Casimir companion: An invariant of motion for Hamiltonian systems

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In this paper an invariant of motion for Hamiltonian systems is introduced: the Casimir companion. For systems with simple dynamical algebras (e.g., coupled spins, harmonic oscillators) our invariant is useful in problems that consider adiabatically varying the parameters in the Hamiltonian. In particular, it has proved useful in optimal control of changes in these parameters. The Casimir companion also allows simple calculation of the entropy of nonequilibrium ensembles.

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I. INTRODUCTION

Classical mechanics as well as quantum mechanics has to solve equations of motion. Finding invariants simplifies these equations. A useful tool to find these invariants is the theory of Lie algebras. Given the Lie algebra associated to the equations of motion, straightforward invariants exist. These so-called Casimir invariants are familiar from quantum treatments of angular momentum.

The Casimir operator was introduced by Hendrik Casimir in 1931 [1]. It is a distinguished element of the enveloping algebra of a Lie algebra that commutes with every element of the algebra. This feature makes it a constant of the motion for any problem having the symmetry of the Lie algebra.

Recent work on the optimal control of quantum systems with low dimensional dynamical algebras [2–14] has turned up a closely related invariant which we here dub the Casimir companion X [15–18]. It appears to be as useful for these problems as the Casimir operator is for problems with traditional, static symmetries. X is calculated using the formula for the Casimir operator but inserting expectation values instead of operators.

In the optimal control problems mentioned above [15,16], the constancy of X reduces the dimension of the problem from 3 to 2—a feature which greatly simplifies the optimal control and facilitates its understanding and interpretation [17,18].

A Hamiltonian problem with Hamiltonian $\mathcal{H}$ is said to have a *dynamical algebra* [19] provided $\mathcal{H}$ can be expressed as a linear combination of elements of the Lie algebra,

$$\mathcal{H} = \sum_{i=1}^{N} h^i(t)\mathcal{B}_i. \tag{1}$$

It then follows that the dynamics of (say) the energy can be reduced to the dynamics of a basis for the algebra and this latter dynamics follows from the commutation relations

$$[\mathcal{B}_i,\mathcal{B}_j] = \sum_{k=1}^{N} c_{ij}{}^k\mathcal{B}_k, \tag{2}$$

defining the algebra.

Optimal control involving only the expectation values of (say) the energy are nicely handled in the Heisenberg representation. The dynamics of any operator $\mathcal{A}$ are then

$$\frac{d\mathcal{A}}{dt} = \frac{i}{\hbar}[\mathcal{H},\mathcal{A}] + \frac{\partial\mathcal{A}}{\partial t}. \tag{3}$$

Taking the trace with the (constant) density matrix leads to ordinary differential equations for the expectation value of $\mathcal{A}$. To describe the dynamics of any operator expressible in terms of the Lie algebra, the required number of coupled differential equations is just the dimension of the algebra. The invariance of the Casimir companion X for these problems reduces the dimension by 1. Furthermore the value of X is related to the entropy and the energy of the system in a way that allows us to express the von Neumann entropy for nonequilibrium states in terms of X.

II. THE CASIMIR COMPANION

Consider a system which is describable by a finite set of operators $\{\mathcal{B}_i\}_{i=1}^N$ forming a closed Lie algebra and where the Hamiltonian is a linear combination of these operators. The equations of motion,

$$\frac{d\mathcal{B}_j}{dt} = \sum_k \gamma_j{}^k(t)\mathcal{B}_k, \tag{4}$$

are easily seen to be closed under this Lie algebra, provided the basis $\{\mathcal{B}_i\}_{i=1}^N$ is not explicitly time dependent. Note that this applies even when parameters in the Hamiltonian are varied. The not explicit time dependence in the basis is not real a restriction because one can always transform the time dependence from the basis to the coefficients, leading to a time-dependent system matrix $\gamma_j{}^k(t)$ and vice versa. This matrix can be calculated directly, knowing the time-dependent coefficients $h^i(t)$ of the linear expansion in Eq. (1) and the time-independent structure constants $c_{ij}{}^k$ of the Lie algebra.

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From Eqs. (3) and (4) we get

$$\gamma_j{}^k(t) = \sum_{i=1}^{N} \frac{i}{\hbar} h^i(t) c_{ij}{}^k. \quad (5)$$

The metric g of the algebra can be calculated directly from the structure constants:

$$g_{ik} = \sum_{m,n=1}^{N} c_{in}{}^m c_{km}{}^n. \quad (6)$$

Now the Casimir invariant $\mathfrak{C}$ [20] is completely determined,

$$\mathfrak{C} = \sum_{i,k=1}^{N} g^{ik} \mathcal{B}_k \mathcal{B}_i, \quad (7)$$

with $g^{ik} = [g^{-1}]_{ki}$. In addition a second dimensionless invariant, the Casimir companion X, naturally exists:

$$X = \sum_{i,k=1}^{N} g^{ik} \langle \mathcal{B}_k \rangle \langle \mathcal{B}_i \rangle. \quad (8)$$

