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Gauge Invariance of Equilibrium Statistical Mechanics

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We identify a recently proposed shifting operation on classical phase space as a gauge transformation for statistical mechanical microstates. The infinitesimal generators of the continuous gauge group form a noncommutative Lie algebra, which induces exact sum rules when thermally averaged. Gauge invariance with respect to finite shifting is demonstrated via Monte Carlo simulation in the transformed phase space which generates identical equilibrium averages. Our results point toward a deeper basis of statistical mechanics than previously known, and they offer avenues for systematic construction of exact identities and of sampling algorithms.

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One of the arguably most important applications of Noether's theorem of invariant variations [1–4] is the systematic treatment of local gauge invariances within the fundamental physical field theories for the electromagnetic, weak, and strong interactions. Using the corresponding continuous gauge groups U(1), SU(2), and SU(3) as fundamental building blocks for theory construction is one of the most successful strategies in modern physics. The nature of the physical mechanisms that underlie the symmetry do not, however, feature explicitly in Noether's theorem. The theorem rather constitutes a power tool to obtain exact equations, usually in the form of global or local conservation laws, from an underlying continuous symmetry that needs to have been identified within (or input into) a variational formulation of the considered physics.

The roots of statistical mechanics are older than the modern gauge field theories. Nevertheless, Noether's theorem has been applied only relatively recently in various different productive ways to the physics of equilibrium and nonequilibrium many-body systems [5–12]. The role that exact sum rules [13–18] play in statistical mechanics is akin to that of conservation laws in dynamical theories, in that they allow one to constrain and rationalize the nature of the physics, without, in general, determining the full solution of the problem at hand.

In a range of recent investigations, Noether's theorem has been applied to a specific shifting operation on phase space [19–25], where, instead of the more usual conservation laws, both well-known and new statistical mechanical sum rules were obtained systematically. Thereby, Noether's concept of invariance against continuous transformation is applied to statistical mechanical functionals, such as the partition sum. While similarities with global spatial translational invariance, as generates linear momentum conservation, were discussed [19,20], neither the physical nature nor the mathematical structure of the general phase space shifting transformation [22–27] have been unraveled.

Here, we identify the phase space shifting transformation [19–25] as a local gauge symmetry transformation that is inherent to the statistical mechanics of particle-based systems. Realizing the defining feature of a gauge transformation, the application of the local shifting has no effect on any physical observables. Despite the shifting being geometric, the transformation is noncommutative, even when displacing only infinitesimally. A noncommutative Lie algebra of generators characterizes infinitesimal transformations. Corresponding exact sum rules follow for thermal averages. Finite transformations retain the gauge invariance, as we demonstrate via Monte Carlo computer simulations.

The shifting operation put forward in Refs. [19–25] affects the positions $\mathbf{r}_i$ and momenta $\mathbf{p}_i$ of each particle $i = 1, \ldots, N$ via the following transformation:

$$\mathbf{r}_i \to \mathbf{r}_i + \boldsymbol{\epsilon}(\mathbf{r}_i) = \tilde{\mathbf{r}}_i, \tag{1}$$

$$\mathbf{p}_i \to [\mathbb{1} + \nabla_i \boldsymbol{\epsilon}(\mathbf{r}_i)]^{-1} \cdot \mathbf{p}_i = \tilde{\mathbf{p}}_i, \tag{2}$$

where the d-dimensional vector field $\boldsymbol{\epsilon}(\mathbf{r}_i)$ is such that Eq. (1) is a diffeomorphism, i.e., together with its inverse is bijective and smooth; d is the spatial dimensionality, and the tilde indicates the new phase space variables. In Eq. (2), the symbol $\mathbb{1}$ denotes the $d \times d$ unit matrix, ∇_i is the derivative with respect to $\mathbf{r}_i$, and the superscript -1 denotes matrix inversion. The transformation is canonical in the sense of classical mechanics [28], and, hence, the differential phase space volume element is preserved, $d\mathbf{r}_i d\mathbf{p}_i = d\tilde{\mathbf{r}}_i d\tilde{\mathbf{p}}_i$. This property is fundamental for thermal averages to arise as invariant under the application of Eqs. (1) and (2).

To be specific, we consider the statistical mechanics of Hamiltonians H with the standard form

$$H = \sum_i \frac{\mathbf{p}_i^2}{2m} + u(\mathbf{r}^N) + \sum_i V_{\text{ext}}(\mathbf{r}_i), \tag{3}$$

where the sums run over all N particle indices i, m denotes the particle mass, $u(\mathbf{r}^N)$ is the interparticle interaction potential, and $V_{\text{ext}}(\mathbf{r})$ is an external one-body potential. We use the shorthand notation $\mathbf{r}^N = \mathbf{r}_1, \ldots, \mathbf{r}_N$ and $\mathbf{p}^N = \mathbf{p}_1, \ldots, \mathbf{p}_N$ to indicate the phase space variables of all particles. The statistical mechanics is based on the grand ensemble with chemical potential μ and temperature T. The grand partition sum is $\Xi = \mathrm{Tr}\, \mathrm{e}^{-\beta(H-\mu N)}$, where the classical trace is defined as $\mathrm{Tr}\cdot = \sum_{N=0}^{\infty}(N!h^{dN})^{-1}\int d\mathbf{r}^N d\mathbf{p}^N \cdot$, with $\int d\mathbf{r}^N d\mathbf{p}^N$ denoting the phase space integral over the position and momentum coordinates of all N particles, $\beta = 1/(k_B T)$, and k_B denoting the Boltzmann constant. The grand potential is $\Omega = -k_B T \ln \Xi$, and thermal averages are obtained as $\langle\cdot\rangle = \mathrm{Tr}\cdot \mathrm{e}^{-\beta(H-\mu N)}/\Xi$.

