CONSTRAINT PROBLEM POSED BY THE CENTER OF MASS CONCEPT

in non-relativistic classical/quantum mechanics

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September 1998

Introduction. Why—to my eye and gross senses—does the quantum world appear classical? Why, even before eyes (and physicists) had been invented, did Jupiter pursue a Keplerian orbit? I will argue that the answer to such questions—seldom asked today, because widely believed to be "understood"—is to be discovered not "in the limit that $\hbar$ becomes small," or "in the limit that quantum numbers become large," but in the circumstance—speculatively evident already to the philosophers of ancient Greece—that the stuff of sensible experience contains many internal degrees of freedom. The systems which yield to, and provide the subject matter of, the methods of classical mechanics are (from a microscoptic point of view) in all cases highly composite, and so also (as Bohr was the first to emphasize) are the instruments with which we undertake quantum measurement. I will argue that classical concepts become relevant to the description of the quantum world for essentially the same reason that thermodynamics becomes relevant to the description of the statistical world—that Newton's laws originate in the Law of Large Numbers.

That, in bald outline, in the program, the source of my motivation. My immediate intention is, however, much more modest. I propose to explore some relatively little known ramifications (it is surprising that there are any such!) of the familiar "center of mass" concept. Quantum mechanics is my destination, but I am will be in no hurry to get there, and expect to stop from time to time, to rest and enjoy the view. Since classical mechanics marks the birthplace of the concept in question, it is with some rudimentary classical mechanics that I will begin.

PART I: CLASSICAL THEORY

1. Classical preliminaries. Let vectors $\boldsymbol{x}_i(t)$ describe, relative to our inertial frame, the instantaneous positions of the constituent elements m_1, m_2,...,m_N

of some N-body system. To describe the motion of the system we might write

$$m_i\ddot{\boldsymbol{x}}_i = \boldsymbol{F}_i + \sum_j \boldsymbol{F}_{ij} \quad : \quad i = 1, 2, \ldots, N \tag{1}$$

on the presumption (soon to be relaxed) that the particles interact only pairwise:

$$\begin{aligned} \bar{\boldsymbol{F}}_i &\equiv \text{force externally impressed upon } m_i \\ \boldsymbol{F}_{ij} &\equiv \text{force exerted upon } m_i \text{ by } m_j \text{ (vanishes when } i = j) \end{aligned}$$

Newton's 3rd Law is standardly interpreted to state that

$$\boldsymbol{F}_{ij} + \boldsymbol{F}_{ji} = \boldsymbol{0} \quad : \quad \text{“action = reaction”} \tag{2}$$

and permits one to draw from $\sum_i(1)$ the mathematical conclusion that

$$\begin{aligned} \tfrac{d^2}{dt^2}\{\textstyle\sum m_i\boldsymbol{x}_i\} &= \boldsymbol{F} \\ \bar{\boldsymbol{F}} \equiv \textstyle\sum \bar{\boldsymbol{F}}_i &= \text{net externally impressed force} \end{aligned} \tag{3}$$

It is this elementary statetment which standardly motivates the introduction of the “center of mass”

$$\begin{aligned} \boldsymbol{X} &\equiv \tfrac{1}{M}\textstyle\sum m_i\boldsymbol{x}_i \\ M &\equiv \textstyle\sum m_i = \text{ total mass of the system} \end{aligned} \tag{4}$$

Returning with (4) to (3) one has

$$M\ddot{\boldsymbol{X}} = \boldsymbol{F} \tag{5}$$

from which all reference to the internal forces has disappeared; the center of mass moves *as if* the system mass were lumped there, and subjected to the net impressed force.

The argument which led to (5) is so elementary, and the result itself basic to our intuitive understanding of such a range of physical problems, that we tend to forget a point which will acquire increasing importance as we proceed: *the center of mass is a mathematical object—a fiction—that lives only in the world of ideas*. One cannot “tie a string to the center of mass” any more than one can tie a string to a puff of smoke,[1] and it becomes “visible” only to the mind's eye, inferentially. It cannot (formally perhaps, but certain not in any instrumental sense) be reckoned among the “observables” of many-body dynamics.

[1] In this respect, rigid bodies with the (exceptional) property that the center of mass lies exposed on the surface provide an exception to the rule.

It is obvious but seldom remarked that the definition (4) is in fact not forced upon us by our desire to get from (3) to (5); we would have enjoyed equal success had we written

$$\boldsymbol{X} \equiv \tfrac{1}{M}\sum m_i \boldsymbol{x}_i + \boldsymbol{a} + \boldsymbol{b}t$$

with $\boldsymbol{a}$ and $\boldsymbol{b}$ arbitrary. It is from certain collateral lines of argument, designed to achieve certain "splitting theorems," that we are led to set $\boldsymbol{a} = \boldsymbol{b} = 0$. Turning now to review of those...

Let $\boldsymbol{\mathfrak{X}}(t)$ describe some abritrarily moving point, at which we have erected a translated (and generally noninertial) moving copy of our inertial Cartesian frame. Writing

$$\boldsymbol{x}_i = \boldsymbol{\mathfrak{X}} + \boldsymbol{r}_i$$

we observe that the *kinetic energy* of our N-particle system can be described

$$\tfrac{1}{2}\sum m_i \dot{\boldsymbol{x}}_i \cdot \dot{\boldsymbol{x}}_i = \tfrac{1}{2}M\dot{\boldsymbol{\mathfrak{X}}}\cdot\dot{\boldsymbol{\mathfrak{X}}} + \dot{\boldsymbol{\mathfrak{X}}}\cdot\Big\{\sum m_i \dot{\boldsymbol{r}}_i\Big\} + \tfrac{1}{2}\sum m_i \dot{\boldsymbol{r}}_i \cdot \dot{\boldsymbol{r}}_i$$

and that the cross term $\big\{\text{etc.}\big\}$ would vanish if it were the case that

$$\sum m_i \dot{\boldsymbol{x}}_i = M\dot{\boldsymbol{\mathfrak{X}}}$$

which entails $\boldsymbol{\mathfrak{X}} \equiv \frac{1}{M}\sum m_i \boldsymbol{x}_i + \boldsymbol{a}$. Looking in this same spirit to the *angular momentum* of the system, we have

$$\sum m_i \boldsymbol{x}_i \times \dot{\boldsymbol{x}}_i = M\boldsymbol{\mathfrak{X}}\times\dot{\boldsymbol{\mathfrak{X}}} + \boldsymbol{\mathfrak{X}}\times\Big\{\sum m_i \dot{\boldsymbol{r}}_i\Big\} + \Big\{\sum m_i \boldsymbol{r}_i\Big\}\times\dot{\boldsymbol{\mathfrak{X}}} + \sum m_i \boldsymbol{r}_i \times \dot{\boldsymbol{r}}_i$$

and find that to eliminate *both* cross terms we are (if unwilling to impose restrictions on the motion of $\boldsymbol{\mathfrak{X}}$) obligated to set $\boldsymbol{a} = \boldsymbol{0}$; i.e., to assume that $\boldsymbol{\mathfrak{X}}$ moves in such a way as to yield

$$\sum m_i \boldsymbol{r}_i = \boldsymbol{0} \quad \Longleftrightarrow \quad \sum m_i \boldsymbol{x}_i = M\boldsymbol{\mathfrak{X}}$$

But we have at this point *enforcedly* obtained $\boldsymbol{\mathfrak{X}} \rightarrow$ center of mass $\boldsymbol{X}$, as defined at (4).

Abandoning temporarily all reference to $\boldsymbol{\mathfrak{X}}$ (which has served its immediate purpose), I linger to recast some of the preceding results; i.e., to render them in the form in which they are most commonly (and usefully) encountered. We observe that (5) can be written

$$\begin{aligned} \boldsymbol{F} = \dot{\boldsymbol{P}} \quad \text{with} \quad \boldsymbol{P} &\equiv M\dot{\boldsymbol{X}} \\ &= \sum m_i \dot{\boldsymbol{x}}_i \\ &= \sum \boldsymbol{p}_i \\ &\equiv \text{total linear momentum of the system} \end{aligned} \tag{6}$$

and that if—writing

$$\boldsymbol{x}_i = \boldsymbol{X} + \boldsymbol{r}_i \tag{7.1}$$

$$\sum m_i \boldsymbol{r}_i = \boldsymbol{0} \tag{7.2}$$

—we erect at the center of mass a (non-rotating, and generally noninertial) copy of our own (inertial) Cartesian frame, then the total kinetic energy of our many-body system can be resolved

$$\begin{aligned} T = \tfrac{1}{2}\sum m_i \dot{\boldsymbol{x}}_i \cdot \dot{\boldsymbol{x}}_i &= \tfrac{1}{2} M \dot{\boldsymbol{X}} \cdot \dot{\boldsymbol{X}} + \tfrac{1}{2}\sum m_i \dot{\boldsymbol{r}}_i \cdot \dot{\boldsymbol{r}}_i \\ &= \tfrac{1}{2M}\boldsymbol{P}\cdot\boldsymbol{P} + \sum \tfrac{1}{2m_i}\boldsymbol{q}_i \cdot \boldsymbol{q}_i \quad \text{with} \quad \boldsymbol{q}_i \equiv m_i \dot{\boldsymbol{r}}_i \\ &= T_{\text{orbital}} + T_{\text{intrinsic}} \end{aligned}$$

while the total angular momentum becomes

$$\begin{aligned} \boldsymbol{L} = \sum m_i \boldsymbol{x}_i \times \boldsymbol{p}_i &= \boldsymbol{X} \times \boldsymbol{P} + \sum \boldsymbol{r}_i \times \boldsymbol{q} \\ &= \boldsymbol{L}_{\text{orbital}} + \boldsymbol{L}_{\text{intrinsic}} \end{aligned}$$

