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Why gauge invariance applies to statistical mechanics

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Abstract

We give an introductory account of the recently identified gauge invariance of the equilibrium statistical mechanics of classical many-body systems (Müller *et al* 2024 *Phys. Rev. Lett.* **133** 217101). The gauge transformation is a non-commutative shifting operation on phase space that keeps the differential phase space volume element and hence the Gibbs integration measure conserved. When thermally averaged any observable is an invariant, including thermodynamic and structural quantities. Shifting transformations are canonical in the sense of classical mechanics. They also form an infinite-dimensional group with generators of infinitesimal transformations that build a non-commutative Lie algebra. We lay out the connections with the underlying geometry of coordinate displacement and with Noether's theorem. Spatial localization of the shifting yields differential operators that satisfy commutator relationships, which we describe both in purely configurational and in full phase space setups. Standard operator calculus yields corresponding equilibrium hyper-force correlation sum rules for general observables and order parameters. Using Monte Carlos simulations we demonstrate explicitly the gauge invariance for finite shifting. We argue in favor of using the gauge invariance as a statistical mechanical construction principle for obtaining exact results and for formulating smart sampling algorithms.

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force sampling, mapped averaging

1. Introduction

Gauge field theories are fundamental for our understanding of nature. Considering the invariance against well-defined gauge transformations constitutes a universal construction principle, which formalizes the independence of the physical predictions that a theory provides from the precise choice of the variables that are in use. The perhaps most well-known case of gauge invariance affects the (scalar and vector) potentials of electrodynamics. While thereby specific choices of gauge can significantly simplify practical calculations, arguably as important are the fundamental consequences of gauge invariance. In the present example it is the intimate connection with the local conservation of electrical charge. We describe this standard case below as a template for the many-body physics that we address in this contribution.

Noether's theorem of invariant variations [1–4] provides the appropriate mathematical framework for systematically addressing the consequences that follow from the juxtaposition of inherent independence and apparent dependence on the choice of gauge. While forming a staple of field theories for many decades, Noether's theorem [1–4] has seen only relatively recently an increasing number of applications to statistical physics [5–16], both in and out-of-equilibrium. As much of statistical physics is based on insightful combination of suitable approximations with exact results, perhaps most notably in the form of equilibrium sum rules [17–25], there is arguably much potential for making progress.

Applications of the Noether theorem were performed in a variety of statistical mechanical settings as follows. In an early study of functional integrals in statistical physics and primarily based on quantum field theory, Revzen derived the continuity equation from Noether's theorem [5]. Baez and Fong formulated a Noether theorem for Markov processes [6]. Marvian and Spekkens provided an extension of Noether's theorem by quantifying the asymmetry of quantum states [7]. Sasa and Yokokura formulated the thermodynamic entropy as a Noether invariant [8]. Their work lead to investigation of the thermodynamical path integral and emergent symmetry [9]. Recently the thermodynamic entropy was viewed as a Noether invariant from contact geometry [10]. Budkov and Kolesnikov carried out a range of studies of complex systems, where the use of Noether's theorem was crucial. This work addressed modified Poisson–Boltzmann equations and macroscopic forces in inhomogeneous ionic fluids [11], as well as a covariant field theory of mechanical stresses in inhomogeneous ionic fluids [12]. The thermomechanical approach was applied to calculating mechanical stresses in inhomogeneous ionic fluids [13] and the surface tension of aqueous electrolyte solutions [14]. In recent work, Beyen and Maes identified the entropy as a Noether charge for quasistatic gradient flow [15] and for more general setups [16].

The statistical mechanics of particle-based systems is well accessible via direct simulation [26]. Thereby inherent statistical uncertainties can be reduced considerably by a range of recent methods, most prominently via mapped averaging [27–39] and force sampling [26, 40–47]. Mapped averaging, as pioneered by Kofke *et al* [27–39], is a systematic means for the reformulation of ensemble averages via flexible (coordinate) mappings [28]. The approach was used in a variety of contexts, including sampling of thermal properties of crystals [27–35], of liquid water [36], and of hard sphere [37] and Lennard–Jones fluids [31]. Force sampling originates from a pioneering early investigation by Borgis *et al* [40] and we refer to the review

by Rotenberg [44] for a comprehensive account of the approach. As a central concept, force sampling is based on using numerical integration methods to invert spatial gradients of correlation functions with the aim to exploit the accompanying smoothening effect. The relationship of force-sampling methods and mapped averaging has been illuminated in [39].

A specific shifting operation on the phase space associated with general interacting many-body systems was recently put forward and shown to be useful in a broad range of statistical mechanical settings [48–54]. These applications include formulating force-based density functional theory [55, 56], self-consistency conditions for neural functionals [57, 58], the formulation of hyperdensity functional theory for the description of the equilibrium behavior of general observables [59, 60], as well as nonequilibrium power functional [61] sum rules [48, 62, 63]. We refer the reader to [48, 54] for discussions of the relationship to the body of existing sum rules in the liquid state literature.

The phase space shifting [48–56] was recently argued to constitute a local gauge transformation of statistical mechanical microstates [64]; see the recent accounts given by Rotenberg [65] and by Miller [66]. Here we provide in-depth background for this gauge shifting transformation [64]. The transformation is geometric in nature and we describe in detail its origins in spatial displacements of particle coordinates. We introduce a purely configurational version and show that including the complementary momentum transformation [64], realized by (position-resolved) matrix multiplication, completes a very specific mathematical structure. As its key features, the shifting transformation is both canonical in the sense of classical mechanics and it constitutes a non-commutative continuous group. Phase space shifting leaves any equilibrium average invariant, which establishes its status as a gauge transformation. Meeting expectations for this role, the shifting unambiguously leads to a breadth of exact identities.

Our gauge theory carries strong similarities in its mathematical structure with the theory of Lie groups and corresponding Lie algebras of infinitesimal transformations. Important examples of nontrivial Lie groups in physics include the rotation matrices of three-dimensional space and the Pauli matrices to describe quantum mechanical spin 1/2 particles [67]. Our theory goes in important ways further than these elementary cases. In particular the tight interweaving with spatial Dirac distributions is notable. This feature provides microscopically sharp resolution and, as we demonstrate, it allows one to retain particle-level precision for all ensuing force and hyperforce correlation functions and their sum rules.

The paper is organized as follows. We describe in section 2 the standard gauge invariance of classical electrodynamics to both provide a discussion of general concepts of gauge invariance and also to formulate a blueprint for the subsequent particle-based physics. Readers who are familiar with this material are welcome to skip forward to section 3 where we describe the statistical mechanical phase space gauge invariance. The underlying phase space shifting transform is presented in section 3.1. Its central properties are derived in section 3.2 and the transform is thereby taken to be in general of finite magnitude. Rich additional mathematical structure is revealed when considering infinitesimal transforms as is described in detail for particle configuration (position) shifting in section 3.3.

We turn to statistical mechanics in section 4 and first define the general concepts, including the partition sum and thermal averages in section 4.1. The relevant standard one-body observables are introduced in section 4.2. Position shifting is applied to derive exact sum rules in section 4.3. General phase space shifting, which includes additional momentum displacement and restores the full canonical phase space transform, is described in section 4.4. We present

implications for and applications to computer simulation work in section 5. We give our conclusions and an outlook on possible future work in section 6.

2. Classical electrodynamics as a precursor

The prototypical and arguably most well-known example of gauge invariance in physics is that of classical electrodynamics [3, 68, 69], where the position- and time-dependent scalar electric potential $V(\mathbf{r},t)$ and the magnetic vector potential $\mathbf{A}(\mathbf{r},t)$ are transformed on the basis of a scalar gauge function $\varphi(\mathbf{r},t)$. The potentials are transformed according to the map:

$$V(\mathbf{r},t) \to V(\mathbf{r},t) - \partial\varphi(\mathbf{r},t)/\partial t, \tag{1}$$

$$\mathbf{A}(\mathbf{r},t) \to \mathbf{A}(\mathbf{r},t) + \nabla\varphi(\mathbf{r},t), \tag{2}$$

where ∇ indicates the derivative with respect to position $\mathbf{r}$.

The form of the gauge function $\varphi(\mathbf{r},t)$ can be arbitrarily chosen, as it has no discernible effect on Maxwell's equations, which govern the dynamics of the magnetic induction $\mathbf{B}(\mathbf{r},t) = \nabla \times \mathbf{A}(\mathbf{r},t)$ and of the electrical field $\mathbf{E}(\mathbf{r},t) = -\nabla V(\mathbf{r},t) - \partial\mathbf{A}(\mathbf{r},t)/\partial t$. This gauge invariance can readily be verified. That the transformation preserves the form of $\mathbf{B}(\mathbf{r},t)$ follows from elementary vector calculus via $\nabla \times \nabla\varphi(\mathbf{r},t) = 0$. Likewise $\mathbf{E}(\mathbf{r},t)$ remains unchanged as the mixed partial derivative of $\varphi(\mathbf{r},t)$ with respect to $\mathbf{r}$ and t can be interchanged and hence the two terms that emerge from the gauge transformation cancel each other such that $\nabla\partial\varphi(\mathbf{r},t)/\partial t - \partial\nabla\varphi(\mathbf{r},t)/\partial t = 0$.

The gauge freedom of choice of the form of $\varphi(\mathbf{r},t)$ has very profound implications quantum mechanically and a rich structure of modern theoretical physics is based on different forms of gauge symmetry. As background here we lay out the gauge freedom for the classical electrodynamical case; Stokes and Nazir [70] review gauge freedom in quantum electrodynamics.

We use the standard covariant formulation with the four-vector potential $A_\nu(x) = (V(\mathbf{r},t)/c, \mathbf{A}(\mathbf{r},t))$ where the four-vector $x_\nu = (ct, \mathbf{r})$ indicates the spacetime point, c is the speed of light, and ν denotes the component of spacetime. The electrical charge density $q(\mathbf{r},t)$ and the electrical current density $\mathbf{J}(\mathbf{r},t)$ form a four-current $J_\nu(x) = (cq(\mathbf{r},t), \mathbf{J}(\mathbf{r},t))$. The electromagnetic field tensor then follows as $F_{\nu\lambda}(x) = \partial_\nu A_\lambda(x) - \partial_\lambda A_\nu(x)$, where ∂_ν indicates the derivative with respect to x^ν, which in explicit form is $\partial_\nu = (c^{-1}\partial/\partial t, -\nabla)$. All Greek indices range from 0 (time-like) to 1, 2, and 3 (all space-like) and the metric has signature $(+,-,-,-)$.

This covariant formalism allows one to express the gauge transformation equations (1) and (2) in the succinct form

$$A_\nu(x) \to A_\nu(x) + \partial_\nu\varphi(x). \tag{3}$$

It is revealing to address the consequences of equation (3) on the standard electromagnetic action S which consists of contributions that arise from free fields (S_{free}) and external influence (S_{ext}) according to the sum $S = S_{\text{free}} + S_{\text{ext}}$. The two individual terms are given by

$$S_{\text{free}} = -\frac{1}{4\mu_0}\int dx F_{\lambda\nu}(x) F^{\nu\lambda}(x), \tag{4}$$

$$S_{\text{ext}} = -\int dx A_\nu(x) J^\nu(x), \tag{5}$$

where μ_0 is the magnetic permeability of the vacuum and we use Einstein summation convention over pairs of Greek spacetime indices. Requiring stationarity of S against changes in $A_\nu(x)$ yields upon multiplying by μ_0 the Maxwell equations in the compact covariant form

$$\partial_\nu F^{\nu\lambda}(x) = \mu_0 J^\lambda(x). \tag{6}$$

The free field action S_{free} is already an invariant and we hence investigate the effects of the gauge transformation on the external action S_{ext}. We apply the transform (3) to equation (5) which yields

$$S_{\text{ext}} \to -\int dx\,[A_\nu(x) + \partial_\nu\varphi(x)]\,J^\nu(x) \tag{7}$$

$$= S_{\text{ext}} + \int dx\varphi(x)\,\partial_\nu J^\nu(x). \tag{8}$$

In equation (7) we have identified the first term in the integral as S_{ext} via equation (5) and in the second term we have integrated by parts and assumed that boundary terms vanish.

Imposing that S_{ext} shall be gauge invariant implies that the second term on the right hand side of equation (8) must vanish. Given that the form of the gauge function $\varphi(x)$ is arbitrary, this can only be true provided that

$$\partial_\nu J^\nu(x) = 0, \tag{9}$$

which is the continuity equation for the charge distribution. When returning to three-vectors equation (9) attains the familiar more elementary form $\partial q(\mathbf{r},t)/\partial t = -\nabla\cdot\mathbf{J}(\mathbf{r},t)$.

The simplicity of the specific form (5) of the external action allowed us to derive equation (9) directly. Instead of relying explicitly on the fundamental lemma of variational calculus, we can equivalently utilize functional differentiation, here with respect to the gauge function $\varphi(x)$. We lay out these connections in appendix, where we also demonstrate the gauge invariance of S_{free} explicitly.

Gauge transformations encompass specific group structure that is associated with repeated application of the transformation. In particular, chaining together two subsequent transforms constitutes again a single transform. This is easy to see when considering two transforms represented by two different gauge functions $\varphi_1(x)$ and $\varphi_2(x)$. Then the composite transform is simply characterized by the sum $\varphi_{21}(x) = \varphi_1(x) + \varphi_2(x)$. Clearly, the order of the first and the second transformations is irrelevant, $\varphi_{21}(x) = \varphi_{12}(x) = \varphi_2(x) + \varphi_1(x)$, and hence the group is commutative (Abelian). For completeness, a transform with given $\varphi_1(x)$ has an inverse transform characterized by $-\varphi_1(x)$, the neutral group element is $\varphi(x) = 0$, and the composition is associative. These properties establish formally the mathematical group structure.

An illustration of the local gauge transformation of the potentials of electrodynamics is shown in figure 1. We also show a depiction of global shifts that displace the coordinates $\mathbf{r}_i$ of particle i in a many-body system. Statistical mechanical averages were shown to be invariant under such transformations of all particles [48–50] and we refer the reader to [12, 71] for similar applications in field theory. In the following we turn to the mathematically much richer local version of phase space shifting [51–56, 64].