Because of the linearity of Eq. (4), the expectation values $B_i = \langle \mathcal{B}_i \rangle$ evolve according to the same equations of motion as the operators $\mathcal{B}_i$. The invariance of X follows,

$$\begin{aligned} \dot{X} &= \sum_{i,k=1}^{N} g^{ik} (\langle \dot{\mathcal{B}}_k \rangle \langle \mathcal{B}_i \rangle + \langle \mathcal{B}_k \rangle \langle \dot{\mathcal{B}}_i \rangle) \\ &= \sum_{i,k=1}^{N} 2 g^{ik} \langle \dot{\mathcal{B}}_k \rangle \langle \mathcal{B}_i \rangle = \sum_{k,n,s=1}^{N} \frac{2i}{\hbar} h^n(t) c_{nk}{}^s \langle \mathcal{B}_s \rangle \langle \mathcal{B}^k \rangle \\ &= \sum_{k,n,m=1}^{N} \frac{2i}{\hbar} h^n(t) c_{nkm} \langle \mathcal{B}^m \rangle \langle \mathcal{B}^k \rangle \\ &= \sum_{k,n,m=1}^{N} \frac{i}{\hbar} h^n(t) \langle \mathcal{B}^m \rangle \langle \mathcal{B}^k \rangle (c_{nkm} + c_{nmk}) = 0, \end{aligned} \quad (9)$$

where we have used the symmetry of the metric, the antisymmetry of the structure constants, and the Jacobi identity. The two invariants $\langle \mathfrak{C} \rangle$ and X are connected by the system's covariance matrix,

$$X = \langle \mathfrak{C} \rangle - \sum_{i,k=1}^{N} g^{ik} \mathrm{Cov}(\mathcal{B}_k, \mathcal{B}_i), \quad (10)$$

with

$$\mathrm{Cov}(\mathcal{B}_i, \mathcal{B}_j) = \tfrac{1}{2} \langle \mathcal{B}_i \mathcal{B}_j + \mathcal{B}_j \mathcal{B}_i \rangle - \langle \mathcal{B}_i \rangle \langle \mathcal{B}_j \rangle. \quad (11)$$

As we shall see from the examples below, for equilibrium states this new invariant X reduces to the energy of the system up to a rescaling factor. Away from equilibrium it measures the stored but marked-for-loss portion of the energy that has accumulated due to quantum friction [21–23]. This energy will thermalize if the system is placed in contact with any thermal reservoir [24]. Before such contact, the right control could recoup this energy. In fact the optimal control solutions found with the aid of X [16–18] require temporary storage and retrieval of energy in such frictional modes, thereby achieving so-called shortcuts to adiabaticity [8–16].

III. EXAMPLE 1: QUANTUM HARMONIC OSCILLATOR

The oscillator evolves according to the Hamiltonian

$$\mathcal{H} = \frac{\mathcal{P}^2}{2m} + \frac{m}{2} \omega(t)^2 \mathcal{Q}^2, \quad (12)$$

where $\mathcal{P}$, $\mathcal{Q}$, m, and $\omega(t)$ are the momentum, position operators, mass of the particle, and frequency of the oscillator, respectively. Adding the operators $\mathcal{L}$ and $\mathcal{C}$ closes the finite Lie algebra induced by $\mathcal{H}$,

$$\mathcal{L} = \frac{\mathcal{P}^2}{2m} - \frac{m}{2} \omega(t)^2 \mathcal{Q}^2 \quad (13)$$

$$\mathcal{C} = \frac{\omega(t)}{2} (\mathcal{Q}\mathcal{P} + \mathcal{P}\mathcal{Q}). \quad (14)$$

Using the commutation relations (from here on $\hbar = 1$ for the rest of the paper)

$$[\mathcal{H},\mathcal{L}] = -i2\omega\mathcal{C} \quad [\mathcal{L},\mathcal{C}] = i2\omega\mathcal{H} \quad [\mathcal{C},\mathcal{H}] = -i2\omega\mathcal{L}, \quad (15)$$

the metric reads

$$[g_{ik}] = 8\,\omega(t)^2 \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \quad (16)$$

This metric is explicitly time dependent, because of the explicitly time-dependent basis $\{\mathcal{H},\mathcal{L},\mathcal{C}\}$. As remarked above, one could transform this basis into a static one, e.g., $\{\mathcal{Q}^2, \mathcal{P}^2, (\mathcal{Q}\mathcal{P} + \mathcal{P}\mathcal{Q})/2\}$. Using Eq. (8) with $E = \langle \mathcal{H} \rangle$, $L = \langle \mathcal{L} \rangle$, and $C = \langle \mathcal{C} \rangle$, the Casimir companion is

$$X = \frac{\langle \mathcal{H} \rangle^2 - \langle \mathcal{L} \rangle^2 - \langle \mathcal{C} \rangle^2}{8\,\omega^2} = \frac{E^2 - L^2 - C^2}{8\,\omega^2}. \quad (17)$$