We here introduce operator methods to capture the essence of the phase space shifting (1) and (2). Specifically, we define the following, at each position $\mathbf{r}$ localized, phase space shifting operators:

$$\boldsymbol{\sigma}(\mathbf{r}) = \sum_i [\delta(\mathbf{r}-\mathbf{r}_i)\nabla_i + \mathbf{p}_i \nabla \delta(\mathbf{r}-\mathbf{r}_i)\cdot\nabla_{\mathbf{p}_i}], \quad (4)$$

where $\delta(\cdot)$ denotes the Dirac distribution in d dimensions, ∇ indicates the derivative with respect to position $\mathbf{r}$, $\nabla_{\mathbf{p}_i}$ is the momentum derivative with respect to $\mathbf{p}_i$, and we recall that ∇_i is the derivative with respect to $\mathbf{r}_i$. The shifting operators (4) possess two key properties. First, $\boldsymbol{\sigma}(\mathbf{r})$ is anti-self-adjoint on phase space:

$$\boldsymbol{\sigma}^\dagger(\mathbf{r}) = -\boldsymbol{\sigma}(\mathbf{r}). \quad (5)$$

The adjoint operator is indicated by the dagger, and it has the standard definition: $\int d\mathbf{r}^N d\mathbf{p}^N f \boldsymbol{\sigma}(\mathbf{r}) g = \int d\mathbf{r}^N d\mathbf{p}^N g \boldsymbol{\sigma}^\dagger(\mathbf{r}) f$ for arbitrary phase space functions $f(\mathbf{r}^N, \mathbf{p}^N)$ and $g(\mathbf{r}^N, \mathbf{p}^N)$. Equation (5) is readily proven via phase space integration by parts and the product rule (for f and g being well behaved).

Second, the consecutive action of two shifting operators that are, respectively, localized at positions $\mathbf{r}$ and $\mathbf{r}'$ satisfies the commutator relation:

$$[\boldsymbol{\sigma}(\mathbf{r}), \boldsymbol{\sigma}(\mathbf{r}')] = \boldsymbol{\sigma}(\mathbf{r}')[\nabla\delta(\mathbf{r}-\mathbf{r}')] + [\nabla\delta(\mathbf{r}-\mathbf{r}')]\boldsymbol{\sigma}(\mathbf{r}). \quad (6)$$

We have used the standard definition of commutators of vectors: $[\boldsymbol{\sigma}(\mathbf{r}), \boldsymbol{\sigma}(\mathbf{r}')] = \boldsymbol{\sigma}(\mathbf{r})\boldsymbol{\sigma}(\mathbf{r}') - \boldsymbol{\sigma}(\mathbf{r}')\boldsymbol{\sigma}(\mathbf{r})^{\mathsf{T}}$, where the superscript T denotes matrix transposition, such that the (Cartesian) ab component is $[\sigma_a(\mathbf{r}), \sigma_b(\mathbf{r}')] = \sigma_a(\mathbf{r})\sigma_b(\mathbf{r}') - \sigma_b(\mathbf{r}')\sigma_a(\mathbf{r})$. Equation (6) follows from explicit calculation via applying the sequence of two shifting operators (4) and simplifying. It is also straightforward to show that the commutator (6) is anti-self-adjoint: $[\boldsymbol{\sigma}(\mathbf{r}), \boldsymbol{\sigma}(\mathbf{r}')]^\dagger = -[\boldsymbol{\sigma}(\mathbf{r}), \boldsymbol{\sigma}(\mathbf{r}')]$, as is a general property of the commutator of two anti-self-adjoint operators. Furthermore, the commutator (6) is antisymmetric: $[\boldsymbol{\sigma}(\mathbf{r}), \boldsymbol{\sigma}(\mathbf{r}')] = -[\boldsymbol{\sigma}(\mathbf{r}'), \boldsymbol{\sigma}(\mathbf{r})]^{\mathsf{T}}$, and it satisfies the Jacobi identity: $[\sigma_a(\mathbf{r}), [\sigma_b(\mathbf{r}'), \sigma_c(\mathbf{r}'')]] + [\sigma_b(\mathbf{r}'), [\sigma_c(\mathbf{r}''), \sigma_a(\mathbf{r})]] + [\sigma_c(\mathbf{r}''), [\sigma_a(\mathbf{r}), \sigma_b(\mathbf{r}')]] = 0$, as can be be proven by explicit calculation.

The above set of distinctive properties of $\boldsymbol{\sigma}(\mathbf{r})$ is closely connected to a Lie algebra structure of infinitesimal phase space shifting, as we lay out in the following. That the operators (6) represent infinitesimal versions of the phase space shifting according to (1) and (2) can be seen by multiplying with a given shifting field $\boldsymbol{\epsilon}(\mathbf{r})$ and integrating over $\mathbf{r}$ to generate an operator $\Sigma[\boldsymbol{\epsilon}] = \int d\mathbf{r} \boldsymbol{\epsilon}(\mathbf{r})\cdot\boldsymbol{\sigma}(\mathbf{r})$ that shifts according to the given form of $\boldsymbol{\epsilon}(\mathbf{r})$. Using $\boldsymbol{\sigma}(\mathbf{r})$ in the form (4) and integrating gives

$$\Sigma[\boldsymbol{\epsilon}] = \sum_i \{\boldsymbol{\epsilon}(\mathbf{r}_i)\cdot\nabla_i - [\nabla_i \boldsymbol{\epsilon}(\mathbf{r}_i)] : \mathbf{p}_i \nabla_{\mathbf{p}_i}\}. \quad (7)$$

The colon in Eq. (7) indicates a double tensor contraction (trace of the product of the two matrices), and the phase space shifting operator $\Sigma[\boldsymbol{\epsilon}]$ depends functionally on the shifting field $\boldsymbol{\epsilon}(\mathbf{r})$ as is indicated by the brackets.