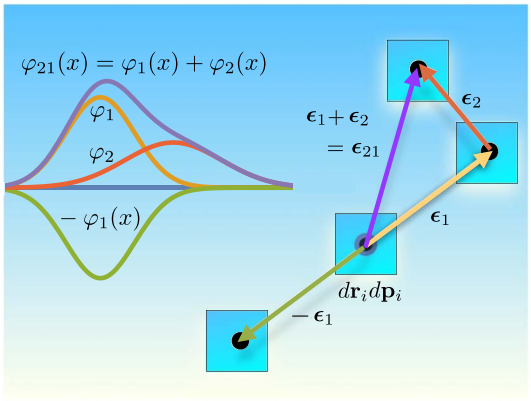


Figure 1. Group structure of the gauge transformations in electrodynamics (curves) and in statistical mechanics (arrows), depicted for global transforms for the latter case. Shown are different forms of the scalar gauge function $\varphi(x)$ that parameterizes the transform in electrodynamics. A given gauge function $\varphi_1(x)$ has an inverse $-\varphi_1(x)$. Two transforms $\varphi_1(x)$ and $\varphi_2(x)$ combine additively to $\varphi_{21}(x) = \varphi_1(x) + \varphi_2(x)$. For the statistical mechanics the global gauge invariance is shown for different realizations of a constant shifting vector $\boldsymbol{\epsilon}_1$. The inverse transform $\boldsymbol{\epsilon}_{-1}$ is represented by the negative shifting vector, $\boldsymbol{\epsilon}_{-1} = -\boldsymbol{\epsilon}_1$. Two transformations that correspond to $\boldsymbol{\epsilon}_1$ and $\boldsymbol{\epsilon}_2$ combine additively to $\boldsymbol{\epsilon}_{21} = \boldsymbol{\epsilon}_1 + \boldsymbol{\epsilon}_2$. Also illustrated is the conserved phase space volume element $d\mathbf{r}_i\, d\mathbf{p}_i$.

3. Gauge invariance of phase space

3.1. Local shifting as a canonical transformation

As laid out in the introduction, Noether's theorem [1–4] has been applied in statistical physics in a variety of settings [5–16]. Here we describe the phase space shifting transformation [48–55] that affects the positions $\mathbf{r}_i$ and the momenta $\mathbf{p}_i$ of a classical many-body system, where the index $i = 1, \ldots, N$ enumerates the N particles. The shifting transform [51] is parameterized by a smooth (infinitely differentiable) three-dimensional vector field $\boldsymbol{\epsilon}(\mathbf{r})$, where $\mathbf{r}$ denotes spatial position.

The position and momentum degrees of freedom of each particle i are affected in the same way. Specifically, the phase space transformation is

$$\mathbf{r}_i \to \mathbf{r}_i + \boldsymbol{\epsilon}(\mathbf{r}_i) = \mathbf{r}_i', \tag{10}$$

$$\mathbf{p}_i \to [\mathbb{1} + \nabla_i \boldsymbol{\epsilon}(\mathbf{r}_i)]^{-1} \cdot \mathbf{p}_i = \mathbf{p}_i', \tag{11}$$

where $\mathbb{1}$ denotes the $d \times d$-unit matrix, with d indicating spatial dimensionality, ∇_i denotes the derivative with respect to particle position $\mathbf{r}_i$, the superscript -1 denotes matrix inversion, and the transformed variables are indicated by a prime (rather than the tilde used in [53, 54, 64]). We adopt the convention that the ab-component of $\nabla_i \boldsymbol{\epsilon}(\mathbf{r}_i)$ is $[\nabla_i \boldsymbol{\epsilon}(\mathbf{r}_i)]_{ab} = \nabla_{i,a} \epsilon_b(\mathbf{r}_i)$, where the indices a,b denote the Cartesian components.

We assume that the shifting field $\boldsymbol{\epsilon}(\mathbf{r}_i)$ has a form that guarantees equation (10) to constitute a diffeomorphism. This implies that: (i) the transform from $\mathbf{r}_i$ to $\mathbf{r}_i'$ is smooth, which follows from $\boldsymbol{\epsilon}(\mathbf{r}_i)$ being smooth, (ii) an inverse exists, such that the map from $\mathbf{r}_i$ to $\mathbf{r}_i'$ is bijective, and (iii) the inverse transform from $\mathbf{r}_i'$ to $\mathbf{r}_i$ is also smooth.

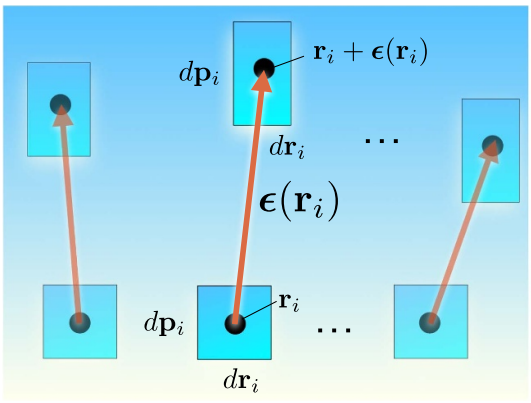


Figure 2. Shifting of microstates. The position and momentum degrees of freedom of each particle i are displaced according to the map (10) and (11). The vector field $\boldsymbol{\epsilon}(\mathbf{r}_i)$ parameterizes the transform, which is in general spatially inhomogeneous and of a form such that $\mathbf{r}_i + \boldsymbol{\epsilon}(\mathbf{r}_i)$ is a diffeomorphism. The transformation keeps the differential phase space volume element $d\mathbf{r}_i\, d\mathbf{p}_i$ conserved for each particle i.

It is straightforward to show that the Jacobian corresponding to the transformation (10) and (11) is unity [51, 55] and hence that the particle-resolved differential phase space volume element $d\mathbf{r}_i d\mathbf{p}_i$ is preserved under the transformation; see figure 2 for an illustration. The variable change expressed by equations (10) and (11) constitutes a canonical transformation in the sense of classical mechanics [67]. This can be seen by considering a generating function $\mathcal{G}$ from which the transformation is obtained by differentiation [67]. The specific form of this generator is $\mathcal{G} = \sum_i \mathbf{p}_i' \cdot [\mathbf{r}_i + \boldsymbol{\epsilon}(\mathbf{r}_i)]$ [55], where the prime denotes the transformed variables. Using the generic transformation equations $\mathbf{r}_i' = \partial\mathcal{G}/\partial\mathbf{p}_i'$ and $\mathbf{p}_i = \partial\mathcal{G}/\partial\mathbf{r}_i$ and solving for the primed variables gives equations (10) and (11).

Alternatively, one can verify that equations (10) and (11) constitute a canonical transformation by explicitly computing the following Poisson bracket identities:

$$\{\mathbf{r}_i', \mathbf{p}_j'\} = \delta_{ij}\mathbb{1}, \tag{12}$$

$$\{\mathbf{r}_i', \mathbf{r}_j'\} = \{\mathbf{p}_i', \mathbf{p}_j'\} = 0, \tag{13}$$

where the Poisson bracket $\{\cdot,\cdot\}$ is expressed in the original coordinates as $\{\hat{A}, \hat{B}\} = \sum_i [(\partial\hat{A}/\partial\mathbf{r}_i)\cdot(\partial\hat{B}/\partial\mathbf{p}_i) - (\partial\hat{A}/\partial\mathbf{p}_i)\cdot(\partial\hat{B}/\partial\mathbf{r}_i)]$, where $\hat{A}(\mathbf{r}^N, \mathbf{p}^N)$ and $\hat{B}(\mathbf{r}^N, \mathbf{p}^N)$ are two general phase space functions.

As a comment on the generality of the phase space shifting given by the joint transformation (10) and (11), this map is constructed to affect individual particles i in an identical way, which is in keeping with the aim of describing the statistical mechanics of identical particles. The position transform (10) is a general smooth map (diffeomorphism) from $\mathbf{r}_i$ to $\mathbf{r}_i'$. Hence the particular additive form $\mathbf{r}_i + \boldsymbol{\epsilon}(\mathbf{r}_i)$ poses no intrinsic restrictions. Note that any map $\mathbf{r}_i \to \mathbf{r}_i'(\mathbf{r}_i)$ can be rewritten trivially in the form of equation (10) as $\mathbf{r}_i \to \mathbf{r}_i + [\mathbf{r}_i'(\mathbf{r}_i) - \mathbf{r}_i]$, where the term in brackets then constitutes the shifting field, $\boldsymbol{\epsilon}(\mathbf{r}_i) = \mathbf{r}_i'(\mathbf{r}_i) - \mathbf{r}_i$. Given the choice of position transform (10), the momentum transform (11) then follows uniquely from imposing that the transformation is canonical and hence needs to satisfy equations (12) and (13). These differential equations leave over free remaining integration constants, which are uniquely determined

by the additional requirement that the identity transformation is recovered in the case of vanishing shifting field, $\boldsymbol{\epsilon}(\mathbf{r}_i) = 0$.

3.2. Finite phase space shifting group

We first demonstrate that the chaining of two shifting operations constitutes again a single shifting operation. Although this might seem obvious based on mere geometric intuition, carrying out a direct verification based on the structure of transformation equations (10) and (11) is worthwhile. We hence consider a second shifting transform, which is parameterized by a new shifting field $\boldsymbol{\epsilon}_2(\mathbf{r}_i')$ and which acts on the already transformed variables $\mathbf{r}_i'$ and $\mathbf{p}_i'$ that result from applying equations (10) and (11). The result of the consecutive shifting is:

$$\mathbf{r}_i'' = \mathbf{r}_i' + \boldsymbol{\epsilon}_2(\mathbf{r}_i'), \tag{14}$$

$$\mathbf{p}_i'' = [\mathbb{1} + \nabla_i' \boldsymbol{\epsilon}_2(\mathbf{r}_i')]^{-1} \cdot \mathbf{p}_i', \tag{15}$$

where ∇_i' denotes the derivative with respect to $\mathbf{r}_i'$. Replacing on the right hand sides of the transformation equations (14) and (15) the variables $\mathbf{r}_i'$ and $\mathbf{p}_i'$ via the transformations (10) and (11) yields the following composite expressions:

$$\mathbf{r}_i'' = \mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i) + \boldsymbol{\epsilon}_2(\mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i)), \tag{16}$$

$$\mathbf{p}_i'' = [\mathbb{1} + \nabla_i' \boldsymbol{\epsilon}_2(\mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i))]^{-1} \cdot [\mathbb{1} + \nabla_i \boldsymbol{\epsilon}_1(\mathbf{r}_i)]^{-1} \cdot \mathbf{p}_i. \tag{17}$$

We have kept the primed derivative in $\nabla_i' \boldsymbol{\epsilon}_2(\mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i))$ in equation (17) to indicate the standard gradient of the given vector field with respect to its argument, evaluated at position $\mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i)$, i.e. $\nabla_i' \boldsymbol{\epsilon}_2(\mathbf{r}_i')|_{\mathbf{r}_i' = \mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i)}$.

The conjecture that the mapping (16) and (17) is again a shifting transform implies that a corresponding shifting field $\boldsymbol{\epsilon}_{21}(\mathbf{r}_i)$ exists, which performs the composite transform in a single step according to:

$$\mathbf{r}_i'' = \mathbf{r}_i + \boldsymbol{\epsilon}_{21}(\mathbf{r}_i), \tag{18}$$

$$\mathbf{p}_i'' = [1 + \nabla_i \boldsymbol{\epsilon}_{21}(\mathbf{r}_i)]^{-1} \cdot \mathbf{p}_i. \tag{19}$$

Comparing the right hand side of the composite position transform (16) with the right hand side of the corresponding single-step position transform (18) allows one to identify:

$$\boldsymbol{\epsilon}_{21}(\mathbf{r}_i) = \boldsymbol{\epsilon}_1(\mathbf{r}_i) + \boldsymbol{\epsilon}_2(\mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i)). \tag{20}$$

Equation (20) is an explicit expression for the specific form of the shifting field $\boldsymbol{\epsilon}_{21}(\mathbf{r}_i)$ that represents the composite transform.

It thus remains to demonstrate the consistency of the single-step momentum transform (19) with the form (20) of the shifting field. Consistency implies that the right hand side of equations (17) and (19) need to be identical, which can only be true in general provided that the following matrices are identical:

$$[\mathbb{1} + \nabla_i \boldsymbol{\epsilon}_{21}(\mathbf{r}_i)]^{-1} = [\mathbb{1} + \nabla_i' \boldsymbol{\epsilon}_2(\mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i))]^{-1} \cdot [\mathbb{1} + \nabla_i \boldsymbol{\epsilon}_1(\mathbf{r}_i)]^{-1}. \tag{21}$$

The validity of equation (21) can be verified straightforwardly by inverting the matrices on both its sides and using the chain rule as follows. Keeping in mind to interchange the order of the matrix product upon matrix inversion gives:

$$\mathbb{1} + \nabla_i \boldsymbol{\epsilon}_{21}(\mathbf{r}_i) = [\mathbb{1} + \nabla_i \boldsymbol{\epsilon}_1(\mathbf{r}_i)] \cdot [\mathbb{1} + \nabla_i' \boldsymbol{\epsilon}_2(\mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i))]. \tag{22}$$

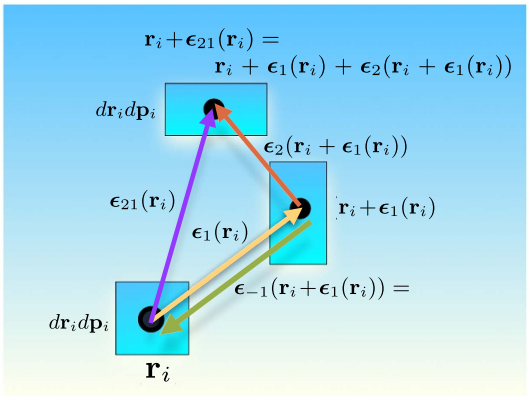


Figure 3. Group structure of local gauge transformations in statistical mechanics. The rich group structure emerges when chaining multiple local shifting operations together. Applying two consecutive transformations $\boldsymbol{\epsilon}_1(\mathbf{r}_i)$ and $\boldsymbol{\epsilon}_2(\mathbf{r}_i)$ results in a new transformation which is parameterized by $\boldsymbol{\epsilon}_{21}(\mathbf{r}_i) = \boldsymbol{\epsilon}_1(\mathbf{r}_i) + \boldsymbol{\epsilon}_2(\mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i))$ according to equation (20). The final destination point is identical such that $\mathbf{r}_i + \boldsymbol{\epsilon}_{21}(\mathbf{r}_i) = \mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i) + \boldsymbol{\epsilon}_2(\mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i))$. For given shifting field $\boldsymbol{\epsilon}_1(\mathbf{r}_i)$ the corresponding inverse shifting field satisfies $\boldsymbol{\epsilon}_{-1}(\mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i)) = -\boldsymbol{\epsilon}_1(\mathbf{r}_i)$ according to equation (23). The phase space volume element $d\mathbf{r}_i\, d\mathbf{p}_i$ is conserved under the transformation, despite its changing shape.

