Strange Lagrangian systems and statistical mechanics

Liu Zhao
School of Physics, Nankai University, Tianjin 300071, People’s Republic of China
E-mail: lzhao@nankai.edu.cn

Received 6 January 2013, in final form 21 April 2013
Published 7 June 2013
Online at stacks.iop.org/JPhysA/46/265002

Abstract
We consider the canonical ensemble of $N$ particles admitting a strange Hamiltonian description. Each of the particles obeys a set of Newtonian equations of motion, which can also be described by standard canonical Hamiltonian mechanics. However, the thermodynamics corresponding to the strange description and canonical description differ drastically from each other. In other words, the strange description and the standard canonical description are inequivalent on the level of thermodynamics.

PACS numbers: 05.20.−y, 05.90.+m, 45.20.−d, 45.20.Jj

1. Introduction

The canonical ensemble in statistical mechanics is deeply rooted in Hamiltonian mechanics. The intimate relationship between statistical mechanics and Hamiltonian mechanics is best illustrated in the definition of the canonical partition function

$$P = Z^N = \left( \frac{1}{\hbar} \int e^{-\beta H} d\Omega \right)^N,$$

where $\beta = 1/kT$ as usual, $N$ is the number of degrees of freedom in the system and $H$ and $d\Omega$ are respectively the Hamiltonian and the symplectic volume element for a single degree of freedom in the system. It is evident that the partition function is invariant under the symplectic group of transformations on the phase space of the underlying Hamiltonian system.

Nowadays it is well known that one can often associate many different Hamiltonian descriptions to the same set of Hamiltonian equations of motion. Under some mild assumptions, it was argued in [1] that different Hamiltonian descriptions give rise to the same canonical partition function in statistical mechanics, yielding the same set of thermodynamical quantities. This novel invariance is beyond the standard symplectic invariance which maintains the Hamiltonian structure, so it seems worth paying some extra attention to it. In particular, it is tempting to ask what happens when the assumptions used in [1] are violated.

Note that, for systems possessing multiple Hamiltonian descriptions, there have been debates in the literature as to the proper choice of Hamiltonian functions. Some insist that the
physical Hamiltonian must be decomposable into kinetic and potential energy parts. However, as far as the equations of motion are concerned, we do not seem be able to justify which description is superior over the others. This indistinguishability between different Hamiltonian descriptions is lifted up by the work of [1] to the level of statistical mechanics.

On the other hand, it has only recently become clear that, for special kinds of mechanical systems, there are choices of Hamiltonian structures in which certain fundamental aspects of classical canonical Hamiltonian mechanics are changed. In [2], Shapere and Wilczek found some Lagrangian systems for which the Hamiltonian become multivalued in terms of the canonical phase space variables. A direct consequence of this multivaluedness is that the time translation symmetry is spontaneously broken in the ground states, even though the Hamiltonian itself is conserved. For an ensemble of such mechanical systems, the canonical partition function as given in (1) is ill defined, because $H$ and $d\Omega$ are not well defined simultaneously. However, as explored in [3, 4], one can change the phase space variables which makes the Hamiltonian and symplectic structures on the phase space simultaneously well defined at the price of introducing a non-canonical symplectic structure. It is interesting to consider whether the corresponding statistical ensemble can be properly defined. Notice that the systems studied in [2–4] belong exactly to the class of models for which the assumptions made in [1] are violated. So, the study of statistical ensembles, consisting of particles as described in [2–4], will enable us to see the consequence of violating the assumptions of [1]. Moreover, if the statistical ensemble for such strange mechanical systems turns out to possess some novel features when compared to the standard canonical ensembles, it will provide us with an experimentally testable—at least in principle—effect for the spontaneous breaking of time translation symmetry, in which great interest is only just emerging [5–10].

2. Strange description of Newtonian particles

To facilitate the discussions to be made below, let us first briefly review the assumptions of [1] based on which the invariance of the partition function (1) with respect to different choices of Hamiltonian structures was proven. Consider a one dimensional Hamiltonian system $\mathcal{H} = \mathcal{H}(p, q)$ with the standard symplectic structure given in terms of the canonical symplectic form $d\Omega = dq \wedge dp$. It is easy to see that a change of Hamiltonian

$$\mathcal{H} \rightarrow \mathcal{H}' = F(\mathcal{H})$$

(2)

together with a change of symplectic structure

$$d\Omega \rightarrow d\Omega' = F'(\mathcal{H}) \, dq \wedge dp$$

(3)

would yield the same set of Hamiltonian equations of motion. The claim of [1] is that, provided $F'(\mathcal{H}) > 0$ on the whole phase space, the above change of Hamiltonian structures will not change the partition function $Z$, and hence all thermodynamic quantities will remain unchanged. As remarked in [1], an important consequence of the condition $F'(\mathcal{H}) > 0$ is that the number of critical points for the Hamiltonian is kept unchanged. In fact, the condition $F'(\mathcal{H}) > 0$ implies more than that. It guarantees that the critical points of the new Hamiltonian are images of those of the original Hamiltonian.

