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A NOTE ON THE VOLUME OCCUPIED IN PHASE SPACE BY A SYSTEM OF GRAVITATIONALLY INTERACTING PARTICLES

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ABSTRACT

We comment on the role played by a confining box in the energy dependence of the phase volume, $g(E)$, of a system. This issue is related to the conservation of the total momentum and the position of the center of mass. A curious behavior of $g(E)$ in the case of gravitationally bound binaries is pointed out.

Subject headings: numerical methods — stars: binaries

I. INTRODUCTION

The purpose of this paper is to point out a curious feature in the energy dependence of the phase volume occupied by a binary system (i.e., a system containing two point masses interacting via gravity). It turns out that the energy dependence of the volume occupied in the phase space depends on whether or not we "confine" the system by a box. This feature arises only for the binary system. For N-body systems with $N \geqq 3$, the phase volume always diverges.

We discuss the general formalism (for $N \geqq 3$) in § II and the behavior of binary system in § III.

II. PHASE VOLUME FOR AN N-BODY SYSTEM INTERACTING VIA NEWTONIAN GRAVITY

Consider a system of N particles interacting via some two-body potential $\phi(|\boldsymbol{x}_i - \boldsymbol{x}_j|)$ where $\boldsymbol{x}_j$ denotes the position of the jth particle. The system can be denoted by a point ($\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N; \boldsymbol{p}_1, \ldots, \boldsymbol{p}_N$) in the $6N$-dimensional phase space at any instant of time. As time goes on, the system evolves and the phase point traces out a complicated trajectory in the phase space. We know that a $6N$-dimensional closed system has $6N - 1$ nontrivial constants (see, e.g., Landau and Lifshitz 1976, p. 13). If the solution to the equations of motion are known, then these $6N - 1$ constants can be determined, thereby confining the system to $[6N - (6N - 1)]$-dimensional—that is, one-dimensional—trajectory in the phase space.

In realistic N-body systems, of course, it is impossible to integrate the equations of motion. The only constants of motion which can be written down are those which follow from the symmetries of the Hamiltonian. For a closed system, which is free from any external influence, we expect the following quantities to be conserved: energy (E), total momentum ($\boldsymbol{P}$), angular momentum ($\boldsymbol{J}$), and the vector $\boldsymbol{Q} = (\boldsymbol{R} - \boldsymbol{P}t)$, where $\boldsymbol{R}$ is the position of the center of mass of the system. (Of these, E, $\boldsymbol{P}$, and $\boldsymbol{J}$ can be expressed entirely in terms of $\boldsymbol{x}_i$'s and $\boldsymbol{p}_i$'s, but $\boldsymbol{Q}$, in general, depends on $\boldsymbol{x}_i$, $\boldsymbol{p}_i$ *and on* t. If $\boldsymbol{P}$ is zero, then—and only then—$\boldsymbol{Q}$ is expressible in terms of $\boldsymbol{x}_i$'s alone. In this case $\boldsymbol{Q}$ is just the center of mass.)

The existence of such conserved quantities, in general, "isolate" the trajectory to some region in phase space of dimension $6N - k$, which is lower than $6N$. We will call the volume of this $6N - K$ dimensional surface as the "phase volume" of the system.

If any one of the N particles can escape to infinite distances from the companions, then the phase volume will clearly be divergent. This is what will happen if $E > 0$ ["unbound" system; we use the convention that $\phi(r)$ is zero for $r \to \infty$, and that energy scale is normalized in such a way that negative E indicates bound systems]. Even if $E < 0$, some particles can escape to infinity ("evaporation") if $N \geqq 3$, *and* the potential is unbounded from below. Consider, for example, the case of three particles interacting via gravity with total energy $E = -|E| < 0$. Two of these particles can come together forming a very tight binary with binding energy $B = -|B|$ and release to the third particle the energy $\epsilon = E - B = |B| - |E|$. This ϵ can be positive and arbitrarily large (because in an infinitely deep potential $|B|$ can be arbitrarily large), allowing the third particle to escape to infinity. Thus, for particles interacting via gravity there is "leakage" of particles if (a) $E > 0$ or if (b) $E < 0$ and $N \geqq 3$.