At fixed ω, the equilibrated state satisfies $\langle \mathcal{L} \rangle = \langle \mathcal{C} \rangle = 0$ [15,25] and $\langle \mathcal{H} \rangle$ achieves its minimum value $\langle \mathcal{H} \rangle_{\text{eq.}}$. For this state, X becomes a scaled minimum energy:

$$X = \frac{\langle \mathcal{H} \rangle_{\text{eq.}}^2}{8\,\omega^2}. \quad (18)$$

All other states reachable with the dynamics have a higher rescaled energy albeit they have the same von Neumann entropy which is a function only of X [15].

The identity (10) and (11) after multiplying through by $8\omega^2$ becomes

$$(\langle \mathcal{H}^2 \rangle - \langle \mathcal{L}^2 \rangle - \langle \mathcal{C}^2 \rangle) - (\langle \mathcal{H} \rangle^2 - \langle \mathcal{L} \rangle^2 - \langle \mathcal{C} \rangle^2) \quad (19)$$

$$= \mathrm{Var}(\mathcal{H}) - \mathrm{Var}(\mathcal{L}) - \mathrm{Var}(\mathcal{C}). \quad (20)$$

IV. EXAMPLE 2: SPIN IN MAGNETIC FIELD

The second example is a spin with its angular momentum operators $\mathcal{S}_\alpha$, where α is the x, y, or z direction. In this case the Hamiltonian of one spin reads

$$\mathcal{H} = J\mathcal{S}_x + \omega(t)\mathcal{S}_z, \quad (21)$$

where J describes a constant external magnetic field in the x direction and $\omega(t)$ its controllable part in z direction. In the same algorithmic way as it was done for the parametric harmonic oscillator, the operators $\mathcal{L}$ and $\mathcal{C}$ are

$$\mathcal{L} = \omega(t)\mathcal{S}_x - J\mathcal{S}_z, \tag{22}$$

$$\mathcal{C} = \sqrt{\omega(t)^2 + J^2}\mathcal{S}_y, \tag{23}$$

which close the Lie algebra. Using the familiar commutation relation of angular momentum operators $[\mathcal{S}_x,\mathcal{S}_y] = i\hbar\mathcal{S}_z$ (and cyclic permutations), the time-dependent metric of the algebra is

$$[g_{ik}] = \frac{\omega(t)^2 + J^2}{2}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{24}$$

Thus, the resulting Casimir companion reads

$$X = 2\frac{\langle\mathcal{H}\rangle^2 + \langle\mathcal{L}\rangle^2 + \langle\mathcal{C}\rangle^2}{\omega(t)^2 + J^2}, \tag{25}$$

and again X can be considered as a scaled minimum energy. Again the von Neumann entropy is a function only of X.

V. NONEQUILIBRIUM ENTROPY

Usually in the control problems mentioned above the initial state is a thermal equilibrium state, i.e., the density operator is $\rho_{\rm eq} = \exp[-\beta\mathcal{H}(\omega)]$. Starting from such a state a time-dependent $\omega(t)$ will excite L-C oscillations through a mechanism that has been dubbed quantum friction [21–23]. The density operator then describes generalized canonical states $\rho_{\rm g}(t)$—now in the Schrödinger picture—which apart from their dependence on $\mathcal{H}$ will also depend on $\mathcal{L}$ and $\mathcal{C}$.

Once these oscillations have been excited, the von Neumann entropy and the energy entropy [15] are no longer equal. The energy entropy is always higher and has the value the von Neumann entropy of the system would have if the extra energy stored in the L-C oscillations were dissipated to thermal energy. This is in fact what happens if thermal contact with another system is allowed.

A direct calculation of the von Neumann entropy via $S_{\rm vN} = {\rm tr}(\rho_{\rm g}\log\rho_{\rm g})$ is quite complicated and can be avoided by making use of the Casimir companion X. To find the von Neumann entropy, we start from the fundamental relation $S_{\rm vN,eq} = S(E,\omega)$ that holds for the system in thermal equilibrium. From dimensional considerations, it follows that $S(E,\omega) = S(\epsilon)$, where $\epsilon = \epsilon(E,\omega)$ is a dimensionless rescaled energy. For instance S is a function of $\epsilon = E/\omega$ only. We then consider any mechanical (and thus reversible) process of our system, i.e., we change $\omega(t)$. The von Neumann entropy does not change nor does Casimir companion X which thus both equal their respective initial values,

$$S_{\rm vN}(t) = S_{\rm vN,i} = S(\epsilon_{\rm i}) = S(\sqrt{X_{\rm i}}) = S(\sqrt{X}). \tag{26}$$

The above result means that we can express the (constant) von Neumann entropy by means of the time-dependent E, L, C, and ω, which evolve due to the Hamiltonian dynamics.