Multiplying out the right hand side and simplifying, we can re-write equation (22) as $\nabla_i \boldsymbol{\epsilon}_{21}(\mathbf{r}_i) = \nabla_i \boldsymbol{\epsilon}_1(\mathbf{r}_i) + \nabla_i' \boldsymbol{\epsilon}_2(\mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i)) + [\nabla_i \boldsymbol{\epsilon}_1(\mathbf{r}_i)] \cdot \nabla_i' \boldsymbol{\epsilon}_2(\mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i))$. This result is identically obtained by building the gradient of equation (20) and using the chain rule on the right hand side. This completes our proof that chaining two shifting transformations parameterized by $\boldsymbol{\epsilon}_1(\mathbf{r})$ and $\boldsymbol{\epsilon}_2(\mathbf{r})$ reduces to a single shifting transformation with shifting field $\boldsymbol{\epsilon}_{21}(\mathbf{r})$ given by equation (20).

It remains to show the existence of an inverse transform, which is also straightforward. For given $\boldsymbol{\epsilon}_1(\mathbf{r}_i)$ the inverse transform $\boldsymbol{\epsilon}_{-1}(\mathbf{r}_i)$ is obtained in the concatenation (20) upon requiring that $\boldsymbol{\epsilon}_{-11}(\mathbf{r}_i) = 0$, which constitutes the neutral group element (identity) and we have replaced the index $2 \to -1$. Hence from equation (20) we obtain the inversion condition

$$\boldsymbol{\epsilon}_{-1}\left(\mathbf{r}_i + \boldsymbol{\epsilon}_1\left(\mathbf{r}_i\right)\right) = -\boldsymbol{\epsilon}_1\left(\mathbf{r}_i\right), \tag{23}$$

which is an implicit equation for the vector field $\boldsymbol{\epsilon}_{-1}(\mathbf{r}_i)$ for given form of $\boldsymbol{\epsilon}_1(\mathbf{r}_i)$. We have to restrict to vector fields $\boldsymbol{\epsilon}_1(\mathbf{r}_i)$ that allow $\boldsymbol{\epsilon}_{-1}(\mathbf{r}_i)$ to exist, which is guaranteed from the assumption that $\mathbf{r}_i + \boldsymbol{\epsilon}(\mathbf{r}_i)$ constitutes a diffeomorphism, as this implies the existence of an inverse. A simple counterexample is $\boldsymbol{\epsilon}_1(\mathbf{r}_i) = -\mathbf{r}_i$ [51] which according to equation (10) maps all $\mathbf{r}_i$ to $\mathbf{r}_i' = 0$ and is hence trivially not bijective. For completeness, we exchange indices 1 and -1 in equation (23) to obtain the equivalent condition $\boldsymbol{\epsilon}_1(\mathbf{r}_i + \boldsymbol{\epsilon}_{-1}(\mathbf{r}_i)) = -\boldsymbol{\epsilon}_{-1}(\mathbf{r}_i)$. Figure 3 depicts an illustration of both the chaining and the inversion of shifting.

Composing together more than two shifting operations is associative, as is a requirement for valid group structure. An illustration is shown in figure 4. Algebraically one has to verify that for three consecutive transforms, as are respectively parameterized by three shifting fields $\boldsymbol{\epsilon}_1(\mathbf{r}_i)$, $\boldsymbol{\epsilon}_2(\mathbf{r}_i)$, and $\boldsymbol{\epsilon}_3(\mathbf{r}_i)$, the order of the grouping of pairs is irrelevant for the final result. We recall that the non-trivial geometrical structure arises from evaluating a subsequent shift to phase space points that have already been displaced by the prior shift.

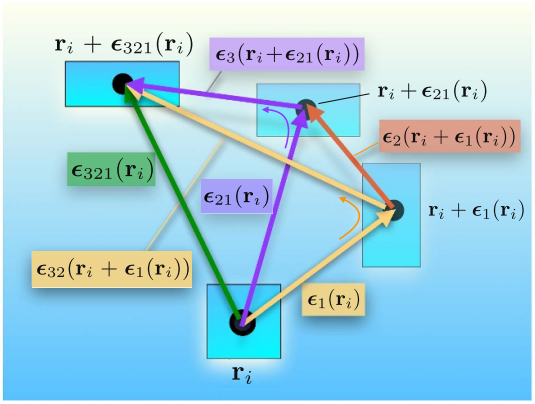


Figure 4. Associativity of the shifting transformation. Shown are different ways of shifting from $\mathbf{r}_i$ to $\mathbf{r}_i + \boldsymbol{\epsilon}_{321}(\mathbf{r}_i)$. Verifying the associative property implies to show that the combined shifting vector $\boldsymbol{\epsilon}_{321}(\mathbf{r}_i)$ of three consecutive transformations has two equivalent forms $\boldsymbol{\epsilon}_{32}(\mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i)) + \boldsymbol{\epsilon}_1(\mathbf{r}_i) = \boldsymbol{\epsilon}_3(\mathbf{r}_i + \boldsymbol{\epsilon}_{21}(\mathbf{r}_i)) + \boldsymbol{\epsilon}_{21}(\mathbf{r}_i)$ (indicated by the two curved arrows). This identity is straightforward to prove from applying equation (20) to the two pairs of consecutive operations, which respectively yield $\boldsymbol{\epsilon}_{21}(\mathbf{r}_i) = \boldsymbol{\epsilon}_1(\mathbf{r}_i) + \boldsymbol{\epsilon}_2(\mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i))$ and $\boldsymbol{\epsilon}_{32}(\mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i)) = \boldsymbol{\epsilon}_2(\mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i)) + \boldsymbol{\epsilon}_3(\mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i) + \boldsymbol{\epsilon}_2(\mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i)))$. Inserting these expressions proves the associativity of shifting.

We demonstrate the equivalence of both groupings explicitly in the following. First, when applying a third transformation to the composite (20), one obtains $\mathbf{r}_i''' = \mathbf{r}_i'' + \boldsymbol{\epsilon}_3(\mathbf{r}_i'') = \mathbf{r}_i'' + \boldsymbol{\epsilon}_3(\mathbf{r}_i + \boldsymbol{\epsilon}_{21}(\mathbf{r}_i)) = \mathbf{r}_i' + \boldsymbol{\epsilon}_2(\mathbf{r}_i') + \boldsymbol{\epsilon}_3(\mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i) + \boldsymbol{\epsilon}_2(\mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i)))$, which can be further made explicit as $\mathbf{r}_i''' = \mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i) + \boldsymbol{\epsilon}_2(\mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i)) + \boldsymbol{\epsilon}_3(\mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i) + \boldsymbol{\epsilon}_2(\mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i)))$. On the other hand, composing the second and third shift gives the displacement vector $\boldsymbol{\epsilon}_{32}(\mathbf{r}_i') = \boldsymbol{\epsilon}_2(\mathbf{r}_i') + \boldsymbol{\epsilon}_3(\mathbf{r}_i' + \boldsymbol{\epsilon}_2(\mathbf{r}_i'))$ as obtained from equation (20) by replacing $1 \to 2$, $2 \to 3$, and $\mathbf{r}_i \to \mathbf{r}_i'$. The overall transformed vector is then $\mathbf{r}_i''' = \mathbf{r}_i' + \boldsymbol{\epsilon}_{32}(\mathbf{r}_i') = \mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i) + \boldsymbol{\epsilon}_{32}(\mathbf{r}_i') = \mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i) + \boldsymbol{\epsilon}_2(\mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i)) + \boldsymbol{\epsilon}_3(\mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i) + \boldsymbol{\epsilon}_2(\mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i)))$, where we have first replaced $\mathbf{r}_i'$ according to equation (10) and have used the prior expression for $\boldsymbol{\epsilon}_{32}(\mathbf{r}_i')$. Both expressions are identical, which proves associativity for both the position and momentum parts of the phase space shifting. Figure 4 depicts an illustration of the associative shifting structure.

Despite the fact that composition, inversion and associativity are all relatively straightforward, the chaining of two finite shifting operations, as specified by the composite shifting field equation (20), is not a commutative operation. This can be seen by interchanging the first and second shifting fields on the right hand side of equation (20), which we reproduce for convenience: $\boldsymbol{\epsilon}_{21}(\mathbf{r}_i) = \boldsymbol{\epsilon}_1(\mathbf{r}_i) + \boldsymbol{\epsilon}_2(\mathbf{r}_i + \boldsymbol{\epsilon}_1(\mathbf{r}_i))$. The result is a composite shift given by $\boldsymbol{\epsilon}_{12}(\mathbf{r}_i) = \boldsymbol{\epsilon}_2(\mathbf{r}_i) + \boldsymbol{\epsilon}_1(\mathbf{r}_i + \boldsymbol{\epsilon}_2(\mathbf{r}_i))$, as obtained from interchanging the indices $1 \leftrightarrow 2$. In general the two results will be different from each other, $\boldsymbol{\epsilon}_{12}(\mathbf{r}) \neq \boldsymbol{\epsilon}_{21}(\mathbf{r})$; see figure 5 for an illustration. We demonstrate in the following section 3.3 that the non-commutative character persists for infinitesimal shifting.

In summary, we have shown that locally resolved shifting transformations on phase space given by equations (10) and (11) constitute a non-commutative group. We recall from section 2 the following requirements: (i) the composite of two group element is again a group element, (ii) the existence of a neutral element, (iii) the existence of an inverse, and (iv) associativity. The group elements are parameterized by the form of their corresponding shifting vector field $\boldsymbol{\epsilon}(\mathbf{r})$, which in general can be of finite magnitude.

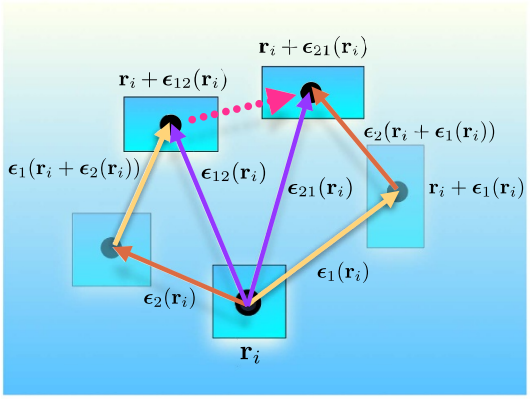


Figure 5. Non-commutative nature of the shifting transformation. Reversing the order of the two shifting operations that are respectively parameterized by $\epsilon_1(\mathbf{r}_i)$ and $\epsilon_2(\mathbf{r}_i)$ creates a spatial mismatch (dotted arrow) between the two destination points $\mathbf{r}_i + \epsilon_{12}(\mathbf{r}_i)$ and $\mathbf{r}_i + \epsilon_{21}(\mathbf{r}_i)$. The non-commutativity is due to the fact that in general $\epsilon_{21}(\mathbf{r}_i) \neq \epsilon_{12}(\mathbf{r}_i)$. Here the combined shifting vectors are given by $\epsilon_{21}(\mathbf{r}_i) = \epsilon_1(\mathbf{r}_i) + \epsilon_2(\mathbf{r}_i + \epsilon_1(\mathbf{r}_i))$, according to equation (20), and by $\epsilon_{12}(\mathbf{r}_i) = \epsilon_2(\mathbf{r}_i) + \epsilon_1(\mathbf{r}_i + \epsilon_2(\mathbf{r}_i))$, as obtained by exchanging the indices $1 \leftrightarrow 2$.

3.3. *Infinitesimal pure position shifting*

It is interesting to consider the infinitesimal version of the shifting transformation and in particular to investigate the algebraic structure that emerges from composite shifting. We first address the inversion operation which to first order in the shifting field and its gradient is given by

$$\epsilon_{-1}(\mathbf{r}_i) = -\epsilon_1(\mathbf{r}_i) + \epsilon_1(\mathbf{r}_i) \cdot \nabla_i \epsilon_1(\mathbf{r}_i). \tag{24}$$

A derivation of equation (24) can be based on expanding the left hand side of the inversion condition (23) to obtain $\epsilon_{-1}(\mathbf{r}_i) + \epsilon_1(\mathbf{r}_i) \cdot \nabla_i \epsilon_{-1}(\mathbf{r}_i) = -\epsilon_1(\mathbf{r}_i)$, which upon re-ordering gives $\epsilon_{-1}(\mathbf{r}_i) = -\epsilon_1(\mathbf{r}_i) \cdot [\mathbb{1} + \nabla_i \epsilon_{-1}(\mathbf{r}_i)]$ and $\epsilon_{-1}(\mathbf{r}_i) \cdot [\mathbb{1} + \nabla_i \epsilon_{-1}(\mathbf{r}_i)]^{-1} = -\epsilon_1(\mathbf{r}_i)$. Expanding the inverse matrix and truncating after the linear term gives $[\mathbb{1} + \nabla_i \epsilon_{-1}(\mathbf{r}_i)]^{-1} = \mathbb{1} - \nabla_i \epsilon_{-1}(\mathbf{r}_i)$ which yields equation (24) upon interchanging $\epsilon_{-1}(\mathbf{r}_i)$ and $\epsilon_1(\mathbf{r}_i)$.

We consider the action of the spatial displacement (10) on a position-dependent function $f(\mathbf{r}_i)$, which is hence moved to $f(\mathbf{r}_i') = f(\mathbf{r}_i + \epsilon_1(\mathbf{r}_i))$, as obtained from using the position transform (10). Taylor expanding in $\epsilon_1(\mathbf{r}_i)$ yields $f(\mathbf{r}_i') = f(\mathbf{r}_i) + \epsilon_1(\mathbf{r}_i) \cdot \nabla_i f(\mathbf{r}_i)$ to linear order in $\epsilon_1(\mathbf{r}_i)$. From the structure of the Taylor expansion we can identify the differential operator $\epsilon_1(\mathbf{r}_i) \cdot \nabla_i$ as performing the change of the function $f(\mathbf{r}_i)$ to $f(\mathbf{r}_i')$ to first order in $\epsilon_1(\mathbf{r}_i)$. Correspondingly, shifting by a vector field $\epsilon_2(\mathbf{r}_i)$ is represented by the operator $\epsilon_2(\mathbf{r}_i) \cdot \nabla_i$.

Successively applying two shifts requires to first expand $f(\mathbf{r}_i'') = f(\mathbf{r}_i' + \epsilon_2(\mathbf{r}_i'))$ around $\mathbf{r}_i'$ and then, after inserting $\mathbf{r}_i' = \mathbf{r}_i + \epsilon_1(\mathbf{r}_i)$, to expand around $\mathbf{r}_i$. The overall result is $f(\mathbf{r}_i'') = [f(\mathbf{r}_i) + \epsilon_2(\mathbf{r}_i) \cdot \nabla_i f(\mathbf{r}_i)] + \epsilon_1(\mathbf{r}_i) \cdot \nabla_i [f(\mathbf{r}_i) + \epsilon_2(\mathbf{r}_i) \cdot \nabla_i f(\mathbf{r}_i)]$, which we re-group as:

$$\begin{aligned} f(\mathbf{r}_i'') = f(\mathbf{r}_i) &+ [\epsilon_1(\mathbf{r}_i) + \epsilon_2(\mathbf{r}_i)] \cdot \nabla_i f(\mathbf{r}_i) \\ &+ \epsilon_1(\mathbf{r}_i) \cdot \nabla_i [\epsilon_2(\mathbf{r}_i) \cdot \nabla_i f(\mathbf{r}_i)]. \end{aligned} \tag{25}$$

Here the order of the two consecutive shifts is imprinted in the specific form of the last term of the sum on the right hand side of equation (25). Reversing the order of the two shifts leads

to a corresponding term $\boldsymbol{\epsilon}_2(\mathbf{r}_i)\cdot\nabla_i[\boldsymbol{\epsilon}_1(\mathbf{r}_i)\cdot\nabla_i f(\mathbf{r}_i)]$, which in general is different from the last term in equation (25).