The above facts are quite self-evident and well known. Usually, we prevent the particles from escaping to infinity by enclosing them in a box of volume V. The integrations over each $\boldsymbol{x}_i$ are now confined to the inside of this volume. Such a confining volume is necessary for all N if $E > 0$ and for all $N \geqq 3$ if $E < 0$. (The case $N = 2$ will be considered separately in next section).

The decision to introduce the confining volume, however, affects the existence of the conserved quantities. Mathematically speaking, the confinement by a box is equivalent to putting the particles in an external potential—which is zero inside the box and infinite outside. But once we apply such a (space-dependent) potential, $\boldsymbol{P}$ is not conserved. (Of course, we can make the momentum transfer to the box negligibly small by making the box very massive, etc., but, *in principle*, $\boldsymbol{P}$ is not conserved.) It follows immediately that $\boldsymbol{R} - \boldsymbol{P}t$ is also not conserved.

Another way of looking at the above result is the following: The conservation of momentum follows from the translational invariance of the system. A confining potential (like "walls") breaks this invariance; momentum is no longer conserved.

Similarly, $\boldsymbol{J}$ is also not conserved if the particles are confined. An arbitrarily shaped box potential (in fact, anything other than a spherical box) will break the rotational invariance of the system, and hence $\boldsymbol{J}$ will not be a constant. We can prevent the exchange of angular momentum between the particles and the box by keeping the box spherical. But this is contrary to the basic principle of statistical mechanics that the results should be independent of the *shape* of the confining volume. Therefore, we must consider a generic shape and drop $\boldsymbol{J}$ from our list.

That leaves us with just one conserved quantity: the total energy E. In the phase space, the system evolves on a constant energy surface described by the equation

$$H(\boldsymbol{p}_i, \boldsymbol{x}_i) = E \,, \tag{1}$$

where $H(p, q)$ is the Hamiltonian for the system. This constant energy surface has the volume given by

$$g(E) \equiv \int_{\boldsymbol{x}_i \in V} \prod_{i=1}^{N} d^3\boldsymbol{p}_i d^3\boldsymbol{x}_i \, \delta[E - H(\boldsymbol{p}_i, \boldsymbol{x}_i)] \,. \tag{2}$$

It is sometimes more convenient to work with the "cumulative volume":

$$\Gamma(E) \equiv \int_{\boldsymbol{x}_i \in V} \prod_{i=1}^{N} d^3\boldsymbol{x}_i d^3\boldsymbol{p}_i \, \theta[E - H(\boldsymbol{p}_i, \boldsymbol{x}_i)] \,, \tag{3}$$

where $\theta(x) = 1$ for $x > 0$ and zero otherwise. Clearly, $g(E) = (d\Gamma/dE)$.

In classical statistical mechanics, the logarithm of $g(E)$ or $\Gamma(E)$ will be defined as the entropy of the system. Systems evolve toward states of larger entropy or—equivalently—toward states of larger $g(E)$. The existence of a "equilibrium state" for the system depends on $g(E)$ being finite. For a system, interacting via r^{-1} forces, such an "equilibrium" is not possible. For such a system $\Gamma(E)$ and $g(E)$ diverge for all E if $N \geqq 3$. Most people accept this result as self-evident. Several equivalent versions of this result exist in literature (see, e.g., Tremaine, Henon, and Lynden-Bell 1986, pp. 286–287; Binney and Tremaine 1987, p. 268). However, there are some papers which claim—erraneously, in our opinion—that $g(E)$ is finite (see, e.g., Miller 1973, 1974). It is, therefore, desirable to have an explicit demonstration that $g(E)$ and $\Gamma(E)$ are divergent. (This demonstration will also help us to understand the results of the next section in proper perspective.)