This gives an easy way to calculate the von Neumann entropy for nonequilibrium states just by replacing the scaled energy with the square root of the Casimir companion, considering some constant scalar factors. Below this is exemplified using the two examples introduced above. In both examples we proceed by determining the rescaled energy as well as the equilibrium entropy as a function of $\beta = \omega/(k_{\rm B}T)$. Then the energy-$\beta$ relation is inverted and reintroduced into the entropy.

In the case of the parametric harmonic oscillator the Hamiltonian has eigenvalues $\epsilon_k = (k + 1/2)$, from which we find

$$\epsilon = \langle H\rangle = \frac{1}{Z}\sum_{k=0}\epsilon_k\, e^{-\beta(k+1/2)}, \tag{27}$$

with the partition function $Z = {\rm csch}(\beta/2)/2$. With $p_k = e^{-\beta(k+1/2)}/Z$ the entropy is

$$S = -k_{\rm B}\sum p_k \ln p_k = k_{\rm B}(\beta\epsilon + \ln Z). \tag{28}$$

Inverting (27) one finds $\beta = 2{\rm arccoth}(2\epsilon)$, which when inserted into (28) leads to

$$S = k_{\rm B}\left[\frac{1}{2}\ln\left(\epsilon^2 - \frac{1}{4}\right) + \epsilon\,{\rm arcsinh}\left(\frac{\epsilon}{\epsilon^2 - 1/4}\right)\right], \tag{29}$$

and thus

$$S_{\rm vN} = k_{\rm B}\left[\frac{1}{2}\ln\left(X - \frac{1}{4}\right) + \sqrt{X}{\rm arcsinh}\left(\frac{\sqrt{X}}{X - 1/4}\right)\right]. \tag{30}$$

For the second example we assume a pair of interacting spins, such that the Hamiltonian has rescaled eigenvalues $(-1,0,0,1)$ with $\beta = (\omega^2 + J^2)/(k_{\rm B}T)$. This system was used to investigate quantum friction in a quantum four-stroke heat engine [21]. Then $Z = 2(1 + \cosh\beta)$, $\beta = \ln[(1-\epsilon)/(1+\epsilon)]$, and $S = k_{\rm B}[\ln Z - \beta\tanh(\beta/2)]$, from which one obtains

$$S = k_{\rm B}\left[\ln\left(\frac{4}{1-\epsilon^2}\right) + \epsilon\ln\left(\frac{1-\epsilon}{1+\epsilon}\right)\right] \tag{31}$$

and thus

$$S_{\rm vN} = k_{\rm B}\left[\ln\left(\frac{4}{1-X}\right) + \sqrt{X}\ln\left(\frac{1-\sqrt{X}}{1+\sqrt{X}}\right)\right]. \tag{32}$$

VI. CONCLUSION

We introduced a dynamic invariant X of an ensemble associated with the dynamic algebra of a Hamiltonian problem. This invariant is related to the Casimir invariant, but reveals insights into nonequilibrium thermodynamic processes. Its many uses include bounding the minimum energy reachable by a system, reduction of the dimension of the system dynamics, and extension of the equilibrium entropy function to nonequilibrium situations to match the von Neumann entropy of the system. Comparison between this von Neumann entropy and the energy entropy measures the amount of work stored in marked-for-loss degrees of freedom excited by quantum friction.

Here we analyzed the harmonic oscillator and the spin system: two three-dimensional examples for which the reduction in dimension from 3 to 2 enabled by the constancy of X makes the difference between complicated formulas and simple geometry. These two examples are two paradigm examples of theoretical physics and the only ones for which shortcuts to adiabatic processes have been found using the very same optimal control that X simplifies. The reduction of the dimension of the problem is a fruitful tool to simplify optimal control problems. For instance, in [7] the former three-dimensional problem of controlling a qubit is reduced to an optimal control problem on the Bloch sphere, a two-dimensional manifold. The shortcuts to adiabaticity were found by lowering the dimension due to an invariant [9]. Dynamical algebras can have more than one Casimir invariant. How the constancy of the associated Casimir companions can aid in the optimal control of other quantum systems remains to be seen. Such optimal control is sure to be important for quantum computing [3] and for NMR [4]. Do fast, effectively adiabatic processes exist for these systems? The Casimir companion is likely to play a significant role in answering these questions. One important role is already clear. Since X enables us to quantify the availability in a quantum state away from equilibrium it tells us the target energy for any effectively adiabatic process.

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