2. Generalized statement of the 3rd Law. Let us now give up the assumption that the particles interact pairwise, writing

$$m_i \ddot{\boldsymbol{x}}_i = \boldsymbol{F}_i + \boldsymbol{F}_{\text{on } i \text{ by others}}$$

The standard "action/reaction" language is now rendered inappropriate: it makes (unfamiliar) sense to speak of "the action on m_i by the others" but no obvious sense to speak of a reaction back upon "the others." The point to which I would draw attention is that to recover (3) we have only to assume that

$$\sum_i \boldsymbol{F}_{\text{on } i \text{ by others}} = \boldsymbol{0} \quad : \quad \text{GENERALIZED } 3^{\text{rd}} \text{ LAW (PART I)}$$

The abandonment of pairwise interaction, however stange it may on first encounter seem, is in fact quite a natural step to take if one imagines the forces of interaction to arise from a potential $U(\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N)$, for then one has

$$\boldsymbol{F}_{\text{on } i \text{ by others}} = -\boldsymbol{\nabla}_i U(\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N)$$

in which light the assumption

$$U(\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N) = \sum U_{ij}(\boldsymbol{x}_i, \boldsymbol{x}_j)$$

that gives rise to pairwise interaction begins to look, from at least the purely function-theoretic point of view, so restrictive as to seem quite *un*natural! Compliance with the 3rd Law (as generalized)

$$\big\{\boldsymbol{\nabla}_1 + \boldsymbol{\nabla}_2 + \cdots + \boldsymbol{\nabla}_N\big\} U = 0$$

is readily seen to entail the gross translational invariance of U:

$$U(\boldsymbol{x}_1 + \boldsymbol{a}, \boldsymbol{x}_2 + \boldsymbol{a}, \ldots, \boldsymbol{x}_N + \boldsymbol{a}) = U(\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N) \quad : \quad \text{all } \boldsymbol{a}$$

This is a condition which is satisfied transparently in cases of the familiar type

$$U = \sum_{ij} U_{ij}(r_{ij}) \tag{8}$$

$$r_{ij} \equiv \text{length of } \boldsymbol{r}_i - \boldsymbol{r}_j = \sqrt{\boldsymbol{r}_i \cdot \boldsymbol{r}_i - 2\,\boldsymbol{r}_i \cdot \boldsymbol{r}_j + \boldsymbol{r}_j \cdot \boldsymbol{r}_j}$$

The statement

$$\boldsymbol{F} = \sum \boldsymbol{F}_i + \underbrace{\sum \boldsymbol{F}_{\text{on } i \text{ by others}}}_{\mathbf{0} \text{ by the } 3^{\text{rd}} \text{ Law}}$$

has the form not so much of a splitting theorem as a "disappearance theorem." But look in this light to the net torque

$$\begin{aligned}
\boldsymbol{N} &= \sum \boldsymbol{x}_i \times \left\{ \boldsymbol{F}_i + \boldsymbol{F}_{\text{on } i \text{ by others}} \right\} \\
&= \sum \left\{ \boldsymbol{X} + \boldsymbol{r}_i \right\} \times \left\{ \boldsymbol{F}_i + \boldsymbol{F}_{\text{on } i \text{ by others}} \right\} \\
&= \boldsymbol{X} \times \boldsymbol{F} + \sum \boldsymbol{r}_i \times \boldsymbol{F}_i + \boldsymbol{X} \times \left\{ \sum \boldsymbol{F}_{\text{on } i \text{ by others}} \right\} + \sum \boldsymbol{r}_i \times \boldsymbol{F}_{\text{on } i \text{ by others}} \\
&= \boldsymbol{N}_{\text{orbital}} + \boldsymbol{N}_{\text{intrinsic}} + \mathbf{0}_{\text{ by } 3^{\text{rd}} \text{ Law}} + \left\{ \sum \boldsymbol{r}_i \times \boldsymbol{F}_{\text{on } i \text{ by others}} \right\}
\end{aligned}$$

In the absence of impressed forces $\boldsymbol{F}_i$ the first two terms on the right vanish. So also does the final term if the particles interact by central 2-body forces[2], but in general its disappearance must be attributed to a seldom-stated law of nature:

$$\sum \boldsymbol{r}_i \times \boldsymbol{F}_{\text{on } i \text{ by others}} = \mathbf{0} \quad : \quad 3^{\text{rd}} \text{ LAW (PART II)}$$

In conservative cases this entails gross rotational invariance of the interaction potential:

$$U(\mathbb{R}\boldsymbol{r}_1, \mathbb{R}\boldsymbol{r}_2, \ldots, \mathbb{R}\boldsymbol{r}_N) = U(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots \boldsymbol{r}_N) \quad : \quad \text{all } \mathbb{R}$$

Translational and rotational invariance conjoin to imply that U is invariant under all Euclidean motions, and permitted therefore to depend upon the vectors $\boldsymbol{r}_i$ only through their dot products $\boldsymbol{r}_i \cdot \boldsymbol{r}_j$. This is, we notice, a property exhibited by all potentials of the form (8).

The familiar upshot of the 3rd Law (Part I) is that "systems do not exert net forces upon themselves," just as—in the degenerate case—isolated particles do not exert net forces upon themselves. The proposed Part II asserts similarly (but quite independently) that "systems do not exert net torques upon themselves." In worlds of contrary design, systems could (like galaxies?) twirl themselves (to point of catastropy?), in violation of several well-established conservation laws, and left/right symmetry would be broken. For a simple instance of an interactive force system of the type which the 3rd Law (Part II) is intended to exclude, see the Figure 1.[3]

I have discovered only one oblique reference to the "3rd Law (Part II)" in the standard literature: into §1.2 of the 2nd edition (1980) of his *Classical Mechanics* Herbert Goldstein has inserted material (absent from the 1st edition)

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[2] We notice that $\boldsymbol{r}_i \times (\boldsymbol{r}_j - \boldsymbol{r}_i) + \boldsymbol{r}_j \times (\boldsymbol{r}_i - \boldsymbol{r}_j) = \boldsymbol{r}_i \times \boldsymbol{r}_j + \boldsymbol{r}_j \times \boldsymbol{r}_i = \mathbf{0}$.

[3] In the *presence* of Part II—which is to say: in the real world—we have $\boldsymbol{N} = \boldsymbol{N}_{\text{"orbital"}} + \boldsymbol{N}_{\text{"intrinsic"}}$, which is the source of the claim that to stabilize a rigid body one must apply both a properly positioned force *and a couple*.

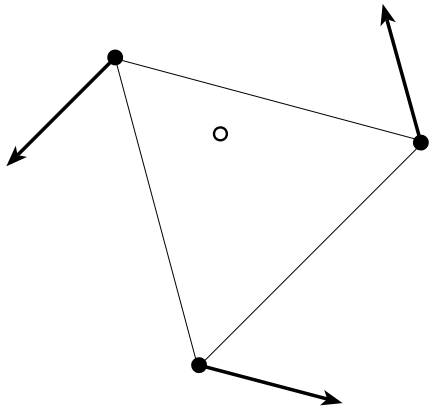

FIGURE 1: *Example of an interactive force system of the type which the* 3rd *Law (Part II) is intended to exclude. The open circle marks the center of mass. The bold arrow at each mass (filled circle) represents the force applied to that mass by conjoint action of the other two. Notice that the forces do vanish when added; i.e., that they do conform to the* 3rd *Law (Part I). The force field experienced by any individual particle has evidently the property that* $\mathrm{curl}\boldsymbol{F} \neq 0$, *and therefore cannot be obtained from a scalar potential.*

culminating in formulation of what he calls the "strong law of action and reaction." Goldstein assumes, however, that interactive forces are necessarily 2-body forces; his "strong law" (for which he cites no source) is intended to render "unphysical" the absurdities (see above) which might otherwise result from *non-central* 2-body forces.

3. Moments of a mass distribution. Let $m(x)$ refer to a 1-dimensional mass distribution. The n^{th} moment of $m(x)$ is defined

$$\begin{aligned}\langle x^n\rangle &\equiv \int x^n m(x)\,dx \\ &\downarrow \\ &= \sum x_i^n m_i \quad \text{in the discrete case } m(x) = \textstyle\sum m_i \delta(x - x_i)\end{aligned}$$

Knowledge of the *moments of all orders* would put one in position to construct the moment generating function

$$w(k) \equiv \textstyle\sum \frac{1}{n!}(ik)^n \langle x^n\rangle = \displaystyle\int e^{ikx} m(x)\,dx$$

and thus to recover the mass distribution itself:

$$m(x) = \tfrac{1}{2\pi}\displaystyle\int e^{-ikx} w(k)\,dk$$

I note in passing that one might, on these grounds, expect to be able to devise a way to discover *by inspection of the moments* whether the distribution is continuous or discrete, and thus to recast information conveyed by (for example) the autocorrelation function $\int m(x)m(x+\xi)\,dx$.

The notions introduced above admit straightforwardly of dimensional generalization, but at cost of some notational encumberance; one has (I look specifically to the 3-dimensional case) a

$$\text{single } 0^{\text{th}} \text{ moment} = \iiint m(x,y,z)\,dxdydz$$

$$\text{vector of } 1^{\text{st}} \text{ moments} = \iiint \begin{pmatrix} x \\ y \\ z \end{pmatrix} m(x,y,z)\,dxdydz$$

$$\text{symmetric matrix of } 2^{\text{nd}} \text{ moments} = \iiint \begin{pmatrix} xx & xy & xz \\ yx & yy & yz \\ zx & zy & zz \end{pmatrix} m(x,y,z)\,dxdydz$$

and higher moments of all orders that become progressively more difficult to describe, especially in the discrete case. Looking back again to (4), we see that the center of mass

$$\boldsymbol{X}(t) = \frac{\text{instantaneous } 1^{\text{st}} \text{ moment of the mass distribution}}{0^{\text{th}} \text{ moment}} \tag{9}$$

I would again emphasize the *mathematical character* of the preceding construction; one can no more touch the center of mass than one can "touch the Pythagorean theorem."