Now consider the following Lagrangian system,

$$\mathcal{L} = \beta_0 \left( \frac{1}{12} m^2 \dot{x}^4 + mU \dot{x}^2 - U^2 \right),$$

(4)
where $\beta_0 > 0$ is a constant which has dimension $[E]^{-1}$ and $U = U(x)$ is a smooth function of $x = x(t)$. This is the special case of $f = m^2/12$ of the $fg\hbar$ model studied in [2]. Naively, the canonical momentum associated with $x$ can be introduced as

$$ p = \frac{\partial L}{\partial \dot{x}} = \beta_0 \left( \frac{1}{3}m^2 \dot{x}^3 + 2mU \dot{x} \right). \tag{5} $$

It is clear that in regions for which $U(x)$ becomes negative, $\dot{x}$ is multivalued in $p$, rendering the Hamiltonian

$$ \mathcal{H} \equiv p\dot{x} - L \tag{6} $$

also multivalued in $p$. Notice that for the Lagrangian (4),

$$ \frac{\partial^2 L}{\partial \dot{x}^2} = \beta_0(m^2 \dot{x}^2 + 2mU(x)), \tag{7} $$

the existence of regions for which $U(x)$ becomes negative implies that $\frac{\partial^2 L}{\partial \dot{x}^2}$ has zeros. Such Lagrangian systems are called singular systems in the literature.

In fact, singular Lagrangian systems can be subdivided into different types. Let $L(q^i, \dot{q}^i)$ be a generic Lagrangian involving generalized coordinates $\{q^i, i = 1, \ldots, n\}$ and generalized velocities $\{\dot{q}^i, i = 1, \ldots, n\}$. Define $\text{Hess}(L) = \det \left( \frac{\partial^2 L}{\partial \dot{q} \partial \dot{q}} \right)$. If $\text{Hess}(L)$ does not have any zeros on the space of states, the system is called regular. If, instead, $\text{Hess}(L) = 0$ everywhere on the space of states, the system is called globally singular, or simply singular. If $\text{Hess}(L) = 0$ only on some proper subset on the space of states, the system is called locally singular, or strange, and the solution to the condition $\text{Hess}(L) = 0$ will be referred to as the strange locus.

According to the above definition, the Lagrangian (4) is strange provided $U \leq 0$. Note that the strange locus for the case with $U = 0$ is different from that for the cases with $U < 0$: in the former case the strange locus consists only of points with $\dot{x} = 0$, while in the latter case the strange locus corresponds to $\dot{x} = \pm \sqrt{-\frac{2U(x)}{m}}$, i.e. the particle can have nontrivial motion along the strange locus.

Let us have a more careful look at the strange system (4) with $U < 0$. For this system, although one can still define the canonical symplectic structure $d\Omega = dx \wedge dp$, the Hamiltonian is not well defined in terms of the canonical variables $(x, p)$. Consequently, the partition function $Z$ associated with the above system seems to be not well defined. However, as was shown in [3, 4], there exists a natural Hamiltonian description for the Lagrangian system (4). The clue is to change from the canonical phase space variables to the set $(x, v)$ (here $v = \dot{x}$) of non-canonical variables. In terms of these, the Hamiltonian (6) is well defined,

$$ \mathcal{H} = \beta_0 \left( \frac{1}{2}mv^2 + U(x) \right)^2, \tag{8} $$

and the associated Poisson structure reads

$$ \{x, v\} = \frac{1}{2m\beta_0} \left( \frac{1}{2mv^2 + U(x)} \right), \quad \{x, x\} = \{v, v\} = 0. $$

1 Notice that when $\frac{1}{2}mv^2 + U(x) = 0$, the Poisson structure becomes singular. However, such singularities will not affect the usefulness of the Poisson structure, because the time evolutions of $x$ and $v$ evaluated using the Poisson structure are never singular. In particular, the evolution equations are satisfied even at the singularities of the Poisson brackets.
Therefore, at least formally, we can make use of the definition (1) to construct a partition function for the ensemble of \( N \) particles governed by the strange Lagrangian (4). The required symplectic form \( d\Omega \) is given by the inverse of the Poisson structure\(^2\)

\[
d\Omega = 2m\beta_0 \left( \frac{1}{2} mv^2 + U(x) \right) dx \wedge dv.
\]

Note that the unusual coefficient in front of \( dx \wedge dv \) in (9) can also be understood as the Jacobian arising from the change of integration variable \( dp \rightarrow dv \).