By construction, a given phase space function $f(\mathbf{r}^N, \mathbf{p}^N)$ is transported from $\mathbf{r}^N$, $\mathbf{p}^N$ to $\tilde{\mathbf{r}}^N, \tilde{\mathbf{p}}^N$ to first order in $\boldsymbol{\epsilon}(\mathbf{r}_i)$ and $\nabla_i \boldsymbol{\epsilon}(\mathbf{r}_i)$ by applying Eq. (7) according to

$$f(\tilde{\mathbf{r}}^N, \tilde{\mathbf{p}}^N) = f(\mathbf{r}^N, \mathbf{p}^N) + \Sigma[\boldsymbol{\epsilon}] f(\mathbf{r}^N, \mathbf{p}^N). \quad (8)$$

Here, the phase space variables with and without tilde are related by the transformation (1) and (2).

Applying two consecutive shifts with respective vector fields $\boldsymbol{\epsilon}_1(\mathbf{r}_i)$ and $\boldsymbol{\epsilon}_2(\mathbf{r}_i)$ constitutes repeated application of the shifting operator according to $\Sigma[\boldsymbol{\epsilon}_2]\Sigma[\boldsymbol{\epsilon}_1]$. As thereby $\Sigma[\boldsymbol{\epsilon}_2]$ acts on the already displaced phase space function $\Sigma[\boldsymbol{\epsilon}_1] f(\mathbf{r}^N, \mathbf{p}^N)$, the order of consecutive shifting is relevant. The noncommutative nature of the displacements is illustrated in Fig. 1.

The commutator of two shifting operators $\Sigma[\boldsymbol{\epsilon}_1]$ and $\Sigma[\boldsymbol{\epsilon}_2]$ quantifies the degree of their noncommutativity. Via explicit calculation on the basis of Eq. (7), one obtains straightforwardly the identity

$$[\Sigma[\boldsymbol{\epsilon}_1], \Sigma[\boldsymbol{\epsilon}_2]] = \Sigma[\boldsymbol{\epsilon}_\Delta]. \quad (9)$$

The difference shifting vector field $\boldsymbol{\epsilon}_\Delta(\mathbf{r}_i)$ is, thereby, obtained from the given forms of $\boldsymbol{\epsilon}_1(\mathbf{r}_i)$ and $\boldsymbol{\epsilon}_2(\mathbf{r}_i)$ via

$$\boldsymbol{\epsilon}_\Delta(\mathbf{r}_i) = \boldsymbol{\epsilon}_1(\mathbf{r}_i)\cdot[\nabla_i \boldsymbol{\epsilon}_2(\mathbf{r}_i)] - \boldsymbol{\epsilon}_2(\mathbf{r}_i)\cdot[\nabla_i \boldsymbol{\epsilon}_1(\mathbf{r}_i)]. \quad (10)$$

The right-hand side of Eq. (10) constitutes the standard form [29] of the Lie bracket $[\boldsymbol{\epsilon}_1(\mathbf{r}_i), \boldsymbol{\epsilon}_2(\mathbf{r}_i)]_{\mathrm{L}}$ of the two vector fields $\boldsymbol{\epsilon}_1(\mathbf{r}_i)$ and $\boldsymbol{\epsilon}_2(\mathbf{r}_i)$. Via replacing the functional argument $\boldsymbol{\epsilon}_\Delta(\mathbf{r}_i)$ on the right-hand side of Eq. (9) by the Lie bracket, we can, hence, alternatively express Eq. (9) compactly as $[\Sigma[\boldsymbol{\epsilon}_1], \Sigma[\boldsymbol{\epsilon}_2]] = \Sigma[[\boldsymbol{\epsilon}_1, \boldsymbol{\epsilon}_2]_{\mathrm{L}}]$.

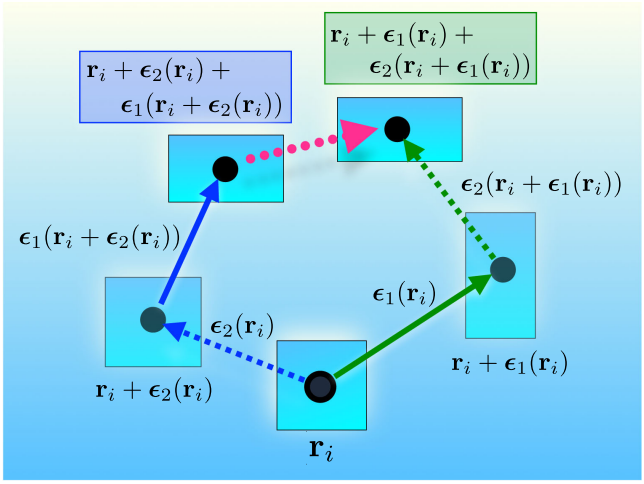

FIG. 1. Illustration of the noncommutative nature of phase space shifting. Given are two different shifting vector fields $\boldsymbol{\epsilon}_1(\mathbf{r}_i)$ (solid arrows) and $\boldsymbol{\epsilon}_2(\mathbf{r}_i)$ (dashed arrows). Starting from $\mathbf{r}_i$, the first shift yields the intermediate position $\mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i)$. At this point, the second shifting field $\boldsymbol{\epsilon}_2(\mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i))$ is used to give $\mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i) + \boldsymbol{\epsilon}_2(\mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i))$ as the final position (two green arrows). Applying the opposite order of shifting and starting again at $\mathbf{r}_i$ gives a different intermediate point $\mathbf{r}_i + \boldsymbol{\epsilon}_2(\mathbf{r}_i)$. Evaluating $\boldsymbol{\epsilon}_1(\mathbf{r}_i + \boldsymbol{\epsilon}_2(\mathbf{r}_i))$ at this position yields $\mathbf{r}_i + \boldsymbol{\epsilon}_2(\mathbf{r}_i) + \boldsymbol{\epsilon}_1(\mathbf{r}_i + \boldsymbol{\epsilon}_2(\mathbf{r}_i))$ as the final location (two blue arrows). The two final destinations mismatch, in general (red dotted arrow), while the differential phase space volume element is conserved (boxes).

