{2}\right)
\end{aligned}
$$

Where we have used $M=m_{j}^{\prime}=m_{j}+m_{k}$. Below, we collect terms and use the fact that $\frac{1}{m_{j}^{\prime}}=\frac{1}{m_{j}}+\frac{1}{m_{k}}$.

$$
\begin{gather*}
=\frac{p_{k}^{2}}{2}\left(\frac{1}{m_{j}^{\prime}} \frac{m_{j}^{2}}{M^{2}}+\frac{1}{M}\right)+\frac{p_{j}^{2}}{2}\left(\frac{1}{m_{j}^{\prime}} \frac{m_{k}^{2}}{M^{2}}+\frac{1}{M}\right)+p_{j} p_{k}\left(\frac{-m_{j} m_{k}}{m_{j}^{\prime} M^{2}}+\frac{1}{M}\right) \\
=\frac{p_{k}^{2}}{2}\left(\frac{m_{j}^{2}}{m_{j} M^{2}}+\frac{m_{j}^{2}}{m_{k} M^{2}}+\frac{1}{M}\right)+\frac{p_{j}^{2}}{2}\left(\frac{m_{k}^{2}}{m_{j} M^{2}}+\frac{m_{k}^{2}}{m_{k} M^{2}}+\frac{1}{M}\right)+p_{j} p_{k}\left(\frac{-m_{j} m_{k}}{m_{j} M^{2}}+\frac{-m_{j} m_{k}}{m_{k} M^{2}}+\frac{1}{M}\right) \\
=\frac{p_{k}^{2}}{2}\left(\frac{m_{j}^{2} m_{k}+m_{j}^{3}+m_{j} m_{k} M}{m_{j} m_{k} M^{2}}\right)+\frac{p_{j}^{2}}{2}\left(\frac{m_{k}^{3}+m_{k}^{2} m_{j}+m_{j} m_{k} M}{m_{j} m_{k} M^{2}}\right)+p_{j} p_{k}\left(\frac{-m_{j} m_{k}^{2}-m_{j}^{2} m_{k}+m_{k} m_{j} M}{m_{k} m_{j} M^{2}}\right) \\
=\frac{p_{k}^{2}}{2}\left(\frac{m_{j} m_{k}+m_{j}^{2}+m_{k} M}{m_{k} M^{2}}\right)+\frac{p_{j}^{2}}{2}\left(\frac{m_{k}^{2}+m_{k} m_{j}+m_{j} M}{m_{j} M^{2}}\right)+p_{j} p_{k}\left(\frac{-m_{k}-m_{j}+M}{M^{2}}\right) \\
=\frac{p_{k}^{2}}{2}\left(\frac{m_{k}^{2}+2 m_{j} m_{k}+m_{j}^{2}}{m_{k} M^{2}}\right)+\frac{p_{j}^{2}}{2}\left(\frac{m_{j}^{2}+m_{k}^{2}+2 m_{k} m_{j}}{m_{j} M^{2}}\right) \\
=\frac{p_{k}^{2}}{2} \frac{\left(m_{j}+m_{k}\right)^{2}}{m_{k} M^{2}}+\frac{p_{j}^{2}}{2} \frac{\left(m_{j}+m_{k}\right)^{2}}{m_{j} M^{2}}=\frac{p_{k}^{2}}{2}\left(\frac{1}{m_{k}}\right)+\frac{p_{j}^{2}}{2}\left(\frac{1}{m_{j}}\right) \tag{4}
\end{gather*}
$$

Which is what we wanted to show.
We call this a "linking" transformation because it stops the distinsguishing the individual position of two particles, and instead treats them as a center of mass of and a relative displacement. As we have shown above, this transformation preserves the sum of squares form of the energy.

Of course, we'd like to ensure that there is a single coordinate that represents the center of mass of the system after a series of transformations. The requirement that there be a single identifiable center of mass term is that the composition of linking transformations link a single specific element with every other one. This way, the $k$-coordinate on the last transformation $\mathcal{L}_{j, k}$ will be the transformed coordinate that corresponds to the center of mass of the system. In a way, it's a "continued weighted averaging" or the coordinates.

The Jacobi transformation has a single center of mass coordinate, and all the other coordinates are decoupled positions relative to an increasingly inclusive center of mass. Thus, any individual coordinate is expressed as the relative difference between all the ones before it and this, along with the center of mass, is enough to specify any configuration.