Interestingly, the Hamiltonian equations of motion in this alternative description are identical to those of a canonical Newtonian particle, i.e.

\[
\dot{x} = v, \quad m\dot{v} = -\frac{dU}{dx}.
\]

So, the same set of equations of motion can also be obtained from the standard canonical Hamiltonian structure (here \( \tilde{p} = mv \))

\[
H_1 = \frac{\tilde{p}^2}{2m} + U(x),
\]

\[
\{x, \tilde{p}\}_1 = 1, \quad \{x, x\}_1 = \{\tilde{p}, \tilde{p}\}_1 = 0,
\]

\[
d\Omega_1 = dx \wedge d\tilde{p}.
\]

The two Hamiltonian descriptions \((H_1, \{\cdot, \cdot\}_1)\) and \((H, \{\cdot, \cdot\})\) for the same set (10) of equations of motion will henceforth be referred to as the first and second Hamiltonian descriptions. Note that the two Hamiltonian descriptions also hold in the case \(U = 0\). What makes the \(U = 0\) case exceptional lies in the fact that, for \(U = 0\), \(\dot{x}\) is actually single-valued in \(p\), so \(H\) is also single-valued and well defined in \((x, p)\). Consequently we can associate with the Hamiltonian

\[
\dot{\tilde{p}} = \{p, H\}_1 = 0
\]

the standard canonical Poisson bracket

\[
\{x, \tilde{p}\}_1 = 1
\]

\[(14)\]

to make a Hamiltonian description \((H, \{\cdot, \cdot\}_1)\) of the system. We have

\[
\dot{x} = \{x, H\}_1 = \left( \frac{3p}{\beta_0 m^2} \right)^{1/3},
\]

\[
\dot{\tilde{p}} = \{p, H\}_1 = 0.
\]

The first of these two equations gives the definition of \(p\) in terms of \(\dot{x}\); the second reproduces the constancy of \(p\). This third Hamiltonian description for the \(U = 0\) case is actually not independent of the previous two descriptions. Writing \(v = \dot{x}\), it can be inferred from (5) (by inserting \(U = 0\)) that \(p = \frac{1}{3} \beta_0 m^2 v^3\). Combining this and (14), we have

\[
\{x, v\}_1 = \frac{1}{\beta_0 m^2 v^2} = \{x, v\},
\]

\[(15)\]

where \(\{x, v\}\) is the Poisson bracket in the second Hamiltonian description. So the third Hamiltonian description for the case \(U = 0\) is actually identical to the second one and we are left with only two independent Hamiltonian descriptions even for the \(U = 0\) case.

\(\text{footnote}^2\) The singularities in the Poisson structure correspond to zeros of the integration measure \(d\Omega\). In [1], the integrations in the partition function are performed under the condition that the critical points of the Hamiltonian are excluded. In our case, the singularities correspond exactly to the critical points of the Hamiltonian (6). Since the integration measure becomes null at the critical points, their contribution to the integration is automatically excluded.
3. Strange statistical ensemble

In this section, we shall consider the statistical ensemble consisting of $N$ particles obeying the Newtonian equations of motion (10). For ease of computation, let us consider the simplest choice $U(x) = -U_0 \leq 0$. The choice $U \leq 0$ is intentional, because only in this case is the original Lagrangian (4) strange.

The partition functions under the first and second Hamiltonian descriptions are given respectively as

$$P_1 = (Z_1)^N, \quad Z_1 = \frac{1}{\hbar} \int e^{-\beta H_1} d\Omega_1,$$

$$P_2 = (Z_2)^N, \quad Z_2 = \frac{1}{\hbar} \int e^{-\beta H} d\Omega.$$  \hfill (16)

$$P_2 = (Z_2)^N, \quad Z_2 = \frac{1}{\hbar} \int e^{-\beta H} d\Omega.$$  \hfill (17)

It is evident that the integrations in both (16) and (17) are well defined. What remains intact is whether these two integrations give rise to the same result.