To systematically capture the emerging difference it is appropriate to consider the commutator of two shifting differential operators $\boldsymbol{\epsilon}_1(\mathbf{r}_i)\cdot\nabla_i$ and $\boldsymbol{\epsilon}_2(\mathbf{r}_i)\cdot\nabla_i$. The following structure is obtained from straightforward calculation:

$$[\boldsymbol{\epsilon}_1(\mathbf{r}_i)\cdot\nabla_i,\boldsymbol{\epsilon}_2(\mathbf{r}_i)\cdot\nabla_i]=\boldsymbol{\epsilon}_\Delta(\mathbf{r}_i)\cdot\nabla_i, \tag{26}$$

where the brackets denote the commutator of two operators $\mathcal{O}_1$ and $\mathcal{O}_2$ in the usual way as $[\mathcal{O}_1,\mathcal{O}_2]=\mathcal{O}_1\mathcal{O}_2-\mathcal{O}_2\mathcal{O}_1$. Hence spelling out equation (26) explicitly gives $[\boldsymbol{\epsilon}_1(\mathbf{r}_i)\cdot\nabla_i,\boldsymbol{\epsilon}_2(\mathbf{r}_i)\cdot\nabla_i]=\boldsymbol{\epsilon}_1(\mathbf{r}_i)\cdot\nabla_i\boldsymbol{\epsilon}_2(\mathbf{r}_i)\cdot\nabla_i-\boldsymbol{\epsilon}_2(\mathbf{r}_i)\cdot\nabla_i\boldsymbol{\epsilon}_1(\mathbf{r}_i)\cdot\nabla_i$, with each derivative ∇_i acting on all functions to its right.

The vector field $\boldsymbol{\epsilon}_\Delta(\mathbf{r})$ in equation (26) that represents the difference between the two composite shifts is given by

$$\boldsymbol{\epsilon}_\Delta(\mathbf{r}_i)=\boldsymbol{\epsilon}_1(\mathbf{r}_i)\cdot[\nabla_i\boldsymbol{\epsilon}_2(\mathbf{r}_i)]-\boldsymbol{\epsilon}_2(\mathbf{r}_i)\cdot[\nabla_i\boldsymbol{\epsilon}_1(\mathbf{r}_i)] \tag{27}$$

$$=[\boldsymbol{\epsilon}_1(\mathbf{r}_i),\boldsymbol{\epsilon}_2(\mathbf{r}_i)]_{\mathrm{L}}, \tag{28}$$

where the matrices $[\nabla_i\boldsymbol{\epsilon}_1(\mathbf{r}_i)]$ and $[\nabla_i\boldsymbol{\epsilon}_2(\mathbf{r}_i)]$ in equation (27) are not differential operators but rather tensor fields. In general the right hand side of equation (27) will not vanish, $\boldsymbol{\epsilon}_\Delta(\mathbf{r}_i)\neq 0$. The particular combination (27) of two given vector fields $\boldsymbol{\epsilon}_1(\mathbf{r}_i)$ and $\boldsymbol{\epsilon}_2(\mathbf{r}_i)$ constitutes the *Lie bracket* $[\boldsymbol{\epsilon}_1(\mathbf{r}_i),\boldsymbol{\epsilon}_2(\mathbf{r}_i)]_{\mathrm{L}}$ as is defined in the standard way [72] in equation (27).

Using the Lie bracket (28) we can rewrite the right hand side of the shifting commutator relation (26) to express the commutator relationship as:

$$[\boldsymbol{\epsilon}_1(\mathbf{r}_i)\cdot\nabla_i,\boldsymbol{\epsilon}_2(\mathbf{r}_i)\cdot\nabla_i]=[\boldsymbol{\epsilon}_1(\mathbf{r}_i),\boldsymbol{\epsilon}_2(\mathbf{r}_i)]_{\mathrm{L}}\cdot\nabla_i, \tag{29}$$

which constitutes a Lie algebra of differential operators.

We have so far formulated the theory on the basis of specific choices of the shifting fields $\boldsymbol{\epsilon}_1(\mathbf{r})$, $\boldsymbol{\epsilon}_2(\mathbf{r})$ and the resulting form of $\boldsymbol{\epsilon}_\Delta(\mathbf{r})$. However, the specific form of these vector fields is not of physical interest, as any observables are independent of the shifting fields, as is consistent with their role as mere gauge functions.

Separating the specificities from the intrinsic nature of the shifting is technically achieved by working with functional differentiation (see [61] for a practitioners' account) and we recall that Noether's theorem addresses such invariant variations [1]. Hence having identified the position shifting operators $\boldsymbol{\epsilon}(\mathbf{r}_i)\cdot\nabla_i$, we functionally differentiate with respect to $\boldsymbol{\epsilon}(\mathbf{r})$ as a measure of the response of the shifting operator $\boldsymbol{\epsilon}(\mathbf{r}_i)\cdot\nabla_i$ against changes in the shifting field at a (new) position $\mathbf{r}$.

The functional derivative is straightforward to carry out and leads to

$$\frac{\delta}{\delta\boldsymbol{\epsilon}(\mathbf{r})}\boldsymbol{\epsilon}(\mathbf{r}_i)\cdot\nabla_i=\delta(\mathbf{r}_i-\mathbf{r})\nabla_i, \tag{30}$$

where we have used that $\delta\boldsymbol{\epsilon}(\mathbf{r}_i)/\delta\boldsymbol{\epsilon}(\mathbf{r})=\mathbb{1}\delta(\mathbf{r}_i-\mathbf{r})$ and $\mathbb{1}\cdot\nabla=\nabla$. Multiplying (via a scalar product) the right hand side of equation (30) with $\boldsymbol{\epsilon}(\mathbf{r})$ and integrating over $\mathbf{r}$ recovers the original position-shifting operator according to:

$$\boldsymbol{\epsilon}(\mathbf{r}_i)\cdot\nabla_i=\int d\mathbf{r}\boldsymbol{\epsilon}(\mathbf{r})\cdot\delta(\mathbf{r}_i-\mathbf{r})\nabla_i. \tag{31}$$

Equation (31) can be viewed as a simple case of functional integration (where here the functional integrand is independent of the functional argument $\boldsymbol{\epsilon}(\mathbf{r})$). We refer to [18, 19, 58–60, 73] both for descriptions and use of functional integration in more general settings, in particular in the context neural functionals [58–60, 73].

The commutator relationship (29) has a simple bilinear dependence on the two shifting fields. It is hence straightforward to build the mixed second functional derivative of equation (26) according to $\delta^2/[\delta\boldsymbol{\epsilon}_1(\mathbf{r})\delta\boldsymbol{\epsilon}_2(\mathbf{r}')]$, where $\mathbf{r}$ and $\mathbf{r}'$ are two new position variables. The functional dependence on the shifting fields is explicit on the left hand side of equation (29). Functionally differentiating the right hand side of equation (29) requires to take into account that $\boldsymbol{\epsilon}_\Delta(\mathbf{r}_i)$ depends on the vector fields $\boldsymbol{\epsilon}_1(\mathbf{r}_i)$ and $\boldsymbol{\epsilon}_2(\mathbf{r}_i)$ via equation (27), which gives $\delta^2\epsilon_{\Delta c}(\mathbf{r}_i)/[\delta\epsilon_{1a}(\mathbf{r})\delta\epsilon_{2b}(\mathbf{r}')] = \delta(\mathbf{r}_i-\mathbf{r})[\nabla_i^a\delta(\mathbf{r}_i-\mathbf{r}')\delta_{bc}] - \delta(\mathbf{r}_i-\mathbf{r}')[\nabla_i^b\delta(\mathbf{r}_i-\mathbf{r})\delta_{ac}]$, where a,b,c denote the Cartesian components and we have used $\delta\epsilon_a(\mathbf{r}_i)/\delta\epsilon_b(\mathbf{r}) = \delta(\mathbf{r}_i-\mathbf{r})\delta_{ab}$. The overall result for the mixed functional derivative of the commutator relationship (29) is:

$$
\begin{aligned}
&[\delta(\mathbf{r}_i-\mathbf{r})\nabla_i, \delta(\mathbf{r}_i-\mathbf{r}')\nabla_i] \\
&= [\nabla_i\delta(\mathbf{r}_i-\mathbf{r}')]\,\delta(\mathbf{r}_i-\mathbf{r})\nabla_i - [\nabla_i\delta(\mathbf{r}_i-\mathbf{r})]\,\delta(\mathbf{r}_i-\mathbf{r}')\nabla_i^{\mathsf{T}} \qquad (32)\\
&= \delta(\mathbf{r}_i-\mathbf{r}')\nabla_i\,[\nabla\delta(\mathbf{r}-\mathbf{r}')] + [\nabla\delta(\mathbf{r}-\mathbf{r}')]\,\delta(\mathbf{r}_i-\mathbf{r})\nabla_i, \qquad (33)
\end{aligned}
$$

where as before ∇ indicates the derivative with respect to $\mathbf{r}$ and the superscript T denotes matrix transposition, here of a dyadic product.

We introduce an integral over $\mathbf{r}''$ on the right hand to express the result as the following operator identity

$$
[\delta(\mathbf{r}_i-\mathbf{r})\nabla_i, \delta(\mathbf{r}_i-\mathbf{r}')\nabla_i] = \int d\mathbf{r}''\mathsf{D}(\mathbf{r},\mathbf{r}',\mathbf{r}'')\cdot\delta(\mathbf{r}_i-\mathbf{r}'')\nabla_i \qquad (34)
$$

where D is a third-rank tensor that plays the role of Lie structure constants. The abc-component of D is given by

$$
D_{abc}(\mathbf{r},\mathbf{r}',\mathbf{r}'') = \delta_{bc}\delta(\mathbf{r}''-\mathbf{r})[\nabla_a''\delta(\mathbf{r}''-\mathbf{r}')] - \delta_{ac}\delta(\mathbf{r}''-\mathbf{r}')[\nabla_b''\delta(\mathbf{r}''-\mathbf{r})], \qquad (35)
$$

where ∇'' denotes the derivative with respect to $\mathbf{r}''$.

In summary we have demonstrated, for the case of position-only shifting, the relationship of the spatial displacement with the action of shifting differential operators. We have shown that the non-commutative nature that is inherent when considering finite displacements persists when Taylor expanding and keeping only the lowest nontrivial terms. The non-commutative aspect is then reflected by algebraic relationships. Specifically, when expressed in the form (35) it is apparent that the particular form of the product of the delta distribution and derivative operator, $\delta(\mathbf{r}_i-\mathbf{r})\nabla_i$, persists as a result of building the commutator.

In section 4.3, we demonstrate that much of this favorable structure can be retained when considering the joint phase space transformation of coordinates and momenta. We recall that this constitutes a canonical transformation, which the present position-only shifting with unchanged momenta does not.

4. Statistical mechanics

4.1. Partition sum and thermal averages

We present the invariance argument [54] for the thermal mean of a phase space function $\hat{A}(\mathbf{r}^N)$, where $\mathbf{r}^N = \mathbf{r}_1, \ldots, \mathbf{r}_N$ is a shorthand for all position coordinates in the system with $\mathbf{r}_i$ denoting the position coordinate of particle $i = 1, \ldots, N$ in d spatial dimensions, and N indicates the total number of particles. The canonical average is given by the classical trace operation $\mathrm{Tr}\cdot = (N!h^{dN})^{-1}\int d\mathbf{r}^N d\mathbf{p}^N \cdot$, where h indicates Planck's constant and $\int d\mathbf{r}^N d\mathbf{p}^N$ denotes the phase space integral over all coordinates $\mathbf{r}^N$ and momentum variables $\mathbf{p}^N = \mathbf{p}_1, \ldots, \mathbf{p}_N$. The partition sum is $Z = \mathrm{Tr}\,\mathrm{e}^{-\beta H(\mathbf{r}^N, \mathbf{p}^N)}$, where $H(\mathbf{r}^N, \mathbf{p}^N)$ denotes the Hamiltonian, with inverse temperature $\beta = 1/(k_\mathrm{B}T)$, where k_B denotes the Boltzmann constant and T the absolute temperature. The Helmholtz free energy is then $F = -k_\mathrm{B}T\ln Z$. Thermal averages are obtained as

$$\langle\cdot\rangle = \mathrm{Tr}\cdot \mathrm{e}^{-\beta H(\mathbf{r}^N, \mathbf{p}^N)}/Z. \tag{36}$$

More explicitly the thermal average of an observable $\hat{A}(\mathbf{r}^N)$ is given by

$$A = \frac{1}{h^{dN}N!}\int d\mathbf{r}^N d\mathbf{p}^N \hat{A}\left(\mathbf{r}^N\right)\mathrm{e}^{-\beta H(\mathbf{r}^N, \mathbf{p}^N)}/Z. \tag{37}$$

We first rewrite the phase space integral in equation (37) in an identical way upon merely renaming the unprimed by primed variables:

$$A = \frac{1}{h^{dN}N!}\int d\mathbf{r}'^N d\mathbf{p}'^N \hat{A}\left(\mathbf{r}'^N\right)\mathrm{e}^{-\beta H(\mathbf{r}'^N, \mathbf{p}'^N)}/Z', \tag{38}$$

where the primed partition sum Z' is expressed in the primed variables and $Z' = Z$.

We next perform the canonical variable transformation given by equations (10) and (11). The phase space volume element is thereby conserved such that $d\mathbf{r}_i d\mathbf{p}_i = d\mathbf{r}'_i d\mathbf{p}'_i$ for each particle i. The result is

$$A = \frac{1}{h^{dN}N!}\int d\mathbf{r}^N d\mathbf{p}^N \hat{A}\left(\mathbf{r}'^N\right)\mathrm{e}^{-\beta H(\mathbf{r}'^N, \mathbf{p}'^N)}/Z', \tag{39}$$

$$= A\left[\boldsymbol{\epsilon}\right]. \tag{40}$$

The dependence of the integrand in equation (39) on the unprimed variables is suppressed in the notation for clarity and it occurs via the transformation equations (10) and (11) that render the $\mathbf{r}'_i$ and $\mathbf{p}'_i$ parametrically dependent on $\mathbf{r}_i$ and $\mathbf{p}_i$ and functionally dependent on the form of the shifting field $\boldsymbol{\epsilon}(\mathbf{r})$. Spelling out these dependencies explicitly we have $\mathbf{r}'_i = \mathbf{r}'_i(\mathbf{r}_i, [\boldsymbol{\epsilon}])$ according to equation (10) and $\mathbf{p}'_i = \mathbf{p}'(\mathbf{r}_i, \mathbf{p}_i, [\boldsymbol{\epsilon}])$ according to equation (11).