The relationship (9) constitutes a noncommutative Lie algebra of infinitesimal generators $\Sigma[\boldsymbol{\epsilon}]$ due to three properties: (i) antisymmetry, (ii) bilinearity, as, respectively, follows from the definition of the commutator and from linearity of the differential operator (7), and (iii) the Jacobi identity: $[\Sigma_1, [\Sigma_2, \Sigma_3]] + [\Sigma_2, [\Sigma_3, \Sigma_1]] + [\Sigma_3, [\Sigma_1, \Sigma_2]] = 0$, as can be verified by explicit calculation on the basis of Eqs. (7)–(10); we have used the shorthand notation $\Sigma_1 = \Sigma[\boldsymbol{\epsilon}_1]$, $\Sigma_2 = \Sigma[\boldsymbol{\epsilon}_2]$, and $\Sigma_3 = \Sigma[\boldsymbol{\epsilon}_3]$.

The variational strategy of Refs. [22–25] is based on eliminating explicit occurrences of the shifting fields. This is in line with their present status as mere gauge functions. Within the functional calculus methods [22–25], one takes appropriate functional derivatives $\delta/\delta\boldsymbol{\epsilon}(\mathbf{r})$ of relevant thermal averages and then sets the shifting field to zero, $\boldsymbol{\epsilon}(\mathbf{r}) = 0$. Applying the concept to the present operator formalism leads to differentiating the shifting operator $\Sigma[\boldsymbol{\epsilon}]$ functionally with respect to $\boldsymbol{\epsilon}(\mathbf{r})$. Calculating $\delta\Sigma[\boldsymbol{\epsilon}]/\delta\boldsymbol{\epsilon}(\mathbf{r}) = \boldsymbol{\sigma}(\mathbf{r})$ on the basis of Eq. (7) is straightforward and reproduces $\boldsymbol{\sigma}(\mathbf{r})$ as defined via Eq. (4). The functional derivative creates spatial localization via the Dirac distribution, as it emerges from the chain rule and the identity $\delta\boldsymbol{\epsilon}(\mathbf{r}_i)/\delta\boldsymbol{\epsilon}(\mathbf{r}) = \delta(\mathbf{r} - \mathbf{r}_i)\mathbb{1}$. Because of the linearity of Eq. (7) in $\boldsymbol{\epsilon}(\mathbf{r})$, the dependence on $\boldsymbol{\epsilon}(\mathbf{r})$ has disappeared in Eq. (4). For how the action of $\boldsymbol{\sigma}(\mathbf{r})$ is related to differentiating by $\boldsymbol{\epsilon}(\mathbf{r})$, see Appendix A.

As an initial demonstration of the prowess of the localized shifting operator (4), we apply it to the Hamiltonian with the result

$$-\boldsymbol{\sigma}(\mathbf{r})H = \hat{\mathbf{F}}(\mathbf{r}), \tag{11}$$

where $\hat{\mathbf{F}}(\mathbf{r})$ is the (total) force density phase space function, which consists of kinetic, interparticle, and external contributions according to [30]

$$\hat{\mathbf{F}}(\mathbf{r}) = \nabla \cdot \hat{\boldsymbol{\tau}}(\mathbf{r}) + \hat{\mathbf{F}}_{\text{int}}(\mathbf{r}) - \hat{\rho}(\mathbf{r})\nabla V_{\text{ext}}(\mathbf{r}). \tag{12}$$

The three terms on the right-hand side represent kinetic stress density $\hat{\boldsymbol{\tau}}(\mathbf{r}) = -\sum_i \mathbf{p}_i\mathbf{p}_i\delta(\mathbf{r} - \mathbf{r}_i)/m$, interparticle force density $\hat{\mathbf{F}}_{\text{int}}(\mathbf{r}) = -\sum_i \delta(\mathbf{r} - \mathbf{r}_i)\nabla_i u(\mathbf{r}^N)$, and particle density $\hat{\rho}(\mathbf{r}) = \sum_i \delta(\mathbf{r} - \mathbf{r}_i)$ as phase space functions.

As a prerequisite for applying the localized shifting operator approach $\boldsymbol{\sigma}(\mathbf{r})$ to the thermal physics, we consider its effect on the Boltzmann factor:

$$\boldsymbol{\sigma}(\mathbf{r})\mathrm{e}^{-\beta H} = \beta\hat{\mathbf{F}}(\mathbf{r})\mathrm{e}^{-\beta H}. \tag{13}$$

The result (13) follows from applying the phase space derivatives in $\boldsymbol{\sigma}(\mathbf{r})$ as given in Eq. (4) to the exponential, using the chain rule, and then generating $\hat{\mathbf{F}}(\mathbf{r})$ via Eq. (11). Applying $\boldsymbol{\sigma}(\mathbf{r})$ to the entire grand ensemble probability distribution $\mathrm{e}^{-\beta(H-\mu N)}/\Xi$ gives no additional terms, as the partition sum Ξ is not a phase space function and is, hence, unaffected by the action of $\boldsymbol{\sigma}(\mathbf{r})$, and the presence of the chemical potential contribution $\mathrm{e}^{\beta\mu N}$ also has no adverse effect. Hence, in full analogy to Eq. (13), $\boldsymbol{\sigma}(\mathbf{r})\mathrm{e}^{-\beta(H-\mu N)}/\Xi = \beta\hat{\mathbf{F}}(\mathbf{r})\mathrm{e}^{-\beta(H-\mu N)}/\Xi$.