We can express the Jacobi transformation as a composition of linking transformations. We want to pick a center of mass element, $x_{0}^{\prime}$, and let the other elements $x_{i}^{\prime}$ to be the relative distance between their original position $x_{i}$ and the center of mass up to that point. Thus, a series of linking transformations which build $x_{0}^{\prime}$ as the successively more inclusive center of mass, and transforms $x_{i}^{\prime}$ to be the relative distance between $x_{i}$ and the new (slightly more inclusive) center of mass $x_{0}^{\prime}$. We see that this can be done with the following series of linking transformations:

$$
\begin{gathered}
\left(\mathcal{L}_{n-1,0} \circ \ldots \circ \mathcal{L}_{1,0}\right)\left(m_{0}, \ldots, m_{n-1} ; x_{0}, \ldots, x_{n-1} ; p_{0}, \ldots, p_{n-1}\right) \\
=\left(m_{0}^{\prime}, \ldots, m_{n-1}^{\prime} ; x_{0}^{\prime}, \ldots, x_{n-1}^{\prime} ; p_{0}^{\prime}, \ldots, p_{n-1}^{\prime}\right)
\end{gathered}
$$

We now explicitly construct the coordinate transforms for the six body problem in the project statement. There are six point particles, divided into left and right triple systems. We denote which triple system a particle is part of with an "L" or "R" subscript, respectively. Each triple system is a binary system (to which we give the subscript "B1" or "B2"), plus a third body (" 3 "). For example, the first particle of the binary system in the triple system on the left is "LB1" with position, momentum and mass $x_{L B 1}, p_{L B 1}$ and $m_{L B 1}$, respectively.

We want to link the particles in each binary system, then link these compositions to the third particle in each triple system, and finally, link these two compositions. Thus, at the end of the transformation, we hope to end up with six coordinate subscripts - " M " for the composition of the entire system, " m " for the relative offset between the two triple systems, $L$ and $R$ for the relative offset of either third body from the binaries, and $l$ and $r$ for the relative coordinate within the binary arrangement.

Let our initial coordinates be

$$
\left(x_{L B 1}, x_{L B 2}, x_{L 3}, x_{R B 1}, x_{R B 2}, x_{R 3} ; p_{L B 1}, \ldots, p_{R 3} ; m_{L B 1}, \ldots, m_{R 3}\right)
$$

We first want to link the two binaries with a $\mathcal{L}_{L B 1, L B 2} \circ \mathcal{L}_{R B 1, R B 2}$ transformation. This changes our subscripts to

$$
\mathcal{L}_{L B 1, L B 2} \circ \mathcal{L}_{R B 1, R B 2}(L B 1, L B 2, L 3, R B 1, R B 2, R 3)=(l, L B, L 3, r, R B, R 3)
$$

Where $L B$ and $R B$ above are the centers of mass of the binaries. Next, we use $\mathcal{L}_{L B, L 3} \circ \mathcal{L}_{R B, R 3}$ to link the composite binary systems with the third element of the triple systems. This changes our subscripts to

$$
\mathcal{L}_{L B, L 3} \circ \mathcal{L}_{R B, R 3}(l, L B, L 3, r, R B, R 3)=\left(l, L, M_{L}, r, R, M_{R}\right)
$$

Where $M_{L}$ and $M_{R}$ above are the centers of mass of the triple systems. Finally, we link these with $\mathcal{L}_{M_{L}, m_{R}}$ to arrive at

$$
\mathcal{L}_{M_{L}, M_{R}}\left(l, L, M_{L}, r, R, M_{R}\right)=(l, L, m, r, R, M)
$$

Following these compositions of transformations, we can find the Jacobi coordinates, mass and momenta for the particles. The first two transformations give us

$$
x_{L B}=\frac{m_{L B 1} x_{L B 1}+m_{L B 2} x_{L B 2}}{m_{L B 1}+m_{L B 2}}, \quad p_{L B}=p_{L B 1}+p_{L B 2}, \quad m_{L B}=m_{L B 1}+m_{L B 2}
$$

$$
\begin{gathered}
x_{l}=x_{L B 2}-x_{L B 1}, \quad p_{l}=\frac{m_{L B 1} p_{L B 2}-m_{L B 2} p_{L B 1}}{m_{L B 1}+m_{L B 2}}, \quad \frac{1}{m_{l}}=\frac{1}{m_{L B 1}}+\frac{1}{m_{L B 2}} \\
x_{R B}=\frac{m_{R B 1} x_{R B 1}+m_{R B 2} x_{R B 2}}{m_{R B 1}+m_{R B 2}}, \quad p_{R B}=p_{R B 1}+p_{R B 2}, \quad m_{R B}=m_{R B 1}+m_{R B 2} \\
x_{r}=x_{R B 2}-x_{R B 1}, \quad p_{r}=\frac{m_{R B 1} p_{R B 2}-m_{R B 2} p_{R B 1}}{m_{R B 1}+m_{R B 2}}, \quad \frac{1}{m_{r}}=\frac{1}{m_{R B 1}}+\frac{1}{m_{R B 2}}
\end{gathered}
$$