And I would emphasize that the construction does not presume the internal "rigidity" of the physical systems to which it is applied; it pertains as well to liquids, gases and globular clusters as to bricks.

The occurance in (9) of the word "instantaneous" alerts us to the fact that in any attempt to incorporate the center of mass concept into a relativistic account of the world we can (owing to the circumstance that in relativity the notion of "distant simultaneity" becomes frame-dependent) expect to encounter grave difficulty; already in my title I have announced my intention to set all such difficulties aside.

It is somewhat surprising that we have thus far encountered explicit dynamical need only of the *moments of lowest order*. In the theory of *rigid* many-body systems[4] one does encounter need also of the matrix of "centered second moments" (i.e., of second moments relative to the center of mass)

$$\text{moment of inertia matrix} \equiv \big\{\text{trace}\,\mathbb{M}\big\}\mathbb{I} - \mathbb{M}$$

[4] See CLASSICAL GYRODYNAMICS (1976), pp. 4–15.

(here $\mathbb{M} = \|M_{ij}\|$ with $\mathbb{M} \equiv \iiint \|r_i r_j\| m(\boldsymbol{r})\, dr_1 dr_2 dr_3$), and higher moments do frequently come into play on the "forcy/torquey side" of the equations of motion (they enter, that is to say, into the description of how a many-body system *senses* an ambient force field), but they do not occur in the expressions that relate to the *response* of the system. This curious circumstance I attribute to the fact that the equations of motion are differential equations of only second order.

Simple though it be, the center of mass concept has in the past inspired the invention of some mathematics of exceptional depth and utility. In his *Der barycentrische Calcul* (1827),[5] August Möbius looked to the point set generated when a "unit mass" is distributed in all possible ways among the points $\{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n\}$

$$\boldsymbol{X} = \mu_1 \boldsymbol{x}_1 + \mu_2 \boldsymbol{x}_2 + \cdots + \mu_n \boldsymbol{x}_n \ : \ \mu_i \text{ all non-negative, and sum to unity}$$

and was led to formulation of the "convex hull" concept,[6] to the topologically important notion of "orientability," and to ideas that contributed valuably to the early development of what was to become "multilinear algebra."[7]

4. Newtonian theory of transported systems. Let us, as a special instance of (1), write

$$m_i \ddot{\boldsymbol{x}}_i = -\boldsymbol{\nabla}_i U(\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N) \tag{10}$$

to describe the interior dynamics of an isolated molecule. My use of the term "molecule" is intended to suggest that the system is bound, and possesses a certain characteristic "size"

$$|\boldsymbol{x}_i - \boldsymbol{x}_j| < \text{some characteristic length } \ell \text{ (all } i \text{ and } j)$$

which is "small" relative to the lengths characteristic of the environment in which the molecule may (before we are done) find itself. We expect ℓ to be energy-dependent, and in realistic cases expect there to exist some "dissociation energy" $\mathcal{E}$ above which ℓ becomes undefined, but will confine our attention to molecular states (motions) with energy $E \ll \mathcal{E}$.

A physical question in which I have independent interest—initial aspects of which bear directly upon issues of immediate concern—can be phrased this way:

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[5] *The Barycentric Calculus*. The full title runs *Der barycentrische Calcul, ein neues Hülfsmittel zur analytischen Behandlung der Geometrie dargestellt und inbesondere auf die Bildung neuer Classen von Aufgaben und die Entwickelung mehrerer Eigenschaften der Kegelschnitte*, and would seem to leave little for further discussion with the text itself.

[6] The center of mass of an object need not lie interior to the object itself, but lies necessarily not outside its convex hull.

[7] For an informative account of Möbius' work and influence, see Michael J. Crowe, *A History of Vector Analysis: The Evolution of the Idea of a Vectorial System* (1967, reissued in 1994).

How is its internal state affected when the molecule is carried from here to there? Suppose, to be more precise, that A and B are molecules of identical design, in identical initial states. A stays home, but B is transported (gently) around a closed loop in physical 3-space. How, after it has returned to its starting point, does the state of B relate to that of A?[8] A moment's thought reveals that the answer to such questions depends critically upon *how the molecule is transported*, and it is that aspect of the problem which at present concerns me.

If I were to borrow one of Professor Dunn's molecular models, I might grab one of its model "atoms," subject that m_1 to extrinsically imposed motion $\boldsymbol{x}_1(t)$ and—being careful to avoid accelerations so large as to risk damage—let the other atoms $\{m_2, m_3, \ldots, m_N\}$ follow along in dynamic response to the elastic forces that serve to bind the model. Under such a scenario, $\boldsymbol{x}_1(t)$ serves no longer to describe the motion of a dynamical variable, but has become a "control function." The system has now only $N-1$ (vectorial) degrees of freedom, and the equations of motion read

$$m_i \ddot{\boldsymbol{x}}_i = -\boldsymbol{\nabla}_i U(\boldsymbol{x}_1(t), \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N) \quad : \quad i = 2, 3, \ldots, N$$

If we write

$$\boldsymbol{x}_i = \boldsymbol{x}_1(t) + \boldsymbol{s}_i \quad : \quad i = 2, 3, \ldots, N$$

and take into account the gross translational invariance of U (enforced by the 3rd Law) we obtain

$$m_i \ddot{\boldsymbol{s}}_i = -m_i \ddot{\boldsymbol{x}}_1(t) - \boldsymbol{\nabla}_i U(\boldsymbol{0}, \boldsymbol{s}_2, \ldots, \boldsymbol{s}_N) \quad : \quad i = 2, 3, \ldots, N \tag{11}$$

where the leading term on the right is a "fictitious force term," an artifact of the transported $\boldsymbol{s}$-frame is (unless $\ddot{\boldsymbol{x}}_1 = \boldsymbol{0}$) non-inertial. The center of mass of the dangling system $\{m_2, m_3, \ldots, m_N\}$ lives at

$$\boldsymbol{S} = \tfrac{1}{M-m_1}\{m_2\boldsymbol{s}_2 + m_3\boldsymbol{s}_3 + \cdots + m_N\boldsymbol{s}_N\}$$

with respect to the $\boldsymbol{s}$-frame, and at

$$\boldsymbol{X}_S = \boldsymbol{x}_1(t) + \boldsymbol{S}$$

with respect to our intertial $\boldsymbol{x}$-frame, while the center of mass of the entire model lives at

$$\begin{aligned} \boldsymbol{X} &= \tfrac{1}{M}\{m_1\boldsymbol{x}_i + (M-m_1)\boldsymbol{X}_S\} \\ &= \boldsymbol{x}_1 + \tfrac{M-m_1}{M}\boldsymbol{S} \end{aligned}$$

[8] The question has much in common with the question that inspired the invention of "Berry's phase"—see Alfred Shapere & Frank Wilczek, *Geometric Phases in Physics* (1989) or §10.2 in David Griffiths' *Introduction to Quantum Mechanics* (1995)—though Michael Berry was concerned with excursions in parameter space, while my interest focuses on the consequences of (necessarily non-inertial) excursions in physical space. Aspects of my problem have been discussed by Boaz Nash in "Getting from here to there: adiabatic transport of single particle classical periodic systems" (Reed College thesis, 1998).

From $\sum_i(11)$ we obtain

$$(M-m_1)\ddot{\boldsymbol{S}} = -(M-m_1)\ddot{\boldsymbol{x}}_1(t) + \boldsymbol{\nabla}_1 U(\boldsymbol{0}, \boldsymbol{s}_2, \ldots, \boldsymbol{s}_N)$$

giving

$$\begin{aligned} M\ddot{\boldsymbol{X}} &= m_1\ddot{\boldsymbol{x}}_1(t) + \boldsymbol{\nabla}_1 U(\boldsymbol{0}, \boldsymbol{s}) \qquad (12)\\ &\equiv \boldsymbol{F}(t) \quad : \quad \text{net force applied to achieve } \boldsymbol{x}(t)\text{-transportation} \end{aligned}$$

the meaning of the first term on the right is obvious, but the second term merits some comment. For the *free* molecule the 3rd Law has been seen to entail the gross translational invariance of $U(\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N)$, which gave

$$\sum_{i=1}^{N} \boldsymbol{\nabla}_i U(\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N) = \boldsymbol{0}$$

and implies the translational invariance also of all the associated force functions. So we have

$$\begin{aligned} \boldsymbol{\nabla}_1 U(\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N) &= -\sum_{i=2}^{N} \boldsymbol{\nabla}_i U(\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N)\\ &= -\boldsymbol{F}_{\text{on } i \text{ by others}}\\ &= +\boldsymbol{F}_{\text{“on others by } i\text{,” so to speak}}\\ &\equiv \boldsymbol{f}(\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N)\\ &= \boldsymbol{f}(\boldsymbol{x}_1, \boldsymbol{x}_1 + \boldsymbol{s}_2, \ldots, \boldsymbol{x}_1 + \boldsymbol{s}_N)\\ &= \boldsymbol{f}(\boldsymbol{0}, \boldsymbol{s}_2, \ldots, \boldsymbol{s}_N) \end{aligned}$$

which makes clear the *mathematical* meaning of the abbreviation $\boldsymbol{\nabla}_1 U(\boldsymbol{0}, \boldsymbol{s})$. Physically, the fact that we have promoted m_1 to a preferred status (it moves now not by the laws of mechanics, but by our whim) means that forces which formerly vanished in a summation process have become precisely the forces by which m_1 drags it's fellows along. From (12) we learn that m_1 acts “on the others” by acting *on their center of mass*. We note that (11) can be written

$$\begin{aligned} m_i\ddot{\boldsymbol{s}}_i &= -\boldsymbol{\nabla}_i \mathcal{U}(\boldsymbol{s}_2, \ldots, \boldsymbol{s}_N; t)\\ \mathcal{U} &\equiv \left\{m_2\boldsymbol{s}_2 + \cdots + m_N\boldsymbol{s}_N\right\}\cdot\ddot{\boldsymbol{x}}(t) + U(\boldsymbol{0}, \boldsymbol{s}_2, \ldots, \boldsymbol{s}_N) \end{aligned}$$

and that it is on account of the t-dependence of $\mathcal{U}$ that the motion of the transported $\left\{m_2, m_3, \ldots, m_N\right\}$-system is not energy-conserving; that, of course, is why we are careful to carry the molecule gently, “adiabatically.” We note finally that we cannot actually know the $\boldsymbol{F}(t)$ introduced at (12) until the system (11) has been solved to yield functions $\boldsymbol{s}_i(t)$; this fact conforms to our kinesthetic experience: to carry a jiggly object is to lurch in unanticipated ways.