We are now ready to apply the operator algebra to the thermal physics. We first demonstrate how prior results follow from the framework and, hence, start with the thermal average $\langle\boldsymbol{\sigma}(\mathbf{r})\rangle = \mathrm{Tr}\,\boldsymbol{\sigma}(\mathbf{r})\mathrm{e}^{-\beta(H-\mu N)}/\Xi = \langle\beta\hat{\mathbf{F}}(\mathbf{r})\rangle$, as is readily obtained from Eq. (13). On the other hand, the anti-self-adjoint property (5) allows, upon inserting a factor 1 before the shifting operator, one to conclude $\langle\boldsymbol{\sigma}(\mathbf{r})\rangle = \langle 1\boldsymbol{\sigma}(\mathbf{r})\rangle = \langle[\boldsymbol{\sigma}^\dagger(\mathbf{r})1]\rangle = -\langle[\boldsymbol{\sigma}(\mathbf{r})1]\rangle = -\langle 0\rangle = 0$. Hence, overall $\langle\hat{\mathbf{F}}(\mathbf{r})\rangle = 0$, which is the exact equilibrium one-body force balance [13,22,26,27,30–32].

Higher-order identities follow with similar ease. Consider the two-point case, where $\langle\boldsymbol{\sigma}(\mathbf{r}')\boldsymbol{\sigma}(\mathbf{r})\rangle = 0$, which follows as above from the adjoint $\boldsymbol{\sigma}^\dagger(\mathbf{r}')1 = 0$. Consecutively applying two operators yields in a first step $\langle\boldsymbol{\sigma}(\mathbf{r}')\boldsymbol{\sigma}(\mathbf{r})\rangle = \langle\boldsymbol{\sigma}(\mathbf{r}')\beta\hat{\mathbf{F}}(\mathbf{r})\rangle$ according to Eq. (13). In the second step applying $\boldsymbol{\sigma}(\mathbf{r}')$, using the product rule, and bearing in mind that the overall result vanishes, one obtains the sum rule $\beta\langle\hat{\mathbf{F}}(\mathbf{r}')\hat{\mathbf{F}}(\mathbf{r})\rangle = -\langle[\boldsymbol{\sigma}(\mathbf{r}')\hat{\mathbf{F}}(\mathbf{r})]\rangle$, as previously identified in Refs. [23,24]. The term on the right-hand side is the mean negative force gradient or, equivalently, the mean Hessian of the Hamiltonian, $-\langle[\boldsymbol{\sigma}(\mathbf{r}')\hat{\mathbf{F}}(\mathbf{r})]\rangle = \langle[\boldsymbol{\sigma}(\mathbf{r}')\boldsymbol{\sigma}(\mathbf{r})H]\rangle = \langle\delta^2 H(\tilde{\mathbf{r}}^N, \tilde{\mathbf{p}}^N)/[\delta\boldsymbol{\epsilon}(\mathbf{r})\delta\boldsymbol{\epsilon}(\mathbf{r}')]|_{\boldsymbol{\epsilon}=0}\rangle$, as rewritten first via

Eq. (11) and then via the functional derivative identity Eq. (A2) given in Appendix A and using that $\langle \hat{\mathbf{F}}(\mathbf{r})\rangle = 0$.

The involved force-force and force-gradient correlation functions were shown to be highly useful measures for the spatial two-body structure of a wide variety of soft matter systems [23,24]. Similarly, by introducing a further physical observable $\hat{A}(\mathbf{r}^N, \mathbf{p}^N)$ of interest [25,33], we consider $\langle \boldsymbol{\sigma}(\mathbf{r})\hat{A}\rangle = 0$, which follows again from using the adjoint (5). Applying the shifting operator to the functions on its right gives $\langle \beta\hat{\mathbf{F}}(\mathbf{r})\hat{A}\rangle + \langle [\boldsymbol{\sigma}(\mathbf{r})\hat{A}]\rangle = 0$, which is the recent general hyperforce sum rule by Robitschko *et al.* [25]. We rewrite the second term as the thermal average $\mathbf{S}_A(\mathbf{r}) = \langle \hat{\mathbf{S}}_A(\mathbf{r})\rangle$, where we have defined the hyperforce phase space function [25] as $\hat{\mathbf{S}}_A(\mathbf{r}) = [\boldsymbol{\sigma}(\mathbf{r})\hat{A}]$ [which is explicitly $\hat{\mathbf{S}}_A(\mathbf{r}) = \sum_i \delta(\mathbf{r}-\mathbf{r}_i)\nabla_i \hat{A}$ in case $\hat{A}$ is independent of momenta]. The one-body hyperforce sum rule [25] can then be expressed in the compact form

$$\langle \beta\hat{\mathbf{F}}(\mathbf{r})\hat{A}\rangle + \mathbf{S}_A(\mathbf{r}) = 0. \tag{14}$$