This result can be demonstrated as follows. Consider the $\Gamma(E)$ for the full system of N particles with phase space coordinates $(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N; \boldsymbol{p}_1, \ldots, \boldsymbol{p}_N)$:

$$\Gamma(E) = \int d^3\boldsymbol{p}_1 \ldots d^3\boldsymbol{p}_N d^3\boldsymbol{x}_1 \ldots d^3\boldsymbol{x}_N \times \theta\left(E + \frac{1}{2}\sum_{i,j} \frac{Gm^2}{|\boldsymbol{x}_1 - \boldsymbol{x}_j|} - \sum_i \frac{p_i^2}{2m}\right) . \tag{4}$$

The $\boldsymbol{p}$-integrations give the volume of a sphere in $3N$-dimensions with the radius $[(E + \frac{1}{2} \sum Gm^2/|\boldsymbol{x}_i - \boldsymbol{x}_j|)2m]^{1/2}$. So we get

$$\Gamma(E) = \int d^3\boldsymbol{x}_1 \ldots d^3\boldsymbol{x}_N \left[E + \frac{1}{2}\sum_{i,j} \frac{Gm^2}{|\boldsymbol{x}_i - \boldsymbol{x}_j|}\right]^{3N/2} . \tag{5}$$

We change the variables of integration from $(\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N)$ to $(\boldsymbol{S}, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N)$, where S is defined via the relation: $\boldsymbol{x}_1 = \boldsymbol{x}_2 + \boldsymbol{S}$. Then

$$\Gamma(E) = \int d^3\boldsymbol{S} d^3\boldsymbol{x}_2 \ldots d^3\boldsymbol{x}_N \left[E + \frac{1}{2}\sum_{i,j} \frac{Gm^2}{|\boldsymbol{x}_i - x_j|}\right]^{3N/2} . \tag{6}$$

The phase volume $g(E)$ is obtained by differentiating $\Gamma(E)$. So

$$\begin{aligned} g(E) &= \frac{d\Gamma}{dE} \\ &= \int d^3\boldsymbol{S} d^3\boldsymbol{x}_2 \ldots d^3\boldsymbol{x}_N \left(\frac{3N}{2}\right)\left(E + \frac{1}{2}\sum_{i,j} \frac{Gm^2}{|\boldsymbol{x}_i - \boldsymbol{x}_j|}\right)^{[(3N/2)-1]} \\ &= \int d^3\boldsymbol{x}_2 \ldots d^3\boldsymbol{x}_N \left(\frac{3N}{2}\right) I(\boldsymbol{x}_2 \ldots \boldsymbol{x}_N) \,, \end{aligned} \tag{7}$$

where

$$I(\boldsymbol{x}_2, \ldots, \boldsymbol{x}_N) = \int d^3\boldsymbol{S}\left(E + \frac{Gm^2}{|\boldsymbol{S}|} + \sum_{j=3}^{N} \frac{Gm^2}{|\boldsymbol{S} + \boldsymbol{x}_2 - \boldsymbol{x}_j|} + \frac{1}{2}\sum_{i,j=2}^{N} \frac{Gm^2}{|\boldsymbol{x}_i - \boldsymbol{x}_j|}\right)^{[3N/2-1]} \tag{8}$$

This integral is divergent. Near $\boldsymbol{S} \approx 0$, the leading order behavior of this integral is

$$I \cong \int_0^{\epsilon} S^2 dS\left(\frac{Gm^2}{S}\right)^{[(3N/2)-1} \cong \epsilon^{[4-(3N/2)]} \quad (\epsilon \to 0) \,, \tag{9}$$

which is divergent for all $N \geqq 3$. The reason for this divergence is also obvious from the above analysis: two particles come close to each other ($\boldsymbol{S}$ goes to zero; $\boldsymbol{x}_1 \to \boldsymbol{x}_2$), releasing large amount of potential energy. This potential energy opens up a large volume in momentum space. Clearly divergence of I implies divergence of $g(E)$. This divergence of $g(E)$ is a *momentum-space effect*. It is *not* due to the fact that some particles can reach *spatial* infinity. In fact, the spatial integration in equations (4)–(8) is confined to the interior of a box of radius R. The result is also independent of the sign of E; in particular, it is true even when E is negative ("bound system").