The theory sketched above does appear to conform to the realities of the procedure I have selected to carry his model from his office to mine. But it

inherits from that procedure a formal asymmetry which seems unfair to the symmetry of the underlying physics. Thus am I led to consider this question: *Is is possible to carry molecule by its center of mass?*

Proceeding again from (10), we write

$$\boldsymbol{x}_i = \boldsymbol{X}(t) + \boldsymbol{r}_i$$

and, using $U(\boldsymbol{x}) = U(\boldsymbol{X}+\boldsymbol{r}) = U(\boldsymbol{r})$, appear to obtain

$$m_i\ddot{\boldsymbol{r}}_i = -m_i\ddot{\boldsymbol{X}}(t) - \boldsymbol{\nabla}_i U(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N)$$

But the variables $\boldsymbol{r}_i$ are subject to a familiar constraint, so the preceding equations are over-determined; they are easily seen to be consistent only when $\ddot{\boldsymbol{X}} = \boldsymbol{0}$. Let us therefore abandon the first of those equations, writing

$$m_i\ddot{\boldsymbol{r}}_i = -m_i\ddot{\boldsymbol{X}}(t) - \boldsymbol{\nabla}_i U(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N) \quad : \quad i = 2, 3, \ldots, N \tag{13}$$

Adding these, and using $m_1\boldsymbol{r}_1 = -\sum_2 m_i\boldsymbol{r}_i$, we obtain this alternative to the abandoned equation:

$$m_1\ddot{\boldsymbol{r}}_1 = (M - m_1)\ddot{\boldsymbol{X}}(t) - \boldsymbol{\nabla}_1 U(\boldsymbol{r})$$

This can be written

$$\begin{aligned} M\ddot{\boldsymbol{X}}(t) &= m_1\ddot{\boldsymbol{x}}_1 + \boldsymbol{\nabla}_1 U(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N) \\ &= m_1\ddot{\boldsymbol{x}}_1 + \boldsymbol{\nabla}_1 U(\boldsymbol{r}_1, \boldsymbol{r}_1 + \boldsymbol{s}_2, \ldots, \boldsymbol{r}_1 + \boldsymbol{s}_N) \\ &= m_1\ddot{\boldsymbol{x}}_1 + \boldsymbol{\nabla}_1 U(\boldsymbol{0}, \boldsymbol{s}_2, \ldots, \boldsymbol{s}_N) \end{aligned} \tag{14}$$

and is therefore equivalent to (12), from which it differs in this regard: in (12) the "control" responsibility has been assigned to $\boldsymbol{x}_1(t)$, but in (14) it has been transferred to $\boldsymbol{X}(t)$.

We have assigned control responsibility to a symmetrically-constructed object (the center of mass), but are disappointed to discover that it exercises its control within an asymmetric population of equations. And we have to wonder: what sense does it make to assign such work to a mathematical abstraction? As I have several times emphasized, one cannot "tie a string to the center of mass." Is it physically/theologically permissible to press the "finger of God" into such service? In reality we are obligated to engage the *constituent particles*, either singly (as above) or severally. I show now that this *can* be done in such a way as to make it seem *as if* one had engaged the center of mass.

Introduce a force field $\boldsymbol{G}(\boldsymbol{x})$ and undertake Taylor expansion about the center of mass:

$$\begin{aligned} \boldsymbol{G}(\boldsymbol{X}+\boldsymbol{r}) &= \left\{1 + (\boldsymbol{r}\cdot\boldsymbol{\nabla}) + \tfrac{1}{2!}(\boldsymbol{r}\cdot\boldsymbol{\nabla})^2 + \cdots\right\}\boldsymbol{G}(\boldsymbol{x})\Big|_{\boldsymbol{x}\to\boldsymbol{X}} \\ &= \boldsymbol{G}(\boldsymbol{X}) + \text{gradient terms or ascending order} \end{aligned}$$

and assume the force experienced by the i^{th} particle is proportional to its inertial mass m_i: $\boldsymbol{F}_i = m_i\boldsymbol{G}$. We have, in effect, assumed the impressed "control field" to be a *gravitational* field, in which context the "gradient terms" are called "tidal terms." Let us agree to abandon such terms, on the ground that field variation is negligible at a scale set by the size ℓ of the molecule. We then have

$$m_i\ddot{\boldsymbol{X}}_i + m_i\ddot{\boldsymbol{r}}_i = m_i\boldsymbol{G}(\boldsymbol{X}) - \boldsymbol{\nabla}_i U(\boldsymbol{X}+\boldsymbol{r}_1, \boldsymbol{X}+\boldsymbol{r}_2, \ldots, \boldsymbol{X}+\boldsymbol{r}_N)$$

which spontaneously splits into a pair of uncoupled systems:

$$\ddot{\boldsymbol{X}} = \boldsymbol{G}(\boldsymbol{X}) \tag{15.1}$$

$$m_i\ddot{\boldsymbol{r}}_i = -\boldsymbol{\nabla}_i U(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N) \quad \text{with} \quad \textstyle\sum m_i\boldsymbol{r}_i = \boldsymbol{0} \tag{15.2}$$

5. Calder's construction. The coupled system (15.2) is consistent but redundant. To manage the implications of this fact, one might abandon (say) the first equation, and feed $\boldsymbol{r}_1 = -\frac{1}{m_1}\{m_2\boldsymbol{r}_2 + \cdots + m_N\boldsymbol{r}_N\}$ into those that remain, as we have several times done. But in the case $N = 2$ both ancient tradition and the physics of the matter recommend a different—less asymmetrically discriminatory—procedure:

Introduce, in addition to the center of mass $\boldsymbol{X} \equiv \frac{1}{m_1+m_2}\{m_1\boldsymbol{x}_1 + m_2\boldsymbol{x}_2\}$, a separation vector $\boldsymbol{R} \equiv \boldsymbol{x}_1 - \boldsymbol{x}_2$. Inversion of the system

$$\begin{aligned} m_1\boldsymbol{x}_1 + m_2\boldsymbol{x}_2 &= (m_1+m_2)\boldsymbol{X} \\ \boldsymbol{x}_1 - \quad \boldsymbol{x}_2 &= \qquad\quad \boldsymbol{R} \end{aligned}$$

gives

$$\left.\begin{aligned} \boldsymbol{x}_1 &= \boldsymbol{X} + \tfrac{m_2}{m_1+m_2}\boldsymbol{R} \\ \boldsymbol{x}_2 &= \boldsymbol{X} - \tfrac{m_1}{m_1+m_2}\boldsymbol{R} \end{aligned}\right\} \quad \text{whence} \quad \left\{\begin{aligned} \boldsymbol{r}_1 &= +\tfrac{m_2}{m_1+m_2}\boldsymbol{R} \\ \boldsymbol{r}_2 &= -\tfrac{m_1}{m_1+m_2}\boldsymbol{R} \end{aligned}\right\} \tag{17}$$

which serve, in effect, to "automate" the constraint $m_1\boldsymbol{r}_1 + m_2\boldsymbol{x}_2 = \boldsymbol{0}$, but favor neither $\boldsymbol{r}$-vector. Returning with (17) to (15.2) we have

$$\begin{aligned} -\tfrac{m_1m_2}{m_1+m_2}\ddot{\boldsymbol{R}} &= -\boldsymbol{\nabla}_1 U(\boldsymbol{r}_1, \boldsymbol{r}_2) \\ +\tfrac{m_1m_2}{m_1+m_2}\ddot{\boldsymbol{R}} &= -\boldsymbol{\nabla}_2 U(\boldsymbol{r}_1, \boldsymbol{r}_2) \end{aligned}$$

—the equivalence of which is assured by the 3rd Law: $(\boldsymbol{\nabla}_1 + \boldsymbol{\nabla}_2)U = \boldsymbol{0}$. In the Kepler Problem (as in all variants of the 2-body problem with central interaction) one has

$$U(\boldsymbol{r}_1, \boldsymbol{r}_2) = U(R) \quad \text{with} \quad R^2 \equiv \boldsymbol{R}\cdot\boldsymbol{R} = |\boldsymbol{x}_1 - \boldsymbol{x}_2|^2 = |\boldsymbol{r}_1 - \boldsymbol{r}_2|^2$$

giving $\mu\ddot{\boldsymbol{R}} = -\boldsymbol{\nabla}U(R)$ where $\mu \equiv \frac{m_1m_2}{m_1+m_2}$ is the so-called "reduced mass."