After the unprimed phase space integral is performed, at face value equation (39) depends functionally on the shifting field, which we have indicated as $A[\boldsymbol{\epsilon}]$ in equation (40). Comparing equation (37) with equation (40) gives the invariance condition $A = A[\boldsymbol{\epsilon}]$, where the left hand side can also be understood as $A[\epsilon]$ being evaluated at vanishing shifting field, $\boldsymbol{\epsilon}(\mathbf{r}) = 0$, such that $A[0] = A[\boldsymbol{\epsilon}]$.

As the phase space shifting affects systems with fixed number of particles, the argumentation carries over to the grand ensemble where each system with N particles is displaced identically. Hence besides the changes in the definition of the grand ensemble averages, no further alterations occur in any of the results.

To be specific, we consider Hamiltonians that consist of kinetic, interparticle, and external energy contributions according to the sum:

$$H\left(\mathbf{r}^N,\mathbf{p}^N\right)=\sum_i\frac{\mathbf{p}_i^2}{2m}+u\left(\mathbf{r}^N\right)+\sum_i V_{\mathrm{ext}}\left(\mathbf{r}_i\right), \tag{41}$$

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 $V_{\mathrm{ext}}(\mathbf{r})$ is an external one-body potential.

4.2. One-body observables

We lay out the relevant one-body observables, which are pertinent in the equilibrium sum rules that follow from the gauge invariance as described above. The one-body level of correlation functions is integral in the classical density functional formulation of statistical mechanics [17–19, 61, 74] and it naturally extends to the dynamical problems, see [61] for systematic (power functional) derivations on the basis of classical Hamiltonian, overdamped Brownian, and quantum many-body time evolution.

The one-body localization enables one to carry out systematic coarse-graining in the sense of reduction of the full phase space information, while it remains microscopically sharp, such that all features on microscopic length scales are resolved without any principal loss. The primary one-body observable is the one-body density distribution or density 'profile' $\rho(\mathbf{r})$. When working with functional relationships two- and higher-body observables are in principle accessible via functional differentiation both in [17–19, 61, 74] and out-of-equilibrium [61].

As an aside, to reach beyond the hierarchy of increasingly higher-order correlation functions, the recent hyperdensity functional theory [59, 60] allows one to treat complex order parameters, including algorithmically defined phase space functions, on the basis of the density profile as the fundamental variable, as is ensured by the Mermin–Evans [18, 75] density functional map.

The response of the Hamiltonian H against changes in the form of the external potential $V_{\mathrm{ext}}(\mathbf{r})$ is measured by the functional derivative $\hat{\rho}(\mathbf{r})=\delta H/\delta V_{\mathrm{ext}}(\mathbf{r})$, where the density 'operator' (phase space function) is obtained as:

$$\hat{\rho}\left(\mathbf{r}\right)=\sum_i\delta\left(\mathbf{r}-\mathbf{r}_i\right). \tag{42}$$

The density profile is the thermal average, $\rho(\mathbf{r})=\langle\hat{\rho}(\mathbf{r})\rangle$. Its use allows one to express the average localized external force density as $-\rho(\mathbf{r})\nabla V_{\mathrm{ext}}(\mathbf{r})$, where we recall that $V_{\mathrm{ext}}(\mathbf{r})$ is the external potential that a particle situated at position $\mathbf{r}$ contributes, and $-\nabla V_{\mathrm{ext}}(\mathbf{r})$ is the corresponding external force field. It is straightforward to show the equality $-\rho(\mathbf{r})\nabla V_{\mathrm{ext}}(\mathbf{r})=\langle\sum_i\delta(\mathbf{r}-\mathbf{r}_i)\mathbf{f}_{\mathrm{ext}}(\mathbf{r}_i)\rangle$, where the external force field is $\mathbf{f}_{\mathrm{ext}}(\mathbf{r})=-\nabla V_{\mathrm{ext}}(\mathbf{r})$.

The localized interparticle force density 'operator' (phase space function) is defined as:

$$\hat{\mathbf{F}}_{\mathrm{int}}\left(\mathbf{r}\right)=-\sum_i\delta\left(\mathbf{r}-\mathbf{r}_i\right)\nabla_i u\left(\mathbf{r}^N\right). \tag{43}$$

The corresponding mean interparticle force density is simply the average $\mathbf{F}_{\mathrm{int}}(\mathbf{r})=\langle\hat{\mathbf{F}}_{\mathrm{int}}(\mathbf{r})\rangle$, with $\hat{\mathbf{F}}_{\mathrm{int}}(\mathbf{r})$ defined by equation (43). Interparticle and external force densities can be combined into a dedicated potential force density:

$$\mathbf{F}_U\left(\mathbf{r}\right)=\mathbf{F}_{\mathrm{int}}\left(\mathbf{r}\right)-\rho\left(\mathbf{r}\right)\nabla V_{\mathrm{ext}}\left(\mathbf{r}\right), \tag{44}$$

where the subscript U refers to total potential energy, as represented by the corresponding phase space function $\hat{U} = u(\mathbf{r}^N) + \sum_i V_{\text{ext}}(\mathbf{r}_i)$. The resulting potential force density 'operator' is analogously defined via

$$\hat{\mathbf{F}}_U(\mathbf{r}) = \hat{\mathbf{F}}_{\text{int}}(\mathbf{r}) - \hat{\rho}(\mathbf{r})\nabla V_{\text{ext}}(\mathbf{r}), \tag{45}$$

and by construction the average is the mean potential force density, $\mathbf{F}_U(\mathbf{r}) = \langle \hat{\mathbf{F}}_U(\mathbf{r}) \rangle$.

In equilibrium the potential forces are balanced by a thermal force density which arises from the kinetic energy contribution to the Hamiltonian (41). The general phase space function that underlies this effect is the localized kinetic stress 'operator' $\hat{\boldsymbol{\tau}}(\mathbf{r})$ which is defined as:

$$\hat{\boldsymbol{\tau}}(\mathbf{r}) = -\sum_i \frac{\mathbf{p}_i \mathbf{p}_i}{m} \delta(\mathbf{r} - \mathbf{r}_i), \tag{46}$$

where $\mathbf{p}_i \mathbf{p}_i$ denotes the dyadic product of the momentum of particle i with itself. It is straightforward to show upon using the properties of the Maxwellian, i.e. the Gaussian distribution of the momenta according to the Boltzmann factor, that $\nabla \cdot \boldsymbol{\tau}(\mathbf{r}) = \nabla \cdot \langle \hat{\boldsymbol{\tau}}(\mathbf{r}) \rangle = -k_{\text{B}} T \nabla \rho(\mathbf{r})$, which acts as a thermal, diffusive force density.

Collecting kinetic, interparticle, and external contributions, we can define a total force density operator:

$$\hat{\mathbf{F}}(\mathbf{r}) = \nabla \cdot \hat{\boldsymbol{\tau}}(\mathbf{r}) + \hat{\mathbf{F}}_{\text{int}}(\mathbf{r}) - \hat{\rho}(\mathbf{r})\nabla V_{\text{ext}}(\mathbf{r}), \tag{47}$$

where we refer the reader to [61] for the derivation from the second time derivative of the density operator (42). In thermal equilibrium the average one-body force density $\mathbf{F}(\mathbf{r}) = \langle \hat{\mathbf{F}}(\mathbf{r}) \rangle$ vanishes,

$$\mathbf{F}(\mathbf{r}) = 0, \tag{48}$$

which upon spelling out the three individual terms is analogous to the more detailed form:

$$-k_{\text{B}} T \nabla \rho(\mathbf{r}) + \mathbf{F}_{\text{int}}(\mathbf{r}) - \rho(\mathbf{r})\nabla V_{\text{ext}}(\mathbf{r}) = 0. \tag{49}$$

The equilibrium force density balance (48) can be verified by explicit calculation of the thermal averages upon using partial integration on phase space to manipulate the occurring coordinate derivatives. In particular when the interparticle force density $\mathbf{F}_{\text{int}}(\mathbf{r})$ is expressed as an integral over the two-body density multiplied by the pair force, equation (48) is commonly referred to as the Yvon–Born–Green equation [17, 76, 77].

Finally, it is useful to define a configurational force density 'operator' as

$$\beta \hat{\mathbf{F}}_c(\mathbf{r}) = -\nabla \hat{\rho}(\mathbf{r}) + \beta \hat{\mathbf{F}}_U(\mathbf{r}), \tag{50}$$

which on average $\langle \hat{\mathbf{F}}_c(\mathbf{r}) \rangle = 0$, which is identical to the equilibrium force density balance (48). Note that for purely configurational observables $\hat{A}(\mathbf{r}^N)$, due to the simplicity of the Maxwellian, we have $\langle \hat{A}(\mathbf{r}^N) \hat{\mathbf{F}}_c(\mathbf{r}) \rangle = \langle \hat{A}(\mathbf{r}^N) \hat{\mathbf{F}}(\mathbf{r}) \rangle$, see e.g. [53] for further details of the thermal average of the kinetic stress operator (46).

4.3. Sum rules from pure position shifting

The mathematical structure of infinitesimal position shifting described in section 3.3 can be directly used to derive statistical mechanical sum rules, as we demonstrate in the following. We define the following localized position-shifting operators

$$\boldsymbol{\sigma}_c(\mathbf{r}) = \sum_i \delta(\mathbf{r} - \mathbf{r}_i)\nabla_i, \tag{51}$$

where the subscript c indicates that only the configuration $\mathbf{r}^N$ is affected, independent of the momentum degrees of freedom $\mathbf{p}^N$.

The adjoint operator is given by

$$\boldsymbol{\sigma}_c^\dagger(\mathbf{r}) = -\boldsymbol{\sigma}_c(\mathbf{r}) + \nabla\hat{\rho}(\mathbf{r}), \tag{52}$$

where the density operator $\hat{\rho}(\mathbf{r})$ is defined via equation (42). Equation (52) follows from configuration space (position) integration by parts, the product rule, and noting that in the resulting expression one can replace $-\nabla_i = \nabla$. Here the adjoint is understood with respect to the phase space integral, such that for any two general phase space functions $f(\mathbf{r}^N, \mathbf{p}^N)$ and $g(\mathbf{r}^N, \mathbf{p}^N)$ the adjoint $\mathcal{O}^\dagger$ of a given operator $\mathcal{O}$ is defined as satisfying $\int d\mathbf{r}^N d\mathbf{p}^N f\mathcal{O}^\dagger g = \int d\mathbf{r}^N d\mathbf{p}^N g\mathcal{O}f$.

The configurational shifting operators at two generic positions $\mathbf{r}$ and $\mathbf{r}'$ satisfy the commutator relationship

$$[\boldsymbol{\sigma}_c(\mathbf{r}), \boldsymbol{\sigma}_c(\mathbf{r}')] = \boldsymbol{\sigma}_c(\mathbf{r}')[\nabla\delta(\mathbf{r} - \mathbf{r}')] + [\nabla\delta(\mathbf{r} - \mathbf{r}')]\boldsymbol{\sigma}_c(\mathbf{r}). \tag{53}$$

Equation (53) follows straightforwardly from the corresponding single-particle commutator (33) upon summing the latter over i, then identifying the explicit form (51) of $\boldsymbol{\sigma}_c(\mathbf{r})$, and noticing that the commutator vanishes for two different particles $i \neq j$. We use the prime in the two different roles to denote the generic position variable $\mathbf{r}'$, which is in general unrelated to $\mathbf{r}$, as well as to indicate the transformed phase space coordinate $\mathbf{r}_i'$, which is related to $\mathbf{r}_i$ via the position transform (10).

It is interesting to apply the localized configuration shift operator (51) to the Hamiltonian, which yields

$$-[\boldsymbol{\sigma}_c(\mathbf{r})H] = \hat{\mathbf{F}}_U(\mathbf{r}), \tag{54}$$

where we recall the potential force density 'operator' $\hat{\mathbf{F}}_U(\mathbf{r})$ as the sum (45) of interparticle and external contributions. The brackets on the left hand side of equation (54) indicate the range of action of $\boldsymbol{\sigma}_c(\mathbf{r})$, i.e. it only operates on H but not beyond. The explicit verification of equation (54) can be based on the definition (51) of $\boldsymbol{\sigma}_c(\mathbf{r})$, the form (41) of the Hamiltonian, and the definition (44) of the potential force operator $\hat{\mathbf{F}}_U(\mathbf{r})$.

Similarly, when applied to the Boltzmann factor, the chain rule together with equation (54) yields straightforwardly

$$\left[\boldsymbol{\sigma}_c(\mathbf{r})\mathrm{e}^{-\beta H}\right] = \beta\hat{\mathbf{F}}_U(\mathbf{r})\mathrm{e}^{-\beta H}. \tag{55}$$

Equation (55) constitutes a fundamental link between spatial shifting of the (equilibrium) many-body probability distribution and the emergence of the localized force density operator. It remains to exploit the specific operator structure of the localized shifting operators, as embodied in equations (52) and (53), and to build the average over the equilibrium ensemble.

To derive hyperforce sum rules we multiply the adjoint identity (52) from the left by a purely coordinate-dependent phase space function $\hat{A}(\mathbf{r}^N)$ and then build the thermal average of the result, which gives:

$$\langle \hat{A}\boldsymbol{\sigma}_c^\dagger(\mathbf{r})\rangle = -\langle \hat{A}\boldsymbol{\sigma}_c(\mathbf{r})\rangle + \nabla\langle \hat{A}\hat{\rho}(\mathbf{r})\rangle. \tag{56}$$

Recalling the thermal average being defined via equation (36) the left hand side of equation (56) is explicitly given by $\langle \hat{A}\boldsymbol{\sigma}_c^\dagger(\mathbf{r})\rangle = \mathrm{Tr}\hat{A}\boldsymbol{\sigma}_c^\dagger(\mathbf{r})\mathrm{e}^{-\beta H}/Z = \mathrm{Tr}\,[\boldsymbol{\sigma}_c(\mathbf{r})\hat{A}]\mathrm{e}^{-\beta H}/Z = \langle[\boldsymbol{\sigma}_c(\mathbf{r})\hat{A}]\rangle$, where in the second step we have made use of the defining property of the adjoint operator. Making also the first term on the right hand side of equation (56) more explicit yields $-\langle \hat{A}\boldsymbol{\sigma}_c(\mathbf{r})\rangle = -\mathrm{Tr}\hat{A}\boldsymbol{\sigma}_c(\mathbf{r})\mathrm{e}^{-\beta H}/Z = -\mathrm{Tr}\hat{A}\beta\hat{\mathbf{F}}_U(\mathbf{r})\mathrm{e}^{-\beta H}/Z = -\langle \hat{A}\beta\hat{\mathbf{F}}_U(\mathbf{r})\rangle$, where we have first used the chain rule and then applied the configuration shift operator to the Boltzmann factor according to equation (55).

