

Quantum statistical mechanical gauge invariance

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We address gauge invariance in the statistical mechanics of quantum many-body systems. The gauge transformation acts on the position and momentum degrees of freedom, and it is represented by a quantum shifting superoperator that maps quantum observables onto each other. The shifting superoperator is anti-self-adjoint, and it has noncommutative Lie algebra structure. These properties induce exact equilibrium sum rules that connect locally resolved force and hyperforce densities for any given observable. We argue that the framework is amenable to tight integration into quantum hyperdensity functional theory and that it generalizes naturally to nonequilibrium.

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The systematic treatment of gauge invariance is key to relating the symmetries that are inherent in a physical theory to the validity of exact identities. Typically such equations have the form of conservation laws that restrict the behavior of the fundamental physical degrees of freedom, which are often taken to be fields. The gauge transformations can carry intricate mathematical structure and have profound consequences for our understanding of nature, and they reside at the core of important modern developments in theoretical physics [1,2].

As a central tool to analyze invariances, Noether's theorem [3] was used in various different statistical mechanical settings [4–11]. A specific “shifting” operation was argued to constitute a gauge transformation for classical statistical mechanics in equilibrium [12–15] and under general Hamiltonian dynamics [16]. The shifting is a canonical transformation both in classical [17,18] and in quantum mechanical form [19]. The classical framework leads to force and generalized “hyperforce” correlation functions that satisfy exact sum rules [12,13,18,20] and it allows one to construct and test novel sampling schemes [12,14]. As a special case the Yvon-Born-Green equation [21–23], which expresses the position-resolved equilibrium force density balance, follows, and it is generalized to a dynamical “hypercurrent” identity [16].

Here we present the generalization of the classical gauge invariance to quantum many-body systems; consequences will be presented in Ref. [24]. We demonstrate that all salient features of the classical gauge theory remain intact, including the validity of exact static hyperforce and dynamical hypercurrent sum rules [see Eq. (18)] provided that the definitions of the occurring quantum correlation functions are appropriately identified, which is nontrivial. The perseverance of the

theoretical structure is remarkable, given the fundamental changes in the underlying microscopic description of the many-body physics.

Quantum statistical mechanics applies to a broad range of diverse systems of current interest. Topical examples include ultracold atomic systems [25], where questions of many-body localization are pertinent from both experimental [26,27] and theoretical [28,29] perspectives. Systems that were initially thermalized and then undergo a sudden change via explicit time dependence of a tuning parameter in the Hamiltonian constitute an important class of setups. Whether then thermalization occurs at long times is a relevant question; see, e.g., Refs. [30,31] for recent work and Ref. [32] for an introduction. Much attention is being paid to the study of spatially nonhomogeneous quantum many-body systems [33–35].

When working with discrete particles instead of fields, then a quantum many-body description involves the position and momentum degrees of freedom of each particle. The quantum nature of the problem is reflected by the algebraic commutator structure of the canonical quantum operators. Formulating a reduced picture can be based efficiently on the density operator $\hat{n}(\mathbf{r}) = \sum_i \delta(\mathbf{r} - \mathbf{r}_i)$; see, e.g., Ref. [36], where the sum runs over all particles $i = 1, \dots, N$, the variable N is the total number of particles, $\delta(\cdot)$ denotes the Dirac distribution in d dimensions, $\mathbf{r}_i$ is the position of particle i , and $\mathbf{r}$ is a generic position.

When considering a general quantum observable $\hat{A}$, the quantum dynamics are given by the associated Heisenberg equation of motion, $\partial \hat{A}(t)/\partial t = (-i/\hbar)[\hat{A}(t), \hat{H}(t)]$, where $[\cdot, \cdot]$ denotes the commutator, $\hat{H}$ is the Hamiltonian, $\hbar$ indicates the reduced Planck constant, i is the imaginary unit, t denotes time, and we let $\hat{A}$ be stationary, such that it carries no mere parametric dependence on time. Choosing the density operator as the observable of interest, $\hat{A} = \hat{n}(\mathbf{r})$, the generic Heisenberg equation of motion reduces to the continuity equation, $\partial \hat{n}(\mathbf{r}, t)/\partial t = -\nabla \cdot \hat{\mathbf{J}}(\mathbf{r}, t)$, where ∇ indicates the derivative with respect to $\mathbf{r}$. Here $\hat{\mathbf{J}}(\mathbf{r}, t)$ is the one-body current operator (defined below). Its dynamics follow again from Heisenberg's equation of motion, which yields $\partial m \hat{\mathbf{J}}(\mathbf{r}, t)/\partial t = \hat{\mathbf{F}}(\mathbf{r}, t)$, where the result is the one-body force

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density operator (also described below) and m indicates the particle mass. Hence one has arrived at a spatially resolved analog of Newton's second law, and upon building the quantum average one recovers Ehrenfest's theorem, again in a spatially resolved version. The crucial step in the derivation is to obtain a microscopic expression for the