I have allowed myself to review such standard stuff in order to pose and address this non-standard question: Can the method be extended to cases $N > 2$? Look to the case $N = 3$: let

$$\begin{aligned}
\boldsymbol{R}_2 &\equiv \text{separation vector directed from } m_2 \text{ to } m_1\\
\boldsymbol{X}_2 &\quad \text{locate center of mass of } \{m_1, m_2\}\\
\boldsymbol{R}_3 &\equiv \text{separation vector directed from } m_3 \text{ to } \boldsymbol{X}_2\\
\boldsymbol{X}_3 &\quad \text{locate center of mass of } \{m_1, m_2, m_3\}
\end{aligned}$$

Then

$$\begin{aligned}
\boldsymbol{R}_2 &= \boldsymbol{x}_1 - \boldsymbol{x}_2\\
\boldsymbol{R}_3 &= \tfrac{1}{m_1+m_2}(m_1\boldsymbol{x}_1 + m_2\boldsymbol{x}_2) - \boldsymbol{x}_3\\
\boldsymbol{X}_3 &= \tfrac{1}{m_1+m_2+m_3}(m_1\boldsymbol{x}_1 + m_2\boldsymbol{x}_2 + m_3\boldsymbol{x}_3)\\
&= \boldsymbol{X} \quad : \quad \text{locates center of mass of entire 3-body system}
\end{aligned}$$

give

$$\left.\begin{aligned}
\boldsymbol{x}_3 &= \boldsymbol{X} - \tfrac{m_1+m_2}{m_1+m_2+m_3}\boldsymbol{R}_3 &&= \boldsymbol{X} + \boldsymbol{r}_3\\
\boldsymbol{x}_2 &= \boldsymbol{X} + \tfrac{m_3}{m_1+m_2+m_3}\boldsymbol{R}_3 - \tfrac{m_1}{m_1+m_2}\boldsymbol{R}_2 &&= \boldsymbol{X} + \boldsymbol{r}_2\\
\boldsymbol{x}_1 &= \boldsymbol{X} + \tfrac{m_3}{m_1+m_2+m_3}\boldsymbol{R}_3 + \tfrac{m_2}{m_1+m_2}\boldsymbol{R}_2 &&= \boldsymbol{X} + \boldsymbol{r}_1
\end{aligned}\right\} \tag{18}$$

Again, we have managed to "automate" the constraint, in the sense that one has $m_1\boldsymbol{r}_1 + m_2\boldsymbol{x}_2 + m_3\boldsymbol{r}_3 = \boldsymbol{0}$ for all values of $\boldsymbol{R}_2$ and $\boldsymbol{R}_3$. In the case $N = 4$ one has

$$\left.\begin{aligned}
\boldsymbol{x}_4 &= \boldsymbol{X} - \tfrac{m_1+m_2+m_3}{m_1+m_2+m_3+m_4}\boldsymbol{R}_4 &&= \boldsymbol{X} + \boldsymbol{r}_4\\
\boldsymbol{x}_3 &= \boldsymbol{X} + \tfrac{m_4}{m_1+m_2+m_3+m_4}\boldsymbol{R}_4 - \tfrac{m_1+m_2}{m_1+m_2+m_3}\boldsymbol{R}_3 &&= \boldsymbol{X} + \boldsymbol{r}_3\\
\boldsymbol{x}_2 &= \boldsymbol{X} + \tfrac{m_4}{m_1+m_2+m_3+m_4}\boldsymbol{R}_4 + \tfrac{m_3}{m_1+m_2+m_3}\boldsymbol{R}_3 - \tfrac{m_1}{m_1+m_2}\boldsymbol{R}_2 &&= \boldsymbol{X} + \boldsymbol{r}_2\\
\boldsymbol{x}_1 &= \boldsymbol{X} + \tfrac{m_4}{m_1+m_2+m_3+m_4}\boldsymbol{R}_4 + \tfrac{m_3}{m_1+m_2+m_3}\boldsymbol{R}_3 + \tfrac{m_2}{m_1+m_2}\boldsymbol{R}_2 &&= \boldsymbol{X} + \boldsymbol{r}_1
\end{aligned}\right\} \tag{19}$$

which I confess I have not actually computed[9] but have simply *read off* from Figure 2, and in the general case that would, I think, be the recommended procedure.

The preceding discussion sprang from a simple idea which has been elevated to a state of (literally) fine art by Alexander Calder, the American sculptor celebrated for his invention of the "mobile." What I call "Calder's construction" has given rise to a change of variables

$$\{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N\} \longrightarrow \{\boldsymbol{X}, \boldsymbol{R}_2, \ldots, \boldsymbol{R}_N\}$$

wherein the variables $\{\boldsymbol{R}_2, \ldots, \boldsymbol{R}_N\}$ serve to "automate" the familiar constraint $\sum m_i\boldsymbol{r}_i = \boldsymbol{0}$, but are themselves *un*constrained. The $\boldsymbol{R}$-variables permit us to avoid the "discriminatory asymmetry" of $\boldsymbol{r}_1 = -\frac{1}{m_1}\{m_2\boldsymbol{r}_2 + \cdots + m_N\boldsymbol{r}_N\}$, but at cost of introducing an asymmetry of a new sort: a population of N masses can be "mobilized" in $N!$ distinct ways; to select one is to reject the others, and to introduce hierarchical order where (typically) none is present in the physics.

[9] The computation would entail tedious inversion of a certain 4×4 matrix.

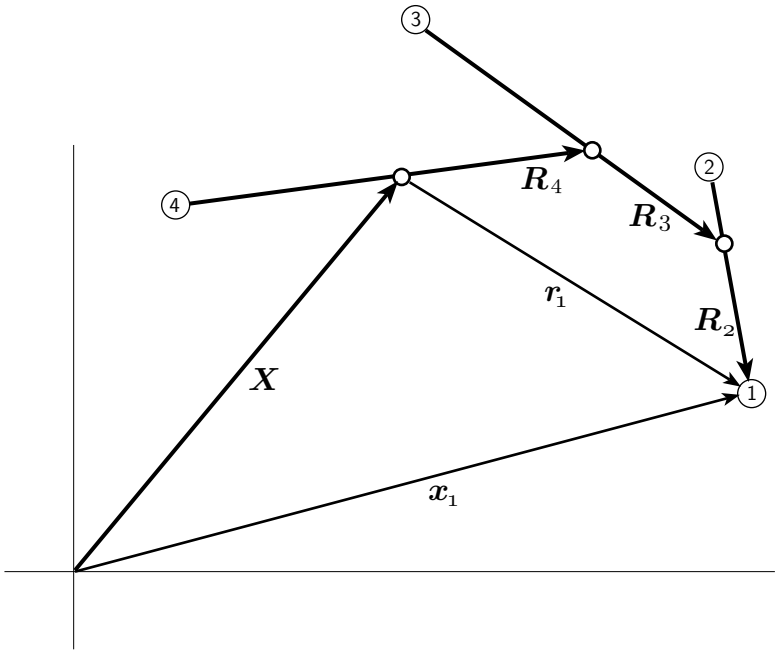

FIGURE 2: *"Calder's construction."* $\boldsymbol{R}_2$ *extends from* ② ⟶ ①, $\boldsymbol{R}_3$ *from* ③ *to the center of mass of the* $\{m_1, m_2\}$ *subsystem (small circle* ∘*), while* $\boldsymbol{X}$ *stands with its tail at the origin of the Cartesian frame.*

So far as concerns the dynamical aspects of that physics, we (with the assistance of *Mathematica*) find

$$\tfrac{1}{2}\{m_1\dot{\boldsymbol{x}}_1\cdot\dot{\boldsymbol{x}}_1+m_2\dot{\boldsymbol{x}}_2\cdot\dot{\boldsymbol{x}}_2\}$$
$$=\tfrac{1}{2}(m_1+m_2)\dot{\boldsymbol{X}}\cdot\dot{\boldsymbol{X}}+\tfrac{1}{2}\mu_2\dot{\boldsymbol{R}}_2\cdot\dot{\boldsymbol{R}}_2$$

$$\tfrac{1}{2}\{m_1\dot{\boldsymbol{x}}_1\cdot\dot{\boldsymbol{x}}_1+m_2\dot{\boldsymbol{x}}_2\cdot\dot{\boldsymbol{x}}_2+m_3\dot{\boldsymbol{x}}_3\cdot\dot{\boldsymbol{x}}_3\}$$
$$=\tfrac{1}{2}(m_1+m_2+m_3)\dot{\boldsymbol{X}}\cdot\dot{\boldsymbol{X}}+\tfrac{1}{2}\mu_2\dot{\boldsymbol{R}}_2\cdot\dot{\boldsymbol{R}}_2+\tfrac{1}{2}\mu_3\dot{\boldsymbol{R}}_3\cdot\dot{\boldsymbol{R}}_3$$

$$\tfrac{1}{2}\{m_1\dot{\boldsymbol{x}}_1\cdot\dot{\boldsymbol{x}}_1+m_2\dot{\boldsymbol{x}}_2\cdot\dot{\boldsymbol{x}}_2+m_3\dot{\boldsymbol{x}}_3\cdot\dot{\boldsymbol{x}}_3+m_4\dot{\boldsymbol{x}}_4\cdot\dot{\boldsymbol{x}}_4\}$$
$$=\tfrac{1}{2}(m_1+m_2+m_3+m_4)\dot{\boldsymbol{X}}\cdot\dot{\boldsymbol{X}}+\tfrac{1}{2}\mu_2\dot{\boldsymbol{R}}_2\cdot\dot{\boldsymbol{R}}_2+\tfrac{1}{2}\mu_3\dot{\boldsymbol{R}}_3\cdot\dot{\boldsymbol{R}}_3+\tfrac{1}{2}\mu_4\dot{\boldsymbol{R}}_4\cdot\dot{\boldsymbol{R}}_4$$
$$\vdots$$