Before proceeding, let us remark that for constant potential $U(x) = -U_0$, although the two Hamiltonian descriptions appear to be very different, the associated Hamiltonian vector fields are actually the same. The canonical Hamiltonian vector field $\Gamma_1$ is given by

$$\Gamma_1 = \frac{\hat{p}}{m} \frac{\partial}{\partial x},$$

which, combined with the canonical symplectic form $d\Omega_1$, gives

$$dH_1 = \langle d\Omega_1, \Gamma_1 \rangle = \frac{\hat{p}}{m} d\hat{p}.$$  

For the non-canonical description, the Hamiltonian vector field is

$$\Gamma = v \frac{\partial}{\partial q},$$

which yields

$$d\mathcal{H} = \langle d\Omega, \Gamma \rangle = 2m\beta_0 \left( \frac{1}{2}mv^2 + U \right) v dv.$$  

Considering the canonical Hamiltonian equations of motion, we can change $\hat{p}$ into $mv$, then it is clear that

$$\Gamma_1 = \Gamma,$$

i.e. the very same $\Gamma_1$ is also the Hamiltonian vector field in the non-canonical description. That the Hamiltonian vector fields remain the same in different Hamiltonian descriptions is a key ingredient in [1] while proving the invariance of partition functions under different Hamiltonian descriptions.

Since the integrands do not depend on $x$, the two integrations in (16) and (17) can be easily evaluated. Assuming $x \in [\frac{-L}{2}, \frac{L}{2}]$, we have

$$Z_1 = \frac{L}{\hbar} \left( \frac{2\pi m}{\beta} \right)^{1/2} e^{\beta U_0}, \quad U_0 \geq 0.$$  \hfill (18)

Also, for (17), we have

$$Z_2|_{U_0>0} = \frac{L}{\hbar} \left( \frac{m}{2} \right)^{1/2} \pi U_0^{3/2} e^{-z} \left( -I_{-1/4}(z) - I_{1/4}(z) + I_{3/4}(z) + I_{5/4}(z) + \frac{1}{2z} I_{1/4}(z) \right).$$  \hfill (19)
for $U_0 > 0$, where $z = \frac{1}{2} (\beta \beta_0) U_0^2$, $J_0(z)$ is the well known modified Bessel function of the first kind, which is always real valued for positive argument $z$. If $U_0 = 0$, the result is much simpler,

$$Z_2|_{U_0=0} = (2m)^{1/2} \Gamma \left( \frac{3}{4} \right) (\beta_0 \beta)^{-3/4}.$$  

(20)

It becomes clear that the partition functions in the two different Hamiltonian descriptions are very different.

4. Why the difference occurs

We have seen in the previous section that the statement ‘the partition function is insensitive to the form of the Hamiltonian as long as the equations of motion remain the same’, quoted from [1], becomes invalid in our example system involving a strange Lagrangian description. It is natural to ask whether this is a consequence of violating the prerequisites of the arguments of [1] or whether we have done something wrong in the construction.

Let us point out that the two descriptions presented in the last section do fit well in the form (2) and (3). Indeed, if we substitute $\beta = m \beta_0$ in (11), then it follows immediately that

$$H = \beta_0 (H_1)^2,$$

(21)

and the symplectic volume element $d\Omega$ as given in (9) is indeed related to $d\Omega_1$ via (3).

What makes the relationship (21) different from the framework of [1] is that the condition $F'(H_1) > 0$ is violated, because in this case, we have $F'(H_1) = 2 \beta_0 H_1$, whose range is $[-2 \beta_0 U_0, \infty)$. Consequently, the number of critical points for the Hamiltonian is changed drastically before and after the change (21) of Hamiltonian descriptions, and most of the critical points of $H$ are not the images of the critical point of $H_1$. In fact, violation of the condition $F'(H_1) > 0$ can happen not only to the quadratic map (21). Any choice of new Hamiltonian which is an even function of the original one will have the same effect, as long as the original Hamiltonian $H_1$ can take negative values in some region in the phase space. Whenever $F'(H_1)$ can have zeros, it would yield an algebraic equation for $H_1$, whose solution in terms of $v = \dot{x}$ will be nonzero in general. In such cases, the time translation symmetry in the ground state of $H = F(H_1)$ will be spontaneously broken.