We argued earlier that it is incorrect to impose conservation of $\boldsymbol{P}$ and $\boldsymbol{Q}$ when the system is confined by a box. Let us ignore this fact for a moment and assume that we can impose the constraints $\boldsymbol{P} = 0$, $\boldsymbol{R} = 0$ on the system. The definition of $\Gamma(E)$ will now change to

$$\Gamma(E)_{\text{modified}} = \int \prod_{i=1}^{N} d^3\boldsymbol{x}_i d^3\boldsymbol{P}_i \, \delta(\boldsymbol{R})\delta(\boldsymbol{P})\theta(E - H) \,. \tag{10}$$

This expression is also divergent for $N \geqq 3$! In doing the momentum integral $\delta(\boldsymbol{P})$ will reduce the dimension of the sphere by 3, changing $(3N/2)$ in equation (5) to $(3/2)(N - 1)$; the $\delta(\boldsymbol{R})$ factor replaces $\boldsymbol{x}_N$ by

$$-\sum_{i=1}^{N-1} \boldsymbol{x}_i \,.$$

The exponent in equation (8) is now changed to $[(3/2)(N - 1) - 1]$. Obviously, both $g(E)$ and $\Gamma(E)$ are divergent for $N \geqq 4$; for $N = 4$, $\Gamma(E)$ is still divergent, but $g(E)$ is finite. Thus for large N, the inclusion of $\delta(\boldsymbol{R})$, $\delta(\boldsymbol{P})$ makes no difference. In any case, this issue is purely academic; for all $N \geqq 3$, it is "illegal" to impose $\delta(\boldsymbol{R})\delta(\boldsymbol{P})$ factors because of reasons explained earlier.

III. PHASE VOLUME FOR BINARIES

Lastly, we would like to mention an interesting curiosity regarding the binary system, with $N = 2$. If $N \geqq 3$, then it is *absolutely essential* to keep a box around the system if no particle should escape to infinity and thus make $g(E)$ infinite. But if $N = 2$, we can keep the system bound, even without any box, provided $E < 0$. Thus we have here the option of either employing a box or not. At first one might think that it really does not matter whether we put a box around a binary system (which is already bound) or not. However, it does matter. It matters because, in the absence of the box, we have to take into account the conservation of $\boldsymbol{P}$ and $\boldsymbol{R}$ as well. This changes the results for $\Gamma(E)$ and $g(E)$.

Let us do the calculation. It is convenient to use—instead of $\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{p}_1, \boldsymbol{p}_2$—the position of center of mass: $\boldsymbol{R} = (\boldsymbol{r}_1 + \boldsymbol{r}_2)/2$, the relative separation $\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2$, the total momentum $\boldsymbol{P} = \boldsymbol{p}_1 + \boldsymbol{p}_2$, and the relative momentum $\boldsymbol{p} = \boldsymbol{p}_1 - \boldsymbol{p}_2$ as the coor-

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dinates. Clearly $\boldsymbol{P}$ is conserved, and we will take it to be zero. Hence, $\boldsymbol{R}$ is also conserved and can also be taken to be zero. The volume of the constant energy surface (with $E < 0$) constrained further by $\boldsymbol{R} = 0, \boldsymbol{P} = 0$ is proportional to

$$\Gamma(E) = \int d^3\boldsymbol{P}\, d^3\boldsymbol{R}\, d^3\boldsymbol{p}\, d^3\boldsymbol{r}\, \delta(\boldsymbol{R})\delta(\boldsymbol{P})\theta \times \left(-|E| + \frac{Gm^2}{|\boldsymbol{r}|} - \frac{P^2}{2M} - \frac{p^2}{2\mu}\right), \quad (11)$$

where $M = 2m$ = total mass and μ is the reduced mass ($\frac{1}{2}m$). We get

$$\begin{aligned}\Gamma(E) &= \int d^3\boldsymbol{p}\, d^3\boldsymbol{r}\, \theta\left(-|E| + \frac{Gm^2}{|\boldsymbol{r}|} - \frac{p^2}{2\mu}\right)\\ &= \int_0^{R_{\max}} 4\pi r^2\, dr\, \frac{4\pi}{3}\left[2\mu\left(\frac{Gm^2}{r} - |E|\right)\right]^{3/2}\\ &= \frac{16\pi^2}{3}\int_0^{R_{\max}} r^2\, dr\left[2\mu\left(\frac{Gm^2}{r} - |E|\right)\right]^{3/2}, \quad (12)\end{aligned}$$

where we have performed the $\boldsymbol{p}$-integration obtaining the volume of a sphere. The r-integration should be confined to the range allowed for the bound state, i.e., $0 \leqq r \leqq R_{\max}$, where $R_{\max} = Gm^2/|E|$. Using this fact, $\Gamma(E)$ becomes (with $r/R_{\max} = x$)