where
$$\begin{aligned}\mu_2&\equiv\left[\tfrac{1}{m_1}+\tfrac{1}{m_2}\right]^{-1}=\tfrac{m_1m_2}{m_1+m_2}\\ \mu_3&\equiv\left[\tfrac{1}{\mu_2}+\tfrac{1}{m_3}\right]^{-1}=\tfrac{(m_1+m_2)m_3}{m_1+m_2+m_3}\\ \mu_4&\equiv\left[\tfrac{1}{\mu_3}+\tfrac{1}{m_4}\right]^{-1}=\tfrac{(m_1+m_2+m_3)m_4}{m_1+m_2+m_3+m_4}\\ &\vdots\end{aligned}\tag{20}$$

serve to generalize the notion of "reduced mass." The fact that *no cross terms*

appear when kinetic energy is described in terms of $\{\boldsymbol{X}, \boldsymbol{R}_2, \ldots, \boldsymbol{R}_N\}$ variables is—though familiar in the case $N = 2$—somewhat surprising in the general case. I look to the underlying mechanism, as illustrated in the case $N = 3$: we have

$$\begin{pmatrix} \boldsymbol{r}_1 \\ \boldsymbol{r}_2 \\ \boldsymbol{r}_3 \end{pmatrix} = \mathbb{M} \begin{pmatrix} \boldsymbol{R}_2 \\ \boldsymbol{R}_3 \end{pmatrix}$$

$$\mathbb{M} \equiv \begin{pmatrix} +\frac{m_2}{m_1+m_2} & +\frac{m_3}{m_1+m_2+m_3} \\ -\frac{m_1}{m_1+m_2} & +\frac{m_3}{m_1+m_2+m_3} \\ 0 & -\frac{m_1+m_2}{m_1+m_2+m_3} \end{pmatrix} \quad : \text{ Note that } \mathbb{M} \text{ is } 3 \times 2$$

The claim—verified by *Mathematica*—is that

$$\mathbb{M}^{\intercal} \begin{pmatrix} m_1 & 0 & 0 \\ 0 & m_2 & 0 \\ 0 & 0 & m_3 \end{pmatrix} \mathbb{M} = \begin{pmatrix} \mu_2 & 0 \\ 0 & \mu_3 \end{pmatrix} \tag{21}$$

But while the $\boldsymbol{R}$-variables are well-adapted to the description of kinetic energy, we see from[10]

$$\begin{aligned}
\boldsymbol{r}_1 - \boldsymbol{r}_2 &= \boldsymbol{R}_2 \\
\boldsymbol{r}_1 - \boldsymbol{r}_3 &= \tfrac{m_2}{m_1+m_2}\boldsymbol{R}_2 + \boldsymbol{R}_3 \\
\boldsymbol{r}_1 - \boldsymbol{r}_4 &= \tfrac{m_2}{m_1+m_2}\boldsymbol{R}_2 + \tfrac{m_3}{m_1+m_2+m_3}\boldsymbol{R}_3 + \boldsymbol{R}_4 \\
\boldsymbol{r}_2 - \boldsymbol{r}_3 &= -\tfrac{m_1}{m_1+m_2}\boldsymbol{R}_2 + \boldsymbol{R}_3 \\
\boldsymbol{r}_2 - \boldsymbol{r}_4 &= -\tfrac{m_1}{m_1+m_2}\boldsymbol{R}_2 + \tfrac{m_3}{m_1+m_2+m_3}\boldsymbol{R}_3 + \boldsymbol{R}_4 \\
\boldsymbol{r}_3 - \boldsymbol{r}_4 &= -\tfrac{m_1+m_2}{m_1+m_2+m_3}\boldsymbol{R}_3 + \boldsymbol{R}_4
\end{aligned}$$

that $\boldsymbol{R}$-variables are (except in the case $N = 2$) not particularly well-adapted to the description of (the distances which separate the masses, whence to the

[10] The following equations can be computed algebraically from (19). But they can also—and more quickly—be read off directly from Figure 2: to compute $\boldsymbol{r}_i - \boldsymbol{r}_j$ one starts at ⓙ and walks along the figure to ⓘ, taking signs to reflect whether one proceeds prograde or retrograde along a given leg, and (when one enters/exits at the "fulcrum" $\circ$ of a leg) taking a fractional factor which conforms to the "teeter-totter principle"

$$\text{factional factor} = \frac{\text{mass to the rear of that leg}}{\text{total mass associated with that leg}}$$

A little practice shows better than any explanation how the procedure works, and how wonderfully efficient it is.

description of) central 2-body interactive forces; one expects in the general case to have

$$\text{interaction potential} = \begin{cases} \text{function of all } \tfrac{1}{2}N(N-1) \text{ dot products} \\ \text{constructable from } \{\boldsymbol{R}_2, \boldsymbol{R}_3 \ldots, \boldsymbol{R}_N\} \end{cases}$$

which is at least not worse than

$$\text{interaction potential} = \begin{cases} \text{function of all } \tfrac{1}{2}N(N+1) \text{ dot products} \\ \text{constructable from } \{\boldsymbol{r}_1, \boldsymbol{r}_2 \ldots, \boldsymbol{r}_N\} \end{cases}$$

and has in fact the advantages that the $\boldsymbol{R}$-variables are fewer in number and unconstrained/independent. In the case of the graviational 3-body problem we now find ourselves led to write

$$\begin{aligned} U = -G\Big\{ & m_1m_2\big[R_2^2\big]^{-\frac{1}{2}} + m_1m_3\big[\big(\tfrac{m_2}{m_1+m_2}\big)^2R_2^2 + \tfrac{m_2}{m_1+m_2}\boldsymbol{R}_2{\cdot}\boldsymbol{R}_3 + R_3^2\big]^{-\frac{1}{2}} \\ & + m_2m_3\big[\big(\tfrac{m_1}{m_1+m_2}\big)^2R_2^2 - \tfrac{m_1}{m_1+m_2}\boldsymbol{R}_2{\cdot}\boldsymbol{R}_3 + R_3^2\big]^{-\frac{1}{2}}\Big\} \\ \downarrow & \\ = -Gm_1m_2/\sqrt{\boldsymbol{R}_2{\cdot}\boldsymbol{R}_2} & \quad \text{when } m_3 \text{ is extinguished} \end{aligned}$$

which serves to remind us why the 2-body problem is so much easier than the 3-body problem, but at the same time suggests that the variables $\boldsymbol{R}_2$ and $\boldsymbol{R}_3$ may be of real use in this physical application. As, apparently, they turn out to be: consulting A. E. Roy's *Orbital Motion* (1978), I discover (see his §5.11.3) that $\boldsymbol{r} \equiv -\boldsymbol{R}_2$ and $\boldsymbol{\rho} \equiv -\boldsymbol{R}_3$ were introduced by Jacobi and Lagrange, and are known to celestial mechanics as "Jacobian coordinates." For an interesting recent application, and modern references, see R. G. Littlejohn & M. Reinseh, "Gauge fields in the separation of rotations and internal motions in the n-body problem," RMP **69**, 213 (1997).

6. Center of mass in Lagrangian theory. Our objective is quantum theory, for which classical Hamiltonian formalism provides standardly the point of departure. It is to gain access to that launch pad that I look now, by way of preparation, to the associated Lagrangian formalism.

To announce our interest in the interior dynamics of a free molecule we might write

$$L = \tfrac{1}{2}\textstyle\sum m_i\dot{\boldsymbol{x}}_i{\cdot}\dot{\boldsymbol{x}}_i - U(\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N)$$

which leads to the equations of motion encountered already at (10).

So informative is the collective variable $\boldsymbol{X}$ (center of mass), and so sharply does it speak to the separation of extrinsic from intrinsic features of the molecular dynamics, that it becomes natural to seek to *promote* $\boldsymbol{X}$ *to the status of an independent variable*. How is that to be accomplished? Writing $\boldsymbol{x}_i = \boldsymbol{X} + \boldsymbol{r}_i$ we confront the fact that the variables $\{\boldsymbol{X}, \boldsymbol{r}_1, \ldots, \boldsymbol{r}_N\}$ are more numerous than the degrees of freedom, so cannot be taken to comprise a set independent variables (generalized coordinates); the vectors $\boldsymbol{r}_i$ are subject to the familiar constraint $\sum m_i\boldsymbol{r}_i = \boldsymbol{0}$, and the question becomes: How is the constraint to be accommodated? Two methods recommend themselves:

We might introduce an $(N-1)$-fold set of variables which serve in effect to "automate" the constraint. If, for example, we appeal to Calder's construction to introduce vectors ("generalized Jacobian coordinates") $\{\boldsymbol{R}_2, \ldots, \boldsymbol{R}_N\}$ then we are led to write

$$L = \tfrac{1}{2} M \dot{\boldsymbol{X}} \cdot \dot{\boldsymbol{X}} + \tfrac{1}{2} \sum_{i=2}^{N} \mu_i \dot{\boldsymbol{R}}_i \cdot \dot{\boldsymbol{R}}_i - \mathcal{U}(\boldsymbol{R}_2, \ldots, \boldsymbol{R}_N) \tag{22}$$

giving

$$\left.\begin{aligned} M\ddot{\boldsymbol{X}} &= \boldsymbol{0} \\ \mu_i \ddot{\boldsymbol{R}}_i &= -\boldsymbol{\nabla}_i \mathcal{U}(\boldsymbol{R}_2, \ldots, \boldsymbol{R}_N) \quad : \quad i = 2, 3, \ldots, N \end{aligned}\right\} \tag{23}$$

This procedure has much to recommend it, but is susceptible to the criticism that the $\boldsymbol{R}$-variables which enter so symmetrically into the design of (at least the kinetic part of) the Lagrangian stand nevertheless in asymmetric relationship to the physics.