Repeated application of the localized shifting can be realized via similar steps as described above. Sketching a typical case for two shifts, we have $0 = \langle [\boldsymbol{\sigma}^\dagger(\mathbf{r}')1]\hat{A}\boldsymbol{\sigma}(\mathbf{r})\rangle = \langle \boldsymbol{\sigma}(\mathbf{r}')\hat{A}\boldsymbol{\sigma}(\mathbf{r})\rangle = \langle [\boldsymbol{\sigma}(\mathbf{r}')\hat{A}]\boldsymbol{\sigma}(\mathbf{r})\rangle + \langle \hat{A}\boldsymbol{\sigma}(\mathbf{r}')\boldsymbol{\sigma}(\mathbf{r})\rangle = \langle [\boldsymbol{\sigma}^\dagger(\mathbf{r})\boldsymbol{\sigma}(\mathbf{r}')\hat{A}]^\mathsf{T}\rangle + \langle \hat{A}\boldsymbol{\sigma}(\mathbf{r}')\boldsymbol{\sigma}(\mathbf{r})\rangle$. The very last term can be made more explicit as $\langle \hat{A}\boldsymbol{\sigma}(\mathbf{r}')\boldsymbol{\sigma}(\mathbf{r})\rangle = \beta^2\langle \hat{A}\,\hat{\mathbf{F}}(\mathbf{r}')\hat{\mathbf{F}}(\mathbf{r})\rangle - \beta\langle \hat{A}[\boldsymbol{\sigma}(\mathbf{r}')\boldsymbol{\sigma}(\mathbf{r})H]\rangle$, which gives upon using Eq. (5) and rearranging the overall result $\beta^2\langle \hat{A}\,\hat{\mathbf{F}}(\mathbf{r}')\hat{\mathbf{F}}(\mathbf{r})\rangle = \beta\langle \hat{A}[\boldsymbol{\sigma}(\mathbf{r}')\boldsymbol{\sigma}(\mathbf{r})H]\rangle + \langle [\boldsymbol{\sigma}(\mathbf{r})\boldsymbol{\sigma}(\mathbf{r}')\hat{A}]^\mathsf{T}\rangle$, which is the two-body hyperforce sum rule of Ref. [25] (the shifting field in Ref. [25] is set to zero after each individual functional derivative is taken).

That these exact correlation identities emerge with relatively little effort from the present operator formalism points to its relevance. Besides technical efficacy, the formalism, however, allows one to reveal the rich additional structure that is generated by the Lie algebra (9). As a demonstration, we multiply Eq. (6) from the left by $\hat{A}(\mathbf{r}^N, \mathbf{p}^N)$ and then build the thermal average. Writing out the resulting sandwich structure of the integral gives for the first term on the left-hand side $\langle \hat{A}\boldsymbol{\sigma}(\mathbf{r})\boldsymbol{\sigma}(\mathbf{r}')\rangle = -\langle [\boldsymbol{\sigma}(\mathbf{r})\hat{A}]\beta\hat{\mathbf{F}}(\mathbf{r}')\rangle = -\langle \hat{\mathbf{S}}_A(\mathbf{r})\beta\hat{\mathbf{F}}(\mathbf{r}')\rangle$. Similar treatment of the second terms yields the following exact Lie sum rule:

$$\begin{aligned}&\langle \hat{\mathbf{S}}_A(\mathbf{r})\beta\hat{\mathbf{F}}(\mathbf{r}')\rangle - \langle \beta\hat{\mathbf{F}}(\mathbf{r})\hat{\mathbf{S}}_A(\mathbf{r}')\rangle \\ &\quad = \mathbf{S}_A(\mathbf{r}')[\nabla\delta(\mathbf{r}-\mathbf{r}')] + [\nabla\delta(\mathbf{r}-\mathbf{r}')]\mathbf{S}_A(\mathbf{r}).\end{aligned} \tag{15}$$

The right-hand side of Eq. (15) follows from the average of the product of $\hat{A}$ with the right-hand side of Eq. (6) and noting that $\langle \hat{A}\boldsymbol{\sigma}(\mathbf{r})\rangle = \langle [-\boldsymbol{\sigma}(\mathbf{r})\hat{A}]\rangle = -\mathbf{S}_A(\mathbf{r})$. The right-hand side of Eq. (15) can alternatively be rewritten via Eq. (14).

The significance of the sum rule (15) is that it imprints the structure of the Lie operator algebra (6) onto measurable spatial correlation functions. There are two immediate consequences. First, for the case $\mathbf{r} \neq \mathbf{r}'$, the right-hand side of Eq. (15) vanishes, and the following nontrivial exchange symmetry emerges:

$$\langle \hat{\mathbf{S}}_A(\mathbf{r})\hat{\mathbf{F}}(\mathbf{r}')\rangle = \langle \hat{\mathbf{F}}(\mathbf{r})\hat{\mathbf{S}}_A(\mathbf{r}')\rangle. \tag{16}$$

Equation (16) implies the invariance of the correlation against exchange of the force and hyperforce densities at two distinct positions $\mathbf{r}$ and $\mathbf{r}'$.

Second, the singular ("self") contribution that occurs for $\mathbf{r} = \mathbf{r}'$ in Eq. (15) does not generate any new one-body correlation functions. Rather, besides the gradient of the delta distribution, the one-body hyperforce correlation function $\mathbf{S}_A(\mathbf{r})$, as it appears in the one-body hyperforce sum rule (14), reemerges. Hence, the present example demonstrates both (i) that the Lie algebra (6) systematically interrelates the different n-body levels of correlation identities and (ii) that, despite possible rewritings of equivalent expressions, the set of relevant correlation functions that is associated with a given observable $\hat{A}$ is closed.

We have thus far considered the infinitesimal structure of phase space shifting. In standard treatments using the exponential map, one generates a Lie group of finite transformations from a given Lie algebra [29]. Here, we use an alternative route to demonstrate directly the invariance of the thermal physics under the general transformation (1) and (2). Via particle-based Monte Carlo simulations, we demonstrate the physical reality of the gauge invariance by considering finite shifting which we perform numerically. We continue to work with the full phase space variables (as are also relevant for equilibrium molecular dynamics) and, hence, resolve both position and momentum.