Careful readers might have already noticed something unusual when the partition function $Z_2$ was evaluated. Indeed, putting in appropriate numeric values for each parameters, a negative value for $Z_2$ can arise from (19). Since the partition function is usually interpreted as the sum of (un-normalized) probability densities corresponding to each micro state in the phase space, a negative result seems difficult to understand. However, we argue that negativity of $Z_2$ can be clearly understood if we take into account the fact that the momentum (5) is nonlinear in the generalized velocity $v$. Inserting $U(x) = -U_0$ into (5), we can see that there are two local extrema of $p$ at $v = v_{\pm} = \pm \sqrt{2U_0/m}$. For $v \in (v_-, v_+)$, $p$ decreases as $v$ increases, therefore, $dp$ and $dv$ will have opposite signs in this region. Moreover, when $v \in (v_-, v_+)$, the value of the Hamiltonian (6) is relatively small, yielding bigger Boltzmann weights $e^{-\beta H}$. When $v$ is beyond the above interval, the value of the Hamiltonian is relatively large, giving rise to smaller Boltzmann weights. Summing over all possible values of $v$, the partition function becomes negative. Let us stress that the negativity of the partition function does not imply that the probability density becomes negative. It just reflects the fact that the symplectic volume element can become negative in the strange description. At this point, please also note that the path integral quantization for systems governed by a strange Lagrangian [11] will also suffer from the same problem of negative measure. Nonetheless, the corresponding path integral is considered to be physically well established.
5. Conclusions

We have considered through a concrete example the construction of the canonical ensemble consisting of $N$ particles admitting a strange Hamiltonian description. It turns out that the partition function and hence the thermodynamic quantities in the strange description differ drastically from their counterparts in the usual canonical Hamiltonian description. A violation of the condition $F'(H_1) > 0$ is identified as the reason for such differences.

Since there is emerging interest in strange systems admitting a spontaneous breaking of time translation symmetry, it is important to ask what will be the experimentally falsifiable criterion for the occurrence of time translation symmetry breaking. In [2], the perpetual motion in the ground state was considered as the signature of the spontaneous breaking of time translation symmetry. However, this statement depends on the choice of a specific Hamiltonian description, because the ground states for the two Hamiltonians do not correspond to each other. The perpetual moving states may be mapped to states with higher energies than the ground state by a change of Hamiltonian (e.g. mapping from $\mathcal{H}$ to $\mathcal{H}_1$ in the present context), thus eliminating the breaking of time translation symmetry. So, one cannot conclude that time translation symmetry is spontaneously broken by simply observing states which undergo perpetual motion—a physical mechanism which determines the preferred choice of the Hamiltonian must also be involved. The research conducted in the present work suggests that one may look at the thermodynamic behavior of the ensemble of strange systems. If one observes thermodynamic behaviors which differ drastically from the predictions of standard canonical ensembles, then this observation might be used as a guide for choosing a physical Hamiltonian description. In other words, the strange description and the standard canonical description are inequivalent on the level of thermodynamics.

Acknowledgments

This work is supported by the National Natural Science Foundation of China (NSFC) through grant no. 10875059. The author would like to thank X-H Meng for useful discussions.

References

[1] Ercolessi E, Marmo G and Morandi G 2002 Alternative Hamiltonian descriptions and statistical mechanics Int. J. Mod. Phys. A 17 20 (arXiv:quant-ph/0107116)
[2] Shapere A and Wilczek F 2012 Classical time crystals arXiv:1202.2537
[3] Zhao L, Yu P-F and Xu W 2012 Hamiltonian description of singular Lagrangian systems with spontaneously broken time translation symmetry arXiv:1206.2985
[4] Zhao L, Xu W and Yu P-F 2012 Landau meets Newton: time translation symmetry breaking in classical mechanics arXiv:1208.5974
[5] Chernodub M N 2012 Permanently rotating devices: extracting rotation from quantum vacuum fluctuations? arXiv:1203.6588
[6] Gong Z-X, Yin Z-Q, Quan H T, Yin X, Zhang P, Duan L M and Zhang X 2012 Space-time crystals of trapped ions Phys. Rev. Lett. 109 163001 (arXiv:1206.4772)
[7] Shapere A and Wilczek F 2012 Branched quantization arXiv:1207.2677
[8] Shapere A, Wilczek F and Xiong Z 2012 Models of topology change arXiv:1210.3545
[9] Chernodub M N 2012 Rotating Casimir systems: magnetic-field-enhanced perpetual motion, possible realization in doped nanotubes, and laws of thermodynamics arXiv:1207.3052
[10] Ghosh S 2012 Emergent discrete space in a generic Lifshitz model arXiv:1208.4438
[11] Henneaux M, Teitelboim C and Zanelli J 1987 Quantum mechanics for multivalued Hamiltonians Phys. Rev. A 36 4417