Alternatively—in an effort to achieve a formalism which better reflects the symmetry of the physics—one might draw upon the "Lagrange multiplier" technique, writing

$$L = \tfrac{1}{2} \textstyle\sum m_i (\dot{\boldsymbol{X}} + \dot{\boldsymbol{r}}_i) \cdot (\dot{\boldsymbol{X}} + \dot{\boldsymbol{r}}_i) - \underbrace{U(\boldsymbol{X} + \boldsymbol{r}_1, \ldots, \boldsymbol{X} + \boldsymbol{r}_N)}_{= U(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N)} + \boldsymbol{q} \cdot \textstyle\sum m_i \boldsymbol{r}_i \tag{24}$$

The $\boldsymbol{X}^{\text{th}}$, $\boldsymbol{r}_i^{\text{th}}$ and $\boldsymbol{q}^{\text{th}}$ equations of motion then read

$$\begin{aligned} \textstyle\sum m_i (\ddot{\boldsymbol{X}} + \ddot{\boldsymbol{r}}_i) &= \boldsymbol{0} \\ m_i (\ddot{\boldsymbol{X}} + \ddot{\boldsymbol{r}}_i) &= -\boldsymbol{\nabla}_i U(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N) + m_i \boldsymbol{q} \\ \textstyle\sum m_i \boldsymbol{r}_i &= \boldsymbol{0} \end{aligned}$$

which can by familiar manipulations be brought to the form

$$\left.\begin{aligned} \boldsymbol{q} &= \ddot{\boldsymbol{X}} \\ M\ddot{\boldsymbol{X}} &= \boldsymbol{0} \\ m_i \ddot{\boldsymbol{r}}_i &= -\boldsymbol{\nabla}_i U(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N) \quad \text{with} \quad \textstyle\sum m_i \boldsymbol{r}_i = \boldsymbol{0} \end{aligned}\right\} \tag{25}$$

These equations are symmetric but redundant, and there appears to be no way to remove that redundancy without at the same time destroying the symmetry; if, for example, one uses equations of the form (see again (18) and (19))

$$\boldsymbol{r}_i = \sum_{j=2}^{N} C_{ij} \boldsymbol{R}_j$$

to "automate" the constraint then one is led back again to (23), which is, as previously remarked, less symmetric than it appears to be.

To describe the "transportation" of a molecule we might (if we are willing to press the "finger of God" once again into service) retain (24) but subject $\boldsymbol{X}$ to reinterpretation:

$$\text{collective dynamical variable } \boldsymbol{X} \longrightarrow \text{autonymous control function } \boldsymbol{X}(t)$$

The equations of motion are then only $N+1$ in number, and read

$$\begin{aligned} m_i\big(\ddot{\boldsymbol{X}}(t) + \ddot{\boldsymbol{r}}_i\big) &= -\boldsymbol{\nabla}_i U(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N) + m_i \boldsymbol{q} \\ \textstyle\sum m_i \boldsymbol{r}_i \ &= \boldsymbol{0} \end{aligned}$$

which entail

$$\left.\begin{aligned} \boldsymbol{q} &= \ddot{\boldsymbol{X}}(t) \\ m_i \ddot{\boldsymbol{r}}_i &= -\boldsymbol{\nabla}_i U(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N) \quad \text{with} \quad \textstyle\sum m_i \boldsymbol{r}_i = \boldsymbol{0} \end{aligned}\right\} \tag{26}$$

Remarkably, no "fictitious forces" are brought into play by the non-inertiality of the $\boldsymbol{r}$-frame; the internal motion of the molecule is unaffected by arbitrary transportation of the center of mass. This conclusion is, however, fictitious in the deeper sense that it refers to an impossible procedure; the best one can in reality hope to do is to apply forces *to the constituent particles* m_i and to arrange for it to appear *as if* the center of mass were being dragged about. The Newtonian implications of this remark were explored in §4; I discuss now its implementation within the Lagrangian formalism:

In place of (24) write

$$\begin{aligned} L = \tfrac{1}{2} \textstyle\sum m_i (\dot{\boldsymbol{X}} + \dot{\boldsymbol{r}}_i)\cdot(\dot{\boldsymbol{X}} + \dot{\boldsymbol{r}}_i) - U(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N) + \boldsymbol{q}\cdot\textstyle\sum m_i \boldsymbol{r}_i \\ - \textstyle\sum V_i(\boldsymbol{X} + \boldsymbol{r}_i) \end{aligned} \tag{27}$$

where $V_i(\bullet)$ refers to a force externally impressed upon m_i. By Taylor expansion we have the generic result

$$\begin{aligned} V(\boldsymbol{X} + \boldsymbol{r}) &= \big\{1 + (\boldsymbol{r}\cdot\boldsymbol{\nabla}) + \tfrac{1}{2}(\boldsymbol{r}\cdot\boldsymbol{\nabla})^2 + \cdots\big\} V(\boldsymbol{X}) \\ &\equiv V(\boldsymbol{X}) - \boldsymbol{r}\cdot\boldsymbol{F}(\boldsymbol{X}) - \tfrac{1}{2}\boldsymbol{r}\cdot\mathbb{F}(\boldsymbol{X})\boldsymbol{r} + \cdots \end{aligned}$$

and are led to equations of motion which can be written

$$\begin{aligned} \textstyle\sum m_i(\ddot{\boldsymbol{X}} + \ddot{\boldsymbol{r}}_i) &= \textstyle\sum\big\{\boldsymbol{F}_i(\boldsymbol{X}) + \mathbb{F}_i(\boldsymbol{X})\boldsymbol{r}_i + \cdots\big\} \\ m_i(\ddot{\boldsymbol{X}} + \ddot{\boldsymbol{r}}_i) &= \quad \big\{\boldsymbol{F}_i(\boldsymbol{X}) + \mathbb{F}_i(\boldsymbol{X})\boldsymbol{r}_i + \cdots\big\} - \boldsymbol{\nabla}_i U(\boldsymbol{r}) + m_i \boldsymbol{q} \\ \textstyle\sum m_i \boldsymbol{r}_i &= \boldsymbol{0} \end{aligned}$$

which after slight rearrangement become

$$\begin{aligned} M\ddot{\boldsymbol{X}} &= \textstyle\sum\big\{\boldsymbol{F}_i(\boldsymbol{X}) + \mathbb{F}_i(\boldsymbol{X})\boldsymbol{r}_i + \cdots\big\} \\ m_i\ddot{\boldsymbol{r}}_i &= -\boldsymbol{\nabla}_i U(\boldsymbol{r}) + m_i\big\{\boldsymbol{q} - \ddot{\boldsymbol{X}}\big\} + \big\{\boldsymbol{F}_i(\boldsymbol{X}) + \mathbb{F}_i(\boldsymbol{X})\boldsymbol{r}_i + \cdots\big\} \end{aligned} \tag{28}$$

Necessarily $\qquad \boldsymbol{q} = \boldsymbol{0}$

It is clear from (28) that enforced dragging of a molecule generally *does* affect its internal dynamics. But assume now more particularly that the impressed force field engages each particle in proportion to its mass; i.e., that it is an impressed *gravitational* field:

$$\boldsymbol{F}_i(\boldsymbol{X}) = m_i \boldsymbol{G}(\boldsymbol{X})$$

The equations of motion then become

$$\begin{aligned}
\ddot{\boldsymbol{X}} &= \boldsymbol{G}(\boldsymbol{X}) + \mathbf{0} + \cdots \\
m_i \ddot{\boldsymbol{r}}_i &= -\boldsymbol{\nabla}_i U(\boldsymbol{r}) + m_i\big\{\mathbf{0} - \ddot{\boldsymbol{X}}\big\} + m_i\big\{\boldsymbol{G}(\boldsymbol{X}) + \mathbb{G}(\boldsymbol{X})\boldsymbol{r}_i + \cdots\big\} \\
&= -\boldsymbol{\nabla}_i U(\boldsymbol{r}) + m_i\big\{\mathbb{G}(\boldsymbol{X})\boldsymbol{r}_i + \cdots\big\} \\
&\downarrow \\
&= -\boldsymbol{\nabla}_i U(\boldsymbol{r}) \quad \text{if "tidal terms" can be neglected}
\end{aligned}$$

We are brought again to the conclusion that *a small molecule in free fall is a free molecule*, and that the action of "God's finger" is, for present purposes, effectively the action of a (locally homogeneous) time-dependent gravitational field $\boldsymbol{G}(t)$.

The Lagrangian formalism draws necessarily upon at least one distinctive analytical device (Lagrange's "method of undetermined multipliers"), but has led to conclusions identical to those achieved previously by Newtonian means. Its particular merit lies in the fact that it places us in position to identify and address certain formal problems which emerge when one looks to the placement of...