As a representative example, we choose the iconic one-dimensional hard rod system, for which analytical solutions exist [34,35]. To induce spatial inhomogeneity, we consider confinement between two hard walls. The hard core nature of this test situation poses a stringent test for the gauge invariance, as the finite particle shifting will, in general, lead to overlapping particle configurations and, consequentially, to a differing sequence of microstates in the Monte Carlo Markov chain. The one-dimensional shifting field is chosen as either $\epsilon(x_i) = 0$, which reproduces the original system and constitutes our reference, or $\epsilon(x_i)/a = 0.5\sin(4\pi x_i/L)$, where $L = 10a$ is the separation distance between the two hard walls, a is the particle diameter, and x_i is the one-dimensional position coordinate of particle i. According to Eqs. (1) and (2), the transformed variables are $\tilde{x}_i = x_i + \epsilon(x_i)$ and $\tilde{p}_i = [1 + \partial\epsilon(x_i)/\partial x_i]^{-1} p_i$. The construction of Monte Carlo trial moves is identical in the shifted and unshifted systems, in that x_i and p_i are displaced uniformly within a maximal cutoff. In the

unshifted system, the new trial state enters the Boltzmann factor to accept or reject the new state according to the Metropolis criterion [36], as is the standard procedure. In the shifted system, the Boltzmann factor is evaluated on the basis of the shifted variables $\tilde{x}_i$ and $\tilde{p}_i$, both before and after the trial move. As a representative observable, we show in Fig. 2 results for the density profile $\rho(x)$ as obtained from histograms of particle positions $\tilde{x}_i$ from separate runs without and with shifting. We also show the position- and momentum-resolved one-body phase space density $f(x,p)$, where p denotes the momentum variable. Consistent with the theoretical structure of the particle gauge invariance, the results in the shifted system are identical to those in the original system with p following the correct Maxwellian. We have ascertained that the same behavior holds when replacing the hard core wall and interparticle potentials by soft potentials, using the Lennard-Jones form as representative. Results are shown in Appendix B together with a confirmation of the gauge invariance in a double well. As expected, the invariance holds already canonically with fixed N.

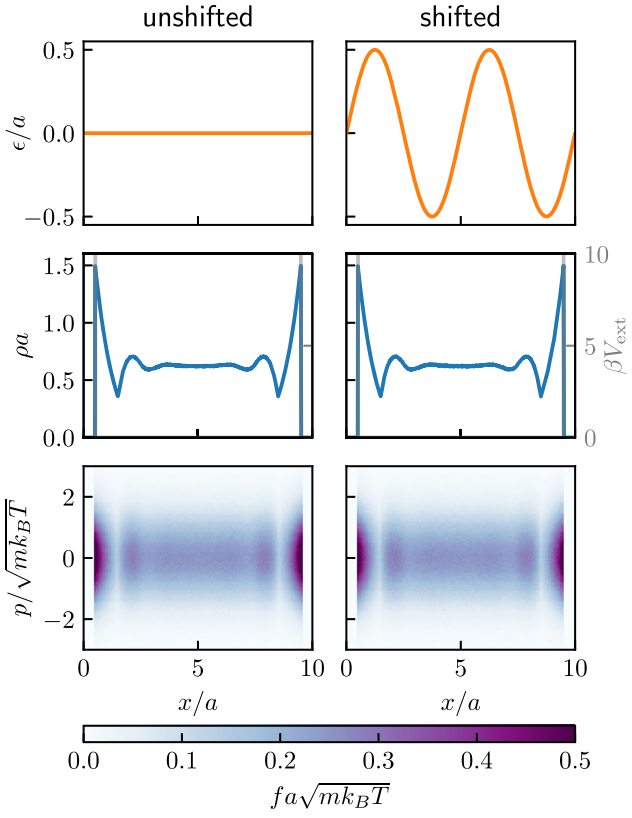

FIG. 2. Monte Carlo results for one-dimensional hard rods confined between two hard walls with separation distance $L = 10a$. Shown are results in the unshifted (left column) and shifted systems (right column). The shifting field ϵ (top panels) displaces both coordinates and momenta. Despite the different sampling and Markov chain, the scaled density profile $\rho(x)a$ (middle panels) and one-body phase space distribution function $f(x,p)a\sqrt{mk_BT}$ (bottom panels) remain numerically identical.

We have restricted ourselves to forms of phase space shifting given by Eqs. (1) and (2) together with Hamiltonians (3) that feature standard kinetic energy. The position transform (1) is a general and freely chosen diffeomorphism. The specific form of the momentum transform (2) then follows uniquely from imposing (i) that the transformation is canonical (and, hence, the Jacobian is unity) and (ii) that the identity transformation is recovered for $\boldsymbol{\epsilon}(\mathbf{r}) = 0$. We leave investigations of possible generalizations to future work. The relationship of the present theory with existing sum rules is recapped in Appendix C. As the shifting operators (4) feature a sum over all particles, with identical terms that involve only a single particle i, the statistical mechanical symmetry with respect to particle index permutation is respected. Hence, applying $\boldsymbol{\sigma}(\mathbf{r})$ commutes with index permutation.

In conclusion, we have shown that statistical mechanical microstates carry an intrinsic ambiguity with respect to the gauge shifting transformation (1) and (2). The Lie algebra (6) for infinitesimal generators (4) is imprinted in measurable physical correlation functions. Numerical implementation of the finite shifting gives additional freedom for particle-based simulation techniques, and one can envisage rich cross fertilization with force sampling schemes [37–42] and the mapped averaging framework [42–45]. Recent progress in microscopy-based measurement of locally resolved forces in colloidal systems [46] offers exciting potential for carrying out corresponding experimental work.