As the second term on the right hand side of equation (56) is already in the form of an explicit average, we can collect all terms to formulate the following exact equilibrium sum rule

$$\mathbf{S}_A(\mathbf{r}) = -\langle \hat{A}\beta\hat{\mathbf{F}}_U(\mathbf{r})\rangle + \nabla\langle \hat{A}\hat{\rho}(\mathbf{r})\rangle, \tag{57}$$

where the hyperforce density $\mathbf{S}_A(\mathbf{r}) = \langle\hat{\mathbf{S}}_A(\mathbf{r})\rangle$ is given in the present case of mere dependence on coordinates (independent of momenta) as

$$\hat{\mathbf{S}}_A(\mathbf{r}) = \left[\boldsymbol{\sigma}_c(\mathbf{r})\hat{A}\left(\mathbf{r}^N\right)\right] \tag{58}$$

$$= \sum_i \delta(\mathbf{r}-\mathbf{r}_i)\left[\nabla_i \hat{A}\left(\mathbf{r}^N\right)\right]. \tag{59}$$

The form (59) follows directly from the definition of the position shift operator (51). Using the configurational force density operator $\hat{\mathbf{F}}_c(\mathbf{r})$ given by equation (50) and rearranging allows one to rewrite the sum rule (57) as

$$\mathbf{S}_A(\mathbf{r}) + \langle \hat{A}\left(\mathbf{r}^N\right)\beta\hat{\mathbf{F}}_c(\mathbf{r})\rangle = 0. \tag{60}$$

The situation becomes even richer when using two (or more) shifting operators due to a larger variety of re-writing of equivalent expressions. This multitude could potentially be useful in concrete applications. We here restrict ourselves to two specific cases and hence first consider the operator algebra (53). To arrive at a sum rule, we multiply equation (53) by $\hat{A}(\mathbf{r}^N)$ from the left and then build the thermal average. The first term of the commutator is $\langle \hat{A}\boldsymbol{\sigma}_c(\mathbf{r})\boldsymbol{\sigma}_c(\mathbf{r}')\rangle = \langle[\boldsymbol{\sigma}_c^\dagger(\mathbf{r})\hat{A}]\boldsymbol{\sigma}_c(\mathbf{r}')\rangle = \langle[-\boldsymbol{\sigma}_c(\mathbf{r})\hat{A} + \nabla\hat{\rho}(\mathbf{r})\hat{A}]\beta\hat{\mathbf{F}}_U(\mathbf{r}')\rangle = -\langle\hat{\mathbf{S}}_A(\mathbf{r})\beta\hat{\mathbf{F}}_U(\mathbf{r}')\rangle + \nabla\langle\hat{A}\hat{\rho}(\mathbf{r})\beta\hat{\mathbf{F}}_U(\mathbf{r}')\rangle$, where we have first re-written via the adjoint $\boldsymbol{\sigma}_c^\dagger(\mathbf{r})$, and then used its relationship (52) and the definition (58) of the configurational hyperforce density operator $\mathbf{S}_A(\mathbf{r})$.

The result for the second term of the commutator either follows from an analogous chain of steps or, equivalently, via simply exchanging $\mathbf{r}$ and $\mathbf{r}'$ and transposing, which yields $\langle \hat{A}\boldsymbol{\sigma}_c(\mathbf{r}')\boldsymbol{\sigma}_c(\mathbf{r})\rangle^\mathsf{T} = -\langle\hat{\mathbf{S}}_A(\mathbf{r}')\beta\hat{\mathbf{F}}_U(\mathbf{r})\rangle^\mathsf{T} + \nabla'\langle\hat{A}\hat{\rho}(\mathbf{r}')\beta\hat{\mathbf{F}}_U(\mathbf{r})\rangle^\mathsf{T}$. Averaging the right hand side of the commutator relationship (53) is straightforward and requires the averages $\langle\hat{A}\boldsymbol{\sigma}_c(\mathbf{r}')\rangle = \langle\hat{A}\beta\hat{\mathbf{F}}_U(\mathbf{r}')\rangle$ and $\langle\hat{A}\boldsymbol{\sigma}_c(\mathbf{r})\rangle = \langle\hat{A}\beta\hat{\mathbf{F}}_U(\mathbf{r})\rangle$.

Collecting all terms we obtain as a result the following equilibrium hyperforce sum rule:

$$\begin{aligned}
&-\langle\hat{\mathbf{S}}_A(\mathbf{r})\,\beta\hat{\mathbf{F}}_U(\mathbf{r}')\rangle+\nabla\langle\hat{A}\rho(\mathbf{r})\,\beta\hat{\mathbf{F}}_U(\mathbf{r}')\rangle\\
&+\langle\hat{\mathbf{S}}_A(\mathbf{r}')\,\beta\hat{\mathbf{F}}_U(\mathbf{r})\rangle^{\mathsf{T}}-\nabla'\langle\hat{A}\rho(\mathbf{r}')\,\beta\hat{\mathbf{F}}_U(\mathbf{r})\rangle^{\mathsf{T}}\\
&\quad=\langle\hat{A}\beta\hat{\mathbf{F}}_U(\mathbf{r}')\rangle\,[\nabla\delta(\mathbf{r}-\mathbf{r}')]+[\nabla\delta(\mathbf{r}-\mathbf{r}')]\,\langle\hat{A}\beta\hat{\mathbf{F}}_U(\mathbf{r})\rangle.
\end{aligned}\tag{61}$$

The right hand side of equation (61) can upon using equation (60) alternatively be expressed as $[\langle\hat{A}\nabla'\hat{\rho}(\mathbf{r}')\rangle-\mathbf{S}_A(\mathbf{r}')][\nabla\delta(\mathbf{r}-\mathbf{r}')]+[\nabla\delta(\mathbf{r}-\mathbf{r}')][\langle\hat{A}\nabla\hat{\rho}(\mathbf{r})\rangle-\mathbf{S}_A(\mathbf{r})]$.

As an alternative starting point we use the adjoint of the commutator relation (53), which is given by

$$-\left[\boldsymbol{\sigma}_c^\dagger(\mathbf{r}),\boldsymbol{\sigma}_c^\dagger(\mathbf{r}')\right]=\boldsymbol{\sigma}_c^\dagger(\mathbf{r}')\,[\nabla\delta(\mathbf{r}-\mathbf{r}')]+[\nabla\delta(\mathbf{r}-\mathbf{r}')]\,\boldsymbol{\sigma}_c^\dagger(\mathbf{r}).\tag{62}$$

Multiplying equation (62) by the configuration-dependent observable $\hat{A}(\mathbf{r}^N)$ from the left and building the thermal average on both sides involves the following three terms: $-\langle\hat{A}\boldsymbol{\sigma}_c^\dagger(\mathbf{r})\boldsymbol{\sigma}_c^\dagger(\mathbf{r}')\rangle=\langle[\boldsymbol{\sigma}_c(\mathbf{r})\hat{A}][\boldsymbol{\sigma}_c(\mathbf{r}')-\nabla'\hat{\rho}(\mathbf{r}')]\rangle=\langle\hat{\mathbf{S}}_A(\mathbf{r})[\beta\hat{\mathbf{F}}_U(\mathbf{r}')-\nabla'\hat{\rho}(\mathbf{r}')]\rangle=\langle\hat{\mathbf{S}}_A(\mathbf{r})\beta\hat{\mathbf{F}}_c(\mathbf{r}')\rangle$, and similarly $-\langle\hat{A}\boldsymbol{\sigma}_c^\dagger(\mathbf{r}')\boldsymbol{\sigma}_c^\dagger(\mathbf{r})\rangle^{\mathsf{T}}=\langle\beta\hat{\mathbf{F}}_c(\mathbf{r})\hat{\mathbf{S}}_A(\mathbf{r}')\rangle$, as well as $\langle\hat{A}\boldsymbol{\sigma}_c^\dagger(\mathbf{r})\rangle=\langle[\boldsymbol{\sigma}_c(\mathbf{r})\hat{A}]\rangle=\langle\hat{\mathbf{S}}_A(\mathbf{r})\rangle=\mathbf{S}_A(\mathbf{r})$. Collecting these results leads to the following sum rule:

$$\langle\hat{\mathbf{S}}_A(\mathbf{r})\,\beta\hat{\mathbf{F}}_c(\mathbf{r}')\rangle-\langle\beta\hat{\mathbf{F}}_c(\mathbf{r})\,\hat{\mathbf{S}}_A(\mathbf{r}')\rangle=\mathbf{S}_A(\mathbf{r}')\,[\nabla\delta(\mathbf{r}-\mathbf{r}')]+[\nabla\delta(\mathbf{r}-\mathbf{r}')]\,\mathbf{S}_A(\mathbf{r}),\tag{63}$$

which is the analogous position-dependent version of the more general (momentum-dependent) result of [64], which features the momentum-dependent force operator $\hat{\mathbf{F}}(\mathbf{r})$, as given by (47), in lieu of its configurational counterpart $\hat{\mathbf{F}}_c(\mathbf{r})$, as given by equation (50).

The examples (57), (61) and (63) demonstrate that an algebraic structure of correlation functions emerges from both the adjoint property (52) and the commutator (53). We have restricted ourselves to considering products of two shifting operators. The present shifting in particle positions does not yet constitute a canonical transform and we next demonstrate that incorporating the momentum transform allows one to obtain canonical shifting transformations which retain the useful commutator structure revealed above for purely configurational shifting.

4.4. Infinitesimal phase space shifts and Lie algebra

We are now in a position to describe the consequence of the full phase space shifting transformation [64], as represented on the level of microstates by the maps that displace particle positions and momentum degrees of freedom according to equations (10) and (11), respectively. Corresponding localized shifting operators displace in position in analogy to the configurational shifting operators $\boldsymbol{\sigma}_c(\mathbf{r})$, as defined in equation (51).

Specifically, the full position-resolved phase space shifting operators are defined as [64]:

$$\boldsymbol{\sigma}(\mathbf{r})=\sum_i\left[\delta(\mathbf{r}-\mathbf{r}_i)\,\nabla_i+\mathbf{p}_i\nabla\delta(\mathbf{r}-\mathbf{r}_i)\cdot\nabla_{\mathbf{p}_i}\right].\tag{64}$$

When applied to a purely configuration-dependent observable $\hat{A}(\mathbf{r}^N)$, the dependence on momentum vanishes and $\boldsymbol{\sigma}(\mathbf{r})\hat{A}(\mathbf{r}^N)=\boldsymbol{\sigma}_c(\mathbf{r})\hat{A}(\mathbf{r}^N)$, where $\boldsymbol{\sigma}_c(\mathbf{r})$ is defined via equation (51). The momentum contribution to the transform (second term in the sum on the right hand side

of equation (64)) constitutes spatially localized momentum shifting operators with the explicit form:

$$\boldsymbol{\sigma}_p(\mathbf{r}) = \sum_i \mathbf{p}_i \nabla\delta(\mathbf{r}-\mathbf{r}_i)\cdot\nabla_{\mathbf{p}_i}. \tag{65}$$

Together with the configurational shifting operator $\boldsymbol{\sigma}_c(\mathbf{r})$, we can express $\boldsymbol{\sigma}(\mathbf{r})$, as given via equation (64), as the sum of configurational and momentum contributions according to:

$$\boldsymbol{\sigma}(\mathbf{r}) = \boldsymbol{\sigma}_c(\mathbf{r}) + \boldsymbol{\sigma}_p(\mathbf{r}). \tag{66}$$

The adjoint momentum shift operator is given as:

$$\boldsymbol{\sigma}_p^\dagger(\mathbf{r}) = -\boldsymbol{\sigma}_p(\mathbf{r}) - \nabla\hat{\rho}(\mathbf{r}), \tag{67}$$

which follows from integration by parts on momentum space, using $\nabla\cdot\nabla_{\mathbf{p}_i}\mathbf{p}_i = \nabla\cdot\mathbb{1} = \nabla$, and identifying the density operator $\hat{\rho}(\mathbf{r})$, see its definition (42).

The adjoint of the full phase space shifting operator $\boldsymbol{\sigma}(\mathbf{r})$ is then the sum of the individual adjoint identities (52) and (67). The result is the simple anti-self adjoint property:

$$\boldsymbol{\sigma}^\dagger(\mathbf{r}) = -\boldsymbol{\sigma}(\mathbf{r}). \tag{68}$$

Despite an increase in apparent structural complexity of $\boldsymbol{\sigma}(\mathbf{r})$ over $\boldsymbol{\sigma}_c(\mathbf{r})$, the corresponding commutator relationship remains simple:

$$[\boldsymbol{\sigma}(\mathbf{r}),\boldsymbol{\sigma}(\mathbf{r}')] = \boldsymbol{\sigma}(\mathbf{r}')[\nabla\delta(\mathbf{r}-\mathbf{r}')] + [\nabla\delta(\mathbf{r}-\mathbf{r}')]\boldsymbol{\sigma}(\mathbf{r}), \tag{69}$$

which is identical in form to the corresponding configurational identity (53).

The following two general properties are straightforward to show:

$$[\boldsymbol{\sigma}(\mathbf{r}),\boldsymbol{\sigma}(\mathbf{r}')]^\dagger = -[\boldsymbol{\sigma}(\mathbf{r}),\boldsymbol{\sigma}(\mathbf{r}')], \tag{70}$$

$$[\boldsymbol{\sigma}(\mathbf{r}),\boldsymbol{\sigma}(\mathbf{r}')] = -[\boldsymbol{\sigma}(\mathbf{r}'),\boldsymbol{\sigma}(\mathbf{r})]^{\mathsf{T}}, \tag{71}$$

where equation (70) holds for two self-adjoint operators and equation (71) is valid for two vectorial operators. Furthermore the Jacobi identity holds:

$$\begin{aligned}&[\sigma_a(\mathbf{r}),[\sigma_b(\mathbf{r}'),\sigma_c(\mathbf{r}'')]] + [\sigma_b(\mathbf{r}'),[\sigma_c(\mathbf{r}''),\sigma_a(\mathbf{r})]]\\ &\quad + [\sigma_c(\mathbf{r}''),[\sigma_a(\mathbf{r}),\sigma_b(\mathbf{r}')]] = 0.\end{aligned} \tag{72}$$

Applying the localized phase space shifting operators to the Hamiltonian and to the Boltzmann factor respectively yields:

$$-[\boldsymbol{\sigma}(\mathbf{r})H] = \hat{\mathbf{F}}(\mathbf{r}), \tag{73}$$

$$\left[\boldsymbol{\sigma}(\mathbf{r})\mathrm{e}^{-\beta H}\right] = \beta\hat{\mathbf{F}}(\mathbf{r})\mathrm{e}^{-\beta H}, \tag{74}$$

where the total force density operator, including the divergences of the explicit momentum-dependent kinetic stress tensor $\nabla\cdot\hat{\boldsymbol{\tau}}(\mathbf{r})$, is given by equation (47). Equations (73) and (74) mirror the corresponding relationships (54) and (55) for configurational shifting on the basis of $\boldsymbol{\sigma}_c(\mathbf{r})$ given by equation (51) and the potential force density $\hat{\mathbf{F}}_U(\mathbf{r})$ given by equation (45).