The "r" and " 1 " terms will not be affected from here on out. Next, we apply the linking transformation to the third element of each triplet and the linked center of mass of their respective triplet. The new " $M_{L}$ ", "L" and " $M_{R}$ ", "R" coordinates in terms of "LB","L3" and "RB","R3", respectively, are

$$
\begin{aligned}
x_{M_{L}} & =\frac{m_{L B} x_{L B}+m_{L 3} x_{L 3}}{m_{L B}+m_{L 3}}, \quad p_{M_{L}}=p_{L B}+p_{L 3}, \quad m_{M_{L}}=m_{L B}+m_{L 3} \\
x_{L} & =x_{L B}-x_{L 3}, \quad p_{L}=\frac{m_{L B} p_{L 3}-m_{L 3} p_{L B}}{m_{L 3}+m_{L B}}, \quad \frac{1}{m_{L}}=\frac{1}{m_{L B}}+\frac{1}{m_{L 3}} \\
x_{M_{R}} & =\frac{m_{R B} x_{R B}+m_{R 3} x_{R 3}}{m_{R B}+m_{R 3}}, \quad p_{M_{R}}=p_{R B}+p_{R 3}, \quad m_{M_{R}}=m_{R B}+m_{R 3} \\
x_{R} & =x_{R B}-x_{R 3}, \quad p_{R}=\frac{m_{R B} p_{R 3}-m_{R 3} p_{R B}}{m_{R 3}+m_{R B}}, \quad \frac{1}{m_{R}}=\frac{1}{m_{R B}}+\frac{1}{m_{R 3}}
\end{aligned}
$$

We keep the relative " L " and " R " coordinates, and merge " $M_{L}$ ", " $M_{R}$ " coordinates into a center of mass term " $M$ " and relative term " $m$ ", as follows:

$$
\begin{aligned}
& x_{M}=\frac{m_{M_{L}} x_{M_{L}}+m_{M_{R}} x_{M_{R}}}{m_{M_{L}}+m_{M_{L}}}, \quad p_{M}=p_{M_{L}}+p_{M_{R}}, \quad m_{M}=m_{M_{L}}+m_{M_{R}} \\
& x_{m}=x_{M_{L}}-x_{M_{R}}, \quad p_{m}=\frac{m_{M_{L}} p_{M_{R}}-m_{M_{R}} p_{M_{L}}}{m_{M_{L}}+m_{M_{R}}}, \quad \frac{1}{m_{m}}=\frac{1}{m_{M_{L}}}+\frac{1}{m_{M_{R}}}
\end{aligned}
$$

We know that the composition of linking transformations preserves the sum of squares form of the kinetic energy, but let's illustrate it below for good measure.

Using the property derived in (4):

$$
\begin{gathered}
T=\left(\frac{1}{2 m_{L B 1}} p_{L B 1}^{2}+\frac{1}{2 m_{L B 2}} p_{L B 2}^{2}\right)+\frac{1}{2 m_{L 3}} p_{L 3}^{2}+\left(\frac{1}{2 m_{R B 1}} p_{R B 1}^{2}+\frac{1}{2 m_{R B 2}} p_{R B 2}^{2}\right)+\frac{1}{2 m_{R 3}} p_{R 3}^{2} \\
T=\frac{1}{2 m_{l}} p_{l}^{2}+\left(\frac{1}{2 m_{L B}} p_{L B}^{2}+\frac{1}{2 m_{L 3}} p_{L 3}^{2}\right)+\frac{1}{2 m_{r}} p_{r}^{2}+\left(\frac{1}{2 m_{R B}} p_{R B}^{2}+\frac{1}{2 m_{R 3}} p_{R 3}^{2}\right) \\
T=\frac{1}{2 m_{l}} p_{l}^{2}+\frac{1}{2 m_{L}} p_{L}^{2}+\left(\frac{1}{2 m_{M_{L}}} p_{M_{L}}^{2}\right)+\frac{1}{2 m_{r}} p_{r}^{2}+\frac{1}{2 m_{R}} p_{R}^{2}+\left(\frac{1}{2 m_{M_{R}}} p_{M_{R}}^{2}\right) \\
T=\frac{1}{2 m_{l}} p_{l}^{2}+\frac{1}{2 m_{L}} p_{L}^{2}+\frac{1}{2 m_{m}} p_{m}^{2}+\frac{1}{2 m_{r}} p_{r}^{2}+\frac{1}{2 m_{R}} p_{R}^{2}+\frac{1}{2 m_{M}} p_{M}^{2}
\end{gathered}
$$

Which is what we wanted to show.


[^0]:    ${ }^{1}$ The exception here is the $n=2$ case, in which the heliocentric and Jacobi transformations are equivalent. But in general, the cross terms do not cancel.