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End Matter

Appendix A: Relationship to functional methods—We can identify the effect of applying $\boldsymbol{\sigma}(\mathbf{r})$ to a generic phase space function $f(\mathbf{r}^N, \mathbf{p}^N)$ to be equivalent to the following functional derivatives of the considered function in the transformed variables:

$$\boldsymbol{\sigma}(\mathbf{r}) f(\mathbf{r}^N, \mathbf{p}^N) = \left. \frac{\delta f(\tilde{\mathbf{r}}^N, \tilde{\mathbf{p}}^N)}{\delta \boldsymbol{\epsilon}(\mathbf{r})} \right|_{\boldsymbol{\epsilon}=0}, \tag{A1}$$

$$\boldsymbol{\sigma}(\mathbf{r})\boldsymbol{\sigma}(\mathbf{r}') f(\mathbf{r}^N, \mathbf{p}^N) = \left. \frac{\delta^2 f(\tilde{\mathbf{r}}^N, \tilde{\mathbf{p}}^N)}{\delta \boldsymbol{\epsilon}(\mathbf{r}) \delta \boldsymbol{\epsilon}(\mathbf{r}')} \right|_{\boldsymbol{\epsilon}=0} + [\nabla \delta(\mathbf{r} - \mathbf{r}')] \boldsymbol{\sigma}(\mathbf{r}) f(\mathbf{r}^N, \mathbf{p}^N). \tag{A2}$$

We recall that the tilde indicates the transformed phase space variables (1) and (2). Equation (A1) follows from differentiating Eq. (8), and the analogous second-order version Eq. (A2) follows iteratively.

Appendix B: Gauge invariance for Lennard-Jones particles—To explicitly demonstrate that the gauge invariance holds beyond the hard core case, shown in Fig. 2, we consider confinement of Lennard-Jones particles between two Lennard-Jones walls, as combined from the single wall potential $\beta V_{\text{ext}}(x) = 4[(a/x)^{12} - (a/x)^6]$. We also consider trapping in a double well with barrier height e_w and separation $2x_m$ between the two potential minima. In this case, the external potential is $V_{\text{ext}}(x) = e_w[(x - L/2)^2 - x_m^2]^2/x_m^4$, where L is the system length, the barrier is located at $L/2$, and we set $\beta e_w = 2$ and $x_m = 2.5a$. Monte Carlo results for the behavior both of a single particle ($N = 1$) and for $N = 5$ particles are shown in Fig. 3. The shifting field $\epsilon(x)$ has the sinusoidal form described in the main text. We find that the results for the shifted and the original system are numerically identical; see Fig. 3.

Appendix C: Relationship to existing sum rules—Several of the sum rules that arise from the present statistical mechanical gauge invariance possess close relationships to the liquid state literature [13–18]. For sum rules that follow from global shifting invariance, we refer the reader to the description in the Methods section in Ref. [19]. Noether two-body force correlation identities such as the "$3g$"-sum rule [23,24] can alternatively to invariance arguments be obtained from

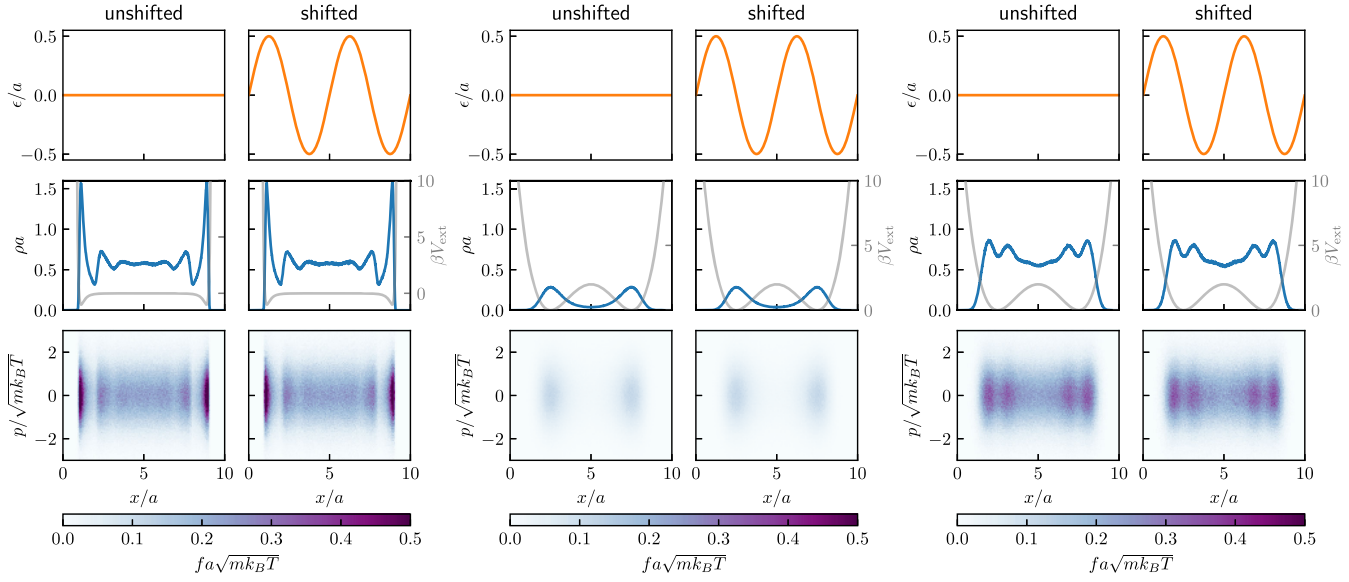

FIG. 3. Computer simulation results for the gauge invariance of Lennard-Jones particles. Shown are three cases: (i) confinement between two Lennard-Jones walls (first and second columns), (ii) trapping inside of a double-well external potential for particle number $N = 1$ (third and fourth columns), and (iii) trapping in the double well for $N = 5$ particles (fifth and sixth columns). Monte Carlo results for the original unshifted system are shown as a reference (first, third, and fifth columns). The simulation results for the scaled density profile $\rho(x)a$ (middle panels) and for the one-body phase space distribution function $f(x, p)a\sqrt{mk_BT}$ (bottom panels) in the shifted system (second, fourth, and sixth columns) are numerically identical to the respective results in the unshifted system.

partial integration on phase space, as described in the Appendix in Ref. [24]. Analogously, global hyperforce sum rules can be derived from Yvon's or from Hirschfelder's theorem, as described in Ref. [25]. Investigating the relationship of the gauge invariance to the (nonequilibrium) fluctuation theorems of stochastic thermodynamics [47] constitutes a highly valuable goal for future work.