The procedure of obtaining sum rules from full phase space shifting is similar in structure to working with configurational shifts described in section 4.3. Application to a phase space

function $\hat{A}(\mathbf{r}^N, \mathbf{p}^N)$ with full configurational dependence on $\mathbf{r}^N$ and momentum dependence on $\mathbf{p}^N$ yields [54, 64]:

$$\hat{\mathbf{S}}_A(\mathbf{r}) = \left[\boldsymbol{\sigma}(\mathbf{r})\hat{A}\right] \tag{75}$$

$$= \sum_i \delta(\mathbf{r}-\mathbf{r}_i)\left(\nabla_i \hat{A}\right) + \nabla \cdot \sum_i \delta(\mathbf{r}-\mathbf{r}_i)\left(\nabla_{\mathbf{p}_i}\hat{A}\right)\mathbf{p}_i. \tag{76}$$

Application in the form $\langle[\boldsymbol{\sigma}^\dagger(\mathbf{r})\hat{A}]\rangle = \langle\hat{A}\boldsymbol{\sigma}(\mathbf{r})\rangle$ yields, upon using the self-adjoint property (68) and the generation of the force density operator via application to the Boltzmann factor (74), the one-body hyperforce sum rule:

$$\mathbf{S}_A(\mathbf{r}) + \langle\hat{A}\beta\hat{\mathbf{F}}(\mathbf{r})\rangle = 0. \tag{77}$$

The exact identity (77) applies to general observables $\hat{A}(\mathbf{r}^N, \mathbf{p}^N)$, with the one-body hyperforce density being the average $\mathbf{S}_A(\mathbf{r}) = \langle\hat{\mathbf{S}}_A(\mathbf{r})\rangle$ of the corresponding hyperforce phase space function (76), and the full force density operator $\hat{\mathbf{F}}(\mathbf{r})$ being given by equation (47). Again we point out the formal similarity of equations (76) and (77) with the corresponding configuration versions (59) and (60).

Building the thermal average of the commutator relationship (69) yields the following hyperforce sum rule:

$$\langle\hat{\mathbf{S}}_A(\mathbf{r})\beta\hat{\mathbf{F}}(\mathbf{r}')\rangle - \langle\beta\hat{\mathbf{F}}(\mathbf{r})\hat{\mathbf{S}}_A(\mathbf{r}')\rangle = \mathbf{S}_A(\mathbf{r}')[\nabla\delta(\mathbf{r}-\mathbf{r}')] + [\nabla\delta(\mathbf{r}-\mathbf{r}')]\mathbf{S}_A(\mathbf{r}), \tag{78}$$

which is in analogy to the configurational version (63). The right hand side of equation (78) vanishes for $\mathbf{r} \neq \mathbf{r}'$ and the following exchange symmetry holds for the case of distinct positions:

$$\langle\hat{\mathbf{S}}_A(\mathbf{r})\hat{\mathbf{F}}(\mathbf{r}')\rangle = \langle\hat{\mathbf{F}}(\mathbf{r})\hat{\mathbf{S}}_A(\mathbf{r}')\rangle. \tag{79}$$

It remains to formulate the Lie algebra for phase space shifting. For prescribed form of the shifting field $\boldsymbol{\epsilon}(\mathbf{r})$ one uses the localized shifting operators (64) to define a global shifting operator via integration:

$$\Sigma[\boldsymbol{\epsilon}] = \int d\mathbf{r}\boldsymbol{\epsilon}(\mathbf{r})\cdot\boldsymbol{\sigma}(\mathbf{r}) \tag{80}$$

$$= \sum_i \left\{\boldsymbol{\epsilon}(\mathbf{r}_i)\cdot\nabla_i - [\nabla_i\boldsymbol{\epsilon}(\mathbf{r}_i)] : \mathbf{p}_i\nabla_{\mathbf{p}_i}\right\}. \tag{81}$$

where the explicit form (81) is obtained from using $\boldsymbol{\sigma}(\mathbf{r})$ according to equation (64) and carrying out the position integral over $\mathbf{r}$. The colon in equation (81) indicates a double tensor contraction, which is equivalently the trace of the product of the two matrices. The phase space shifting operator $\Sigma[\boldsymbol{\epsilon}]$ depends functionally on the shifting field $\boldsymbol{\epsilon}(\mathbf{r})$ as is indicated by the brackets.

The commutator relationship for full phase space shifting is given by

$$[\Sigma[\boldsymbol{\epsilon}_1], \Sigma[\boldsymbol{\epsilon}_2]] = \Sigma[\boldsymbol{\epsilon}_\Delta]. \tag{82}$$

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 the relation (27), as previously obtained for pure position shifting, which we reproduce for convenience: $\boldsymbol{\epsilon}_\Delta(\mathbf{r}_i) = \boldsymbol{\epsilon}_1(\mathbf{r}_i)\cdot[\nabla_i\boldsymbol{\epsilon}_2(\mathbf{r}_i)] - \boldsymbol{\epsilon}_2(\mathbf{r}_i)\cdot[\nabla_i\boldsymbol{\epsilon}_1(\mathbf{r}_i)]$.

The commutator relationship (82) forms a non-commutative Lie algebra due to the following three features: (i) anti-symmetry, which originates from the very definition of the commutator, (ii) bilinearity, which is induced by the linearity of the differential operator (81), and (iii) the Jacobi identity: $[\Sigma_1,[\Sigma_2,\Sigma_3]]+[\Sigma_2,[\Sigma_3,\Sigma_1]]+[\Sigma_3,[\Sigma_1,\Sigma_2]]=0$, which can be shown by direct manipulation using equation (81). The functional arguments are suppressed in the notation such that $\Sigma_1=\Sigma[\boldsymbol{\epsilon}_1]$, $\Sigma_2=\Sigma[\boldsymbol{\epsilon}_2]$, and $\Sigma_3=\Sigma[\boldsymbol{\epsilon}_3]$.

By construction, the shifting operators perform the following phase space displacement to lowest order in the shifting field and its gradient:

$$f\left(\mathbf{r}'^N,\mathbf{p}'^N\right)=f\left(\mathbf{r}^N,\mathbf{p}^N\right)+\Sigma\left[\boldsymbol{\epsilon}\right]f\left(\mathbf{r}^N,\mathbf{p}^N\right). \tag{83}$$

We recall the relationship of original phase space variables $\mathbf{r}^N,\mathbf{p}^N$ and their displaced versions $\mathbf{r}'^N$ and $\mathbf{p}'^N$ via the joint particle-resolved transformation (10) and (11).

For completeness, we can restore the localized shifting operators $\boldsymbol{\sigma}(\mathbf{r})$ from $\Sigma[\boldsymbol{\epsilon}]$ by functional differentiation with respect to the shifting field according to:

$$\boldsymbol{\sigma}\left(\mathbf{r}\right)=\frac{\delta\Sigma\left[\boldsymbol{\epsilon}\right]}{\delta\boldsymbol{\epsilon}\left(\mathbf{r}\right)}. \tag{84}$$

As a consequence, the following relationships hold between single and successive application of localized shifting and functional derivatives with respect to the shifting field:

$$\boldsymbol{\sigma}\left(\mathbf{r}\right)f\left(\mathbf{r}^N,\mathbf{p}^N\right)=\left.\frac{\delta f\left(\mathbf{r}'^N,\mathbf{p}'^N\right)}{\delta\boldsymbol{\epsilon}\left(\mathbf{r}\right)}\right|_{\boldsymbol{\epsilon}=0}, \tag{85}$$

$$\boldsymbol{\sigma}\left(\mathbf{r}\right)\boldsymbol{\sigma}\left(\mathbf{r}'\right)f\left(\mathbf{r}^N,\mathbf{p}^N\right)=\left.\frac{\delta^2 f\left(\mathbf{r}'^N,\mathbf{p}'^N\right)}{\delta\boldsymbol{\epsilon}\left(\mathbf{r}\right)\delta\boldsymbol{\epsilon}\left(\mathbf{r}'\right)}\right|_{\boldsymbol{\epsilon}=0}+\left[\nabla\delta\left(\mathbf{r}-\mathbf{r}'\right)\right]\boldsymbol{\sigma}\left(\mathbf{r}\right)f\left(\mathbf{r}^N,\mathbf{p}^N\right). \tag{86}$$

We have hence demonstrated that much of the favorable structure of coordinate shifting, as described in section 4.3, is not only retained, see e.g. the corresponding operator algebra for phase space shifting (69) and coordinate shifting (53), but even formally simplified, see the simple self-adjoint nature of phase space shifting (68), as compared to the (slightly) more complex version (52) for coordinate shifting.

The mathematical structure that is encoded in the behavior of the differential transformations allows one to derive exact sum rules, as we have demonstrated. That the gauge invariance against phase space shifting is not a mere formal device but an intrinsic property of the statistical mechanics of many-body systems is arguably most strikingly demonstrated for finite shifting, as we turn to next.

5. Computer simulations in the shifted phase space

Finite phase space shifting is expressed by the general coordinate and momentum map (10) and (11) described in section 3.2. We wish to demonstrate that phase space averages are *in practice* invariant under this gauge transformation. As a prototypical example we consider hard rod particles of size a in one spatial dimension. The hard core interaction assigns vanishing statistical weight to any configuration with two particles i and j having spatial distance $|x_i-x_j|<a$, where x_i and x_j are one-dimensional position coordinates. We refer the reader to [58] for a description of the emerging collective physics as described on the basis of classical density functional theory and using neural functionals. We deem the hard rod model

to constitute a fundamental test case. The results presented in [64] for soft interparticle and external interaction potentials demonstrate the generality of our conclusions.

We use Monte Carlo simulations and choose two representative observables. One is the density 'operator', $\hat{A} = \hat{\rho}(x) = \sum_i \delta(x - x_i)$ where x denotes a generic position and we have cast the general definition (42) of $\hat{\rho}(\mathbf{r})$ in one-dimensional form. We furthermore address the one-body phase space distribution function $f(x,p) = \langle \hat{f}(x,p) \rangle$, where the observable under consideration is $\hat{A} = \hat{f}(x,p) = \sum_i \delta(x - x_i)\delta(p - p_i)$, with p being a generic momentum variable.

To carry out the simulations in the displaced system we use a one-dimensional shifting field given by the following specific form:

$$\epsilon(x) = \epsilon_0 \sin(4\pi x/L), \tag{87}$$

where ϵ_0 is an amplitude that governs the overall magnitude of the displacement, L denotes the system size, which we choose as $L = 10a$. The system is confined between two hard walls. Setting $\epsilon_0 = 0$ leads to vanishing shift and constitutes our baseline. We compare the corresponding results with those obtained for two different chosen values of ϵ_0. We first set $\epsilon_0/a = 0.5$, which is a safe choice below the threshold of invertibility and the resulting phase space transformation is bijective. As a further choice we take $\epsilon_0/a = 1.5$, which is above the invertibility threshold, which we obtain in the present simple geometry as $\epsilon_0 = L/(4\pi) = 0.796$ from the requirement $d(x + \epsilon(x))/dx > 0$.

The simulation results shown in figure 6 indicate that sampling in the validly displaced system $\epsilon_0/a = 0.5$ (middle column) generates results that are numerically identical to those of the original system with $\epsilon_0/a = 0$ (left column). The invalid transformation, upon using identical code and merely changing the amplitude of the shifting field to the value of $\epsilon_0/a = 1.5$, yields corrupted results (right column). Such behavior is expected for this case of a transform that is not bijective.

Pseudocode for the corresponding Metropolis Monte Carlo algorithm based on single particle moves is described in figure 7. We lay out the standard procedure (algorithm 1), together with the changes that implement phase space shifting both for the generation of the microstates and for the data acquisition via histogram filling (algorithm 2).

6. Conclusions

In conclusion we have described background and details for the gauge transformation of statistical mechanical microstates [64]. Thereby the thermal invariance against phase space shifting implies exact sum rules, as previously identified in a variety of different settings [48–55]. These include inhomogeneous thermal quantum systems [51], as well as classical liquids and more general soft matter states [52, 53]. Previous work was based on variational methods and using invariance against the specific form of the displacement field $\boldsymbol{\epsilon}(\mathbf{r})$ that parameterizes the phase space transformation. Here we have given background and details about the structure of the underlying invariance group including the algebra of phase space differential operators identified in [64]. The relevant phase space operators represent infinitesimal versions of finite gauge transformations and the analysis of their properties allows one to reveal rich mathematical structure.