$$\begin{aligned}\Gamma(E) &= \frac{16\pi^2}{3}(2\mu|E|)^{3/2}\int_0^{R_{\max}} r^2\, dr\left(\frac{Gm^2}{r|E|} - 1\right)^{3/2}\\ &= \frac{16\pi^2}{3}(2\mu|E|)^{3/2}\left(\frac{Gm^2}{|E|}\right)^3\int_0^1 x^2\, dx\left(\frac{1}{x} - 1\right)^{3/2}\\ &= (\text{constant})|E|^{-3/2}\,. \quad (13)\end{aligned}$$

Note that $\Gamma(E)$ is finite and is proportional to $|E|^{-3/2}$. The $g(E)$ will be

$$g(E) = \frac{d\Gamma}{dE} = (\text{constant})|E|^{-5/2}\,. \quad (14)$$

This is the result we get without the box and is well-known (see, e.g., Lynden-Bell 1969).

When there is a box around the system, we do not have $\delta(R)$, $\delta(\boldsymbol{P})$ factors. $\Gamma(E)$ is given by equation (5) with $E = -|E|$ and $N = 2$:

$$\Gamma(E) = \int d^3\boldsymbol{r}_1\, d^3\boldsymbol{r}_2\left(\frac{Gm^2}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|} - |E|\right)^3. \quad (15)$$

We introduce the variables $\boldsymbol{R} = (\boldsymbol{r}_1 + \boldsymbol{r}_2)/2$ and $\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2$ and note that R-integration is over the volume of the box (V) and r-integral is up to $R_{\max} = Gm^2/|E|$. We get

$$\Gamma(E) = (\text{constant})V\int_0^{R_{\max}} r^2\, dr\left(\frac{Gm^2}{r} - |E|\right)^3. \quad (16)$$

This expression diverges near $r = 0$! In equation (12), because $\boldsymbol{P}$ was conserved, the momentum integration was three-dimensional, giving an index 3/2. But in equation (15) since $\boldsymbol{p}_1$ and $\boldsymbol{p}_2$ are unconstrained, the momentum integration is six-dimensional, giving an index 3.

The last surprise is that, even though $\Gamma(E)$ diverges, $g(E)$ does not! From equation (16) we see that

$$\begin{aligned}g(E) = \frac{d\Gamma}{dE} &= (\text{constant})\int_0^{R_{\max}} r^2\, dr\left(\frac{Gm^2}{r} - |E|\right)^2\\ &= (\text{constant})|E|^2\left(\frac{Gm^2}{|E|}\right)^3\int_0^1 x^2\, dx\left(\frac{1}{x} - 1\right)^2\\ &= (\text{constant})|E|^{-1}\,, \quad (17)\end{aligned}$$

which is perfectly finite. Thus we arrive at the following conclusion: for $N = 2$, $g(E)$ is finite with and without the confining box; without the box it varies as $|E|^{-5/2}$, and with the box it varies as $|E|^{-1}$. The $\Gamma(E)$ is finite without the box (and varies as $|E|^{-3/2}$), while it is divergent (logarithmically) with the box.

This change of $g(E)$ from $|E|^{-5/2}$ to $|E|^{-1}$ can also be interpreted in the following manner. Once we confine the binary by a box, we effectively release the translational degree of freedom of the binary. We will expect this increase in the number of degrees of freedom of the system to be accompanied by an increase in the specific heat by $3/2k$. This is indeed the case, if we define the specific heat to be

$$C_v = \frac{dE}{dT} = T\frac{dS}{dT} = T\frac{d}{dT}[k\ln g(E)]\,, \quad (18)$$

where we have defined $T \equiv dE/dS$. Simple calculation shows that

$$C_v = \begin{cases} -\frac{5}{2}k & (\text{without the box})\,,\\ -k & (\text{with the box})\,.\end{cases} \quad (19)$$

Thus the box has increased the C_v by $(3/2)k$. Note that it is still negative. (I thank the referee for pointing out this interpretation).

There is not much point in doing statistical mechanics with $N = 2$, but the above analysis clarifies the role of $\boldsymbol{P}$, $\boldsymbol{R}$ conservation in a simple setting.

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