7. Center of mass in Hamiltonian theory. It is, in view of some of what is to follow, gratifying to note that *no* formal problem intrudes if one proceeds from

$$L = \tfrac{1}{2}\textstyle\sum m_i \dot{\boldsymbol{x}}_i \cdot \dot{\boldsymbol{x}}_i - V(\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N)$$

and agrees to look upon the center of mass as an auxilliary construction, to be assembled and studied "after the fact." For then one has

$$\boldsymbol{p}_i \equiv \frac{\partial L}{\partial \dot{\boldsymbol{x}}_i} = m_i \dot{\boldsymbol{x}}_i \quad : \quad \text{momentum conjugate to } \boldsymbol{x}_i$$

giving

$$H = \textstyle\sum \boldsymbol{p}_i \dot{\boldsymbol{x}}_i - L = \sum \frac{1}{2m_i} \boldsymbol{p}_i \cdot \boldsymbol{p}_i + V(\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N) \tag{29}$$

which leads to a formally quite unexceptionable Hamiltonian theory. Our agreement to look upon center of mass as an "auxilliary construction" is in fact recommended by Noether's theorem, of which it is a particular implication that—to the extent that we may have interest in *gross translation* of the system; i.e, in maps of the form

$$\boldsymbol{x}_i \longmapsto \boldsymbol{x}_i + \delta\boldsymbol{\omega} \quad : \quad (\text{all } i)$$

—to that extent we have implicit interest in the construct

$$\boldsymbol{P} \equiv \sum m_i \dot{\boldsymbol{x}}_i = M \tfrac{d}{dt}\big\{\boldsymbol{X} + \text{any constant vector}\big\}$$

and that such maps will describe a symmetry of the dynamical action (the "total momentum" $\boldsymbol{P} = \sum \boldsymbol{p}_i$ will, in other words, be a constant of the motion) if and only if

$$V(\boldsymbol{x}_1 + \delta\boldsymbol{\omega}, \boldsymbol{x}_2 + \delta\boldsymbol{\omega}, \ldots, \boldsymbol{x}_N + \delta\boldsymbol{\omega}) = V(\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N)$$

It was that circumstance which led us to write $\boldsymbol{x}_i = \boldsymbol{X} + \boldsymbol{r}_i$, and

$$\begin{aligned} &\downarrow \\ &= U(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N) \end{aligned}$$

when we have wished to emphasize that the system has been isolated: all forces are internal forces, and conform to the 3rd Law; "total momentum" $\boldsymbol{P}$ is conserved. These remarks[11] provide relatively formal grounds on which to base the claim that $\boldsymbol{X}$ and $\boldsymbol{P}$ are "natural constructs," of continuing interest even when $\boldsymbol{P}$ is (owing to the presence of net impressed forces) *not* conserved.

That $\big\{\boldsymbol{X}, \boldsymbol{P}\big\}$ comprise a pair (actually three pairs) of "conjugate variables" in the sense standard to Hamiltonian mechanics is anticipated and not difficult to prove, but discussion of the details forces us to confront and resolve certain fussy notational matters. An N-particle molecule has $3N$ literal degrees of freedom, but I have on occasion found it more natural to employ the phrase "N vectorial degrees of freedom" to say the same thing. The dynamical state of such a system is represented by a point—coordinatized

$$\big\{x_{i\alpha}\,, p_{i\alpha}\big\} \quad : \quad \begin{cases} i = 1, 2, 3, \ldots, N \\ \alpha = 1, 2, 3 \end{cases}$$

—in $6N$-dimensional phase space, but in many contexts I find it more natural to speak of the point

$$\big\{\boldsymbol{x}_i\,, \boldsymbol{p}_i\big\} \quad : \quad i = 1, 2, 3, \ldots, N$$

in a phase space of $2N$ "vectorial dimensions." If an "observable" $A(x, p)$ is assembled in such a way as to reflect the transformation properties of its lumped arguments I find it more natural to write $A(\boldsymbol{x}, \boldsymbol{p})$. The Poisson bracket of a pair of observables can be described

$$[A(x,p), B(x,p)] \equiv \sum_{k=1}^{N} \sum_{\alpha=1}^{3} \left\{ \frac{\partial A}{\partial x_{k\alpha}} \frac{\partial B}{\partial p_{k\alpha}} - \frac{\partial B}{\partial x_{k\alpha}} \frac{\partial A}{\partial p_{k\alpha}} \right\} \tag{30.1}$$

[11] See also CLASSICAL MECHANICS (1983), p. 163.

but when the observables have been assembled from vectors (and not just their individual components) I find it more illuminating to write

$$[A(\boldsymbol{x},\boldsymbol{p}),B(\boldsymbol{x},\boldsymbol{p})]=\sum_{k=1}^{N}\mathrm{tr}\left\{\frac{\partial A}{\partial \boldsymbol{x}_k}\frac{\partial B}{\partial \boldsymbol{p}_k}-\frac{\partial B}{\partial \boldsymbol{x}_k}\frac{\partial A}{\partial \boldsymbol{p}_k}\right\} \tag{30.2}$$

where

$$\frac{\partial A}{\partial \boldsymbol{x}}\frac{\partial B}{\partial \boldsymbol{p}}\equiv 3\times 3 \text{ matrix with elements } \frac{\partial A}{\partial x_\alpha}\frac{\partial B}{\partial p_\beta}$$

accounts for the occurance of the trace. The fundamental brackets

$$\begin{gathered}[x_{i\alpha},x_{j\beta}]=[p_{i\alpha},p_{j\beta}]=0\\ [x_{i\alpha},p_{j\beta}]=\delta_{ij}\delta_{\alpha\beta}\end{gathered}$$

can be recovered as $\alpha\beta$-components of these matrix-valued statements

$$\begin{gathered}[\boldsymbol{x}_i,\boldsymbol{x}_j]=[\boldsymbol{p}_i,\boldsymbol{p}_j]=\mathbb{O}\\ [\boldsymbol{x}_i,\boldsymbol{p}_j]=\delta_{ij}\mathbb{I}\end{gathered}$$

Looking with the aid of the latter to $[\boldsymbol{X},\boldsymbol{P}]$, we have

$$[\boldsymbol{X},\boldsymbol{P}]=[\tfrac{1}{M}\textstyle\sum m_i\boldsymbol{x}_i,\sum\boldsymbol{p}_j]=\ \tfrac{1}{M}\sum m_i\mathbb{I}=\mathbb{I} \tag{31}$$

Were we to take (22) as our point of departure

$$L=\tfrac{1}{2}M\dot{\boldsymbol{X}}\cdot\dot{\boldsymbol{X}}+\tfrac{1}{2}\sum_{i=2}^{N}\mu_i\dot{\boldsymbol{R}}_i\cdot\dot{\boldsymbol{R}}_i-\mathcal{U}(\boldsymbol{R}_2,\ldots,\boldsymbol{R}_N)$$

we would have

$$\left.\begin{aligned}\boldsymbol{P}\ &\equiv\ \frac{\partial L}{\partial\dot{\boldsymbol{X}}}=M\dot{\boldsymbol{X}}\quad &:\quad &\text{momentum conjugate to } \boldsymbol{X}\\ \boldsymbol{P}_i&\equiv\frac{\partial L}{\partial\dot{\boldsymbol{R}}_i}=\mu_i\dot{\boldsymbol{R}}_i\quad &:\quad &\text{momentum conjugate to } \boldsymbol{R}_i\end{aligned}\right\} \tag{32}$$

giving

$$H=\tfrac{1}{2M}\boldsymbol{P}\cdot\boldsymbol{P}+\sum_{i=2}^{N}\tfrac{1}{2\mu_i}\boldsymbol{P}_i\cdot\boldsymbol{P}_i+\mathcal{U}(\boldsymbol{R}_2,\ldots,\boldsymbol{R}_N) \tag{33}$$

The resulting theory is again "formally unexceptionable" and appears, in fact, to be in several applications the "Hamiltonian formalism of choice:" it is encountered standardly in connection with the Kepler problem, and has the property that it yields $\boldsymbol{P}$-conservation not as a statement deduced from the equations of motion, but *as* an equation of motion:

$$\begin{aligned}\dot{\boldsymbol{X}}&=+\frac{\partial H}{\partial\boldsymbol{P}}=\tfrac{1}{M}\boldsymbol{P}\\ \dot{\boldsymbol{P}}&=+\frac{\partial H}{\partial\boldsymbol{X}}=\quad\boldsymbol{0}\end{aligned}$$

The transformation $\{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N\} \rightarrow \{\boldsymbol{X}, \boldsymbol{R}_2, \ldots, \boldsymbol{R}_N\}$—described in particular cases by (18)/(19) and in the general case by equations of the form

$$\boldsymbol{x}_i = \boldsymbol{X} + \sum_{j=2}^{N} C_{ij}\boldsymbol{R}_j \tag{34}$$

—has the character of a "linear point transformation" (linear recoordinatization of $3N$-dimensional configuration space) so the induced linear recoordinatization of of $6N$-dimensional phase space

$$\{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N; \boldsymbol{p}_1, \boldsymbol{p}_2, \ldots, \boldsymbol{p}_N\} \rightarrow \{\boldsymbol{X}, \boldsymbol{R}_2, \ldots, \boldsymbol{R}_N; \boldsymbol{P}, \boldsymbol{P}_2, \ldots, \boldsymbol{P}_N\} \tag{35}$$

is *necessarily canonical*, a linear instance of what are called "extended point transformations."[12]

The preceding remarks, elementary though they are, do serve to bring into focus a seldom-noted circumstance which will, I anticipate, come back to haunt us. The variables which stand on the right side of (35) are (by inversion of (34)) presented to us as functions of the $\boldsymbol{x}$'s and $\boldsymbol{p}$'s that stand on the left; they are, in short, presented to us as "observables," in the mathematical sense of the term. But they are *not "observables" in the laboratory sense*. One cannot "tie a string to the center of mass," neither can one see it; it lives in the world of ideas, and its location is revealed only by analysis of data obtained from other more literally observable sources. Similar remarks pertain to the Jacobean vectors $\boldsymbol{R}_i$ and their conjugates, all of which refer to collective properties of the many-body system. We appear to confront an implied distinction between

- "formal observables," and
- "true observables" (those susceptible to direct physical measurement)

but at present lack means to make the distinction sharp and precise. In quantum mechanics we standardly pretend that every self-adjoint operator A can in principle be associated with a possible "measurement device," but confront now the possibility that (unless one is willing to admit data analysis routines into the definition of "measurement device") such associations may only contingently be possible. "Contingent upon what?" is the embarrassing question.

[12] See CLASSICAL MECHANICS (1983), pp. 250–253 for discussion of where the "necessarily canonical" comes from.