The gauge transformation affects particle position (10) and momentum (11) degrees of freedom. The vector field $\boldsymbol{\epsilon}(\mathbf{r})$ that parameterizes the transform needs to be smooth and of a form that allows the transformation to be bijective. Specifically we require that the function $\mathbf{r}_i + \boldsymbol{\epsilon}(\mathbf{r}_i)$ is a diffeomorphism. With the position transform being very general, the momentum transform ensures that the differential phase space volume element is conserved and that the

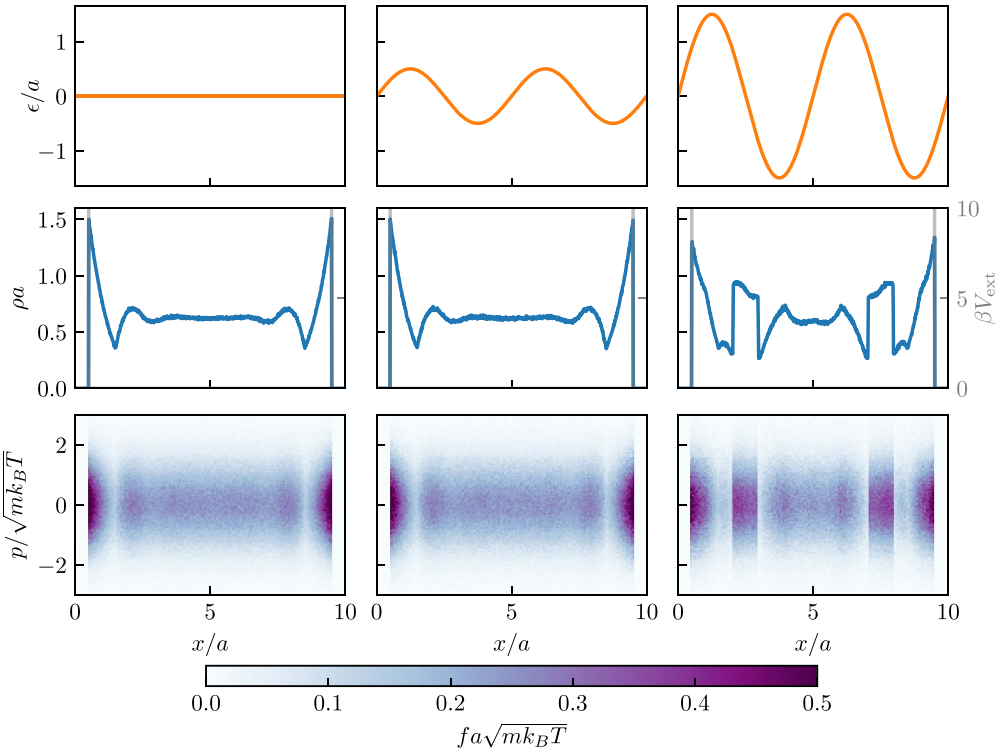
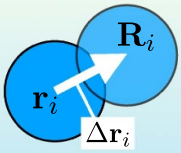


Figure 6. Demonstration of particle gauge invariance via Monte Carlo simulations. Hard rod particles of size a are confined between two hard walls, as represented by a scaled external potential $\beta V_{\mathrm{ext}}(\mathbf{r})$ (gray lines) that vanishes for $0.5a \leqslant x \leqslant 9.5a$ and is ∞ otherwise. Results are shown for the unshifted system (left column), a shifted system (middle column), and a corrupted system (right column). In the latter case the amplitude of the shifting field is beyond the threshold of invertibility, such that the transformation fails to be bijective and is hence no longer a gauge transformation. Shown is the scaled sinusoidal shifting field $\epsilon(x)/a$ as a function of scaled position x/a (top panels), the scaled density profile $\rho(x)a$ (middle panels), and the scaled one-body phase space distribution $f(x,p)a\sqrt{mk_{\mathrm{B}}T}$ (bottom panels), where the variables are the scaled position x/a and scaled momentum $p/\sqrt{mk_{\mathrm{B}}T}$. The shifting transformation displaces both coordinates and momenta. Despite the difference in Monte Carlo simulation moves and acceptance events, the results in the original system (left column) and in the transformed system (middle column) are numerically identical to each other, while the invalidly transformed system develops artifacts (right column).

Algorithm 1 Conventional Monte Carlo sweep and sampling

for $i \leftarrow 1 \ldots N$ **do** ▷ Monte Carlo sweep
  draw random displacement $\Delta\mathbf{r}_i$
  do trial move: $\mathbf{R}_i \leftarrow \mathbf{r}_i + \Delta\mathbf{r}_i$
  calculate configurational energy difference: $\Delta E = U(\mathbf{R}^N) - U(\mathbf{r}^N)$
  draw random number $0 < \xi < 1$
  if $\exp(-\beta\Delta E) > \xi$ **then**
    accept trial move: $\mathbf{r}_i \leftarrow \mathbf{R}_i$
  end if
end for
for $i \leftarrow 1 \ldots N$ **do** ▷ Histogram sampling
  calculate histogram bin b_i for particle position $\mathbf{r}_i$
  increment density histogram at bin b_i
end for



Algorithm 2 Monte Carlo sweep and sampling with shifting

for $i \leftarrow 1 \ldots N$ **do** ▷ Monte Carlo sweep
  draw random displacement $\Delta\mathbf{r}_i$ and momentum change $\Delta\mathbf{p}_i$
  do trial move: $\mathbf{R}_i \leftarrow \mathbf{r}_i + \Delta\mathbf{r}_i$, $\mathbf{P}_i \leftarrow \mathbf{p}_i + \Delta\mathbf{p}_i$
  transform original and trial variables to shifted system:
    $\mathbf{r}'_i \leftarrow \mathbf{r}_i + \boldsymbol{\epsilon}(\mathbf{r}_i)$, $\mathbf{p}'_i \leftarrow [\mathbb{1} + \nabla\boldsymbol{\epsilon}(\mathbf{r}_i)]^{-1} \cdot \mathbf{p}_i$,
    $\mathbf{R}'_i \leftarrow \mathbf{R}_i + \boldsymbol{\epsilon}(\mathbf{R}_i)$, $\mathbf{P}'_i \leftarrow [\mathbb{1} + \nabla\boldsymbol{\epsilon}(\mathbf{R}_i)]^{-1} \cdot \mathbf{P}_i$
  calculate energy difference: $\Delta E = H(\mathbf{R}'^N, \mathbf{P}'^N) - H(\mathbf{r}'^N, \mathbf{p}'^N)$
  draw random number $0 < \xi < 1$
  if $\exp(-\beta\Delta E) > \xi$ **then**
    accept trial move: $\mathbf{r}_i \leftarrow \mathbf{R}_i$, $\mathbf{p}_i \leftarrow \mathbf{P}_i$
  end if
end for
for $i \leftarrow 1 \ldots N$ **do** ▷ Histogram sampling
  apply shift: $\mathbf{r}'_i \leftarrow \mathbf{r}_i + \epsilon(\mathbf{r}_i)$
  calculate histogram bin b_i for *shifted* particle position $\mathbf{r}'_i$
  increment density histogram at bin b_i
end for

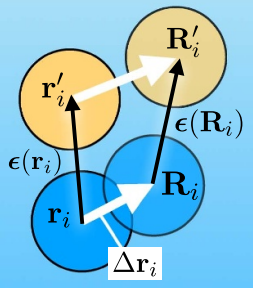


Figure 7. Pseudocodes that describe Monte Carlo simulations in the standard form (algorithm 1) and using phase space shifting (algorithm 2). The standard Metropolis algorithm is based on trial displacement from $\mathbf{r}_i, \mathbf{p}_i$ to $\mathbf{R}_i, \mathbf{P}_i$, where the capitalization indicates the trial variables. In the shifted system the transformation is applied both to the current state, resulting in $\mathbf{r}'_i, \mathbf{p}'_i$, as well as to the trial state, resulting in $\mathbf{R}'_i, \mathbf{P}'_i$. The Metropolis criterion is then evaluated with respect to the shifted variables and these then also form the basis for the sampling of observables. The illustrations of the shifted system only display configurational degrees of freedom with the momentum variables being treated accordingly. The pseudocode for histogram sampling in the shifted system only describes the configurational strategy with corresponding momentum sampling being required for obtaining, e.g. the one-body phase space distribution function $f(\mathbf{r}, \mathbf{p})$ shown in figure 6.

joint transformation (10) and (11) is canonical in the sense of classical mechanics [67]. This is not the case in an early contribution by Baus and Lovett [78], who have worked with functional differentiation methods based on only the position transformation (10), rather than the present phase space operators and their algebraic commutator structure.

For finite displacement we have described in detail the geometric nature of position shifting. This transformation can be inverted and chained and hence establishes a group structure. Notwithstanding the apparent geometric simplicity, the group is non-commutative with the order of two consecutive shifts being relevant. Despite its more complex matrix multiplication structure, the corresponding momentum transform (11) remains entirely compatible with the mathematical structure of the position transform.

When considering the infinitesimal version of shifting much additional structure is revealed by formalizing relationships for differential operators that perform the shifting. The transformations are functionally dependent on the vector field $\boldsymbol{\epsilon}(\mathbf{r})$ that parameterizes the transform. Functional differentiation yields corresponding commutator relationships for position-localized differential operators that act on the phase space of a many-body system. We have laid out the properties of pure position shifting and have compared against those of full phase space gauge transformation. Both versions of corresponding localized differential operators can be used as a basis for deriving exact statistical mechanical sum rules, as we have demonstrated. The mathematical derivation of these correlation function identities (sum rules) is greatly simplified by the use of the differential operator formalism.

The classical gauge theory that we have presented carries strong similarities with the theory of Lie groups and associated Lie algebras. In particular, the phase space shifting operators $\Sigma[\boldsymbol{\epsilon}]$ given by equation (81) form a non-commutative Lie algebra, as described by the commutator relation (82). For pure configuration shifting the corresponding Lie algebra is given by equation (29). The dependence on the shifting field $\boldsymbol{\epsilon}(\mathbf{r})$ remains thereby explicit and it acts to identify the elements of the algebra.

In the present statistical mechanical setting it is useful to go further and eliminate the dependence on $\boldsymbol{\epsilon}(\mathbf{r})$. We recall that $\boldsymbol{\epsilon}(\mathbf{r})$ possesses the status of a mere gauge function, which does not affect the actual physics; see the similarities with gauge invariance in electrodynamics as described in section 2. Functional differentiation of the Lie algebra with respect to the shifting field constitutes a well-characterized route to eliminate the dependence on $\boldsymbol{\epsilon}(\mathbf{r})$, which in turn generates spatial localization via Dirac distributions. The resulting operator commutator identities, see equation (69) for full phase space shifting and equation (34) for the purely configurational version, retain much of the favorable structure of a Lie algebra, see the occurrence of structure constants equation (35). However, the distribution character reaches beyond elementary Lie theory [72] and it would be interesting in future work to explore connections with more abstract Lie concepts in modern mathematical treatments of the subject.

We have described several implications of the gauge invariance for simulation methods focusing on Monte Carlo sampling. Choosing a specific form of the shifting field and displacing the particles in a prototypical confined one-dimensional hard core system allows one to give a standalone demonstration of gauge invariance. Applying the transformation (10) and (11) goes in practice beyond a mere change of phase space variables, as this procedure genuinely alters the resulting Markov chain due to the evaluation of acceptance probabilities in the virtually displaced system. Nevertheless, the invariance property ensures that thermal averages remain valid despite the seemingly violated requirement of detailed balance. That the acceptance rates differ in the displaced and original systems serves as a practical indicator for the algorithmic differences. The sampled states retain, as theoretically predicted, identical one-body density profile and phase space distribution function, which we took as representative of the behavior of general observables.

In future work, it would be interesting to investigate the potential use of gauge invariance in machine learning of neural density functionals [57, 58], for constructing analytical density functional approximations [25], for cross fertilization with hyperdensity functional theory [59, 60], for the construction of advanced simulation schemes [28, 37–44] in particular based on mapped averaging [27–39], and for the application to mixtures [79].

Data availability statement

The data that support the findings of this study are openly available at the following URL/DOI: https://github.com/sfalmo/gauge-mc.

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Appendix. Functional derivatives in electrodynamics

We denote the transformed action by $S_{\text{ext}}[\varphi]$, as given via the right hand side of equation (8). The brackets indicate functional dependence, which arises as the value of the action depends *a priori* on the specific form of the gauge function $\varphi(x)$. We can express the gauge invariance as the identity

$$S_{\text{ext}} = S_{\text{ext}}\,[\varphi]\,, \tag{A1}$$

where the left hand side denotes the original action (5), which is clearly independent of $\varphi(x)$. The invariance equation (A1) holds irrespective of the form of the gauge function $\varphi(x)$. Hence a valid identity is retained upon functionally differentiating both sides by $\varphi(x)$. The left hand side of equation (A1) then vanishes as there is no dependence on the gauge function.

Differentiating also on the right hand side of equation (A1) gives $0 = \delta S_{\text{ext}}[\varphi]/\delta\varphi(x) = \delta[S_{\text{ext}} + \int dx'\varphi(x')\partial'_\nu J^\nu(x')]/\delta\varphi(x)$, where the prime indicates a new spacetime integration variable and ∂'_ν is the corresponding spacetime derivative. The first term in the sum vanishes, as argued above. Exchanging in the second term the order of the functional derivative and the spacetime integral gives $0 = \int dx'[\delta\varphi(x')/\delta\varphi(x)]\partial'_\nu J^\nu(x') = \int dx'\delta(x-x')\partial'_\nu J^\nu(x') = \partial_\nu J^\nu(x)$. Here we have used that functionally differentiating a function by itself gives the Dirac distribution, $\delta\varphi(x')/\delta\varphi(x) = \delta(x-x')$, which is here in four dimensions. Recalling that the result of the functional derivative vanishes, we have hence rederived the charge continuity equation (9).

While requiring slightly more steps than the route considered in the main text, the present method via functional calculus is arguably as generally applicable as is ordinary multivariate calculus and hence there are no principal limits in terms of complexity of the functional dependence under investigation. Moreover, as was demonstrated recently for statistical functionals [57, 58, 80], powerful software tools that implement automatic differentiation [81] can be used.

For completeness, the free field action (4) is unaffected by the gauge transformation, as $F_{\lambda\nu}(x)$ is already an invariant. We demonstrate this explicitly as follows. The free field

action (4) acquires the following apparent change under the gauge transformation (3) according to

$$S_{\text{free}} \to S_{\text{free}} + \mu_0^{-1} \int dx \varphi(x)\, \partial_\lambda \partial_\nu F^{\lambda\nu}(x)\,. \tag{A2}$$

From invariance of the free field action one can conclude that $\partial_\lambda \partial_\nu F^{\lambda\nu}(x) = 0$, which already follows in an elementary way from the antisymmetry $F^{\lambda\nu}(x) = -F^{\nu\lambda}(x)$.

Again an alternative derivation can be based on functional differentiation which, following steps analogous to those described above for the external action, gives the same result: $\delta S_{\text{free}}[\varphi]/\delta\varphi(x) = \partial_\lambda \partial_\nu F^{\lambda\nu}(x)/\mu_0 = 0$.

To make the covariant formulation more explicit, the relationship of $F_{\nu\lambda}(x)$ to the electrical field and to the magnetic induction is via the explicit components: $F_{0\lambda}(x) = (0, E_x/c, E_y/c, E_z/c)$, $F_{1\lambda}(x) = (-E_x/c, 0, -B_z, B_y)$, $F_{2\lambda}(x) = (-E_y/c, B_z, 0, -B_x)$ $F_{3\lambda}(x) = (-E_z/c, -B_y, B_x, 0)$, where $\mathbf{E}(\mathbf{r},t) = (E_x, E_y, E_z)$ and $\mathbf{B}(\mathbf{r},t) = (B_x, B_y, B_z)$. For completeness, the entire field tensor reads as follows:

$$F_{\nu\lambda}(x) = \begin{pmatrix} 0 & E_x/c & E_y/c & E_z/c \\ -E_x/c & 0 & -B_z & B_y \\ -E_y/c & B_z & 0 & -B_x \\ -E_z/c & -B_y & B_x & 0 \end{pmatrix}. \tag{A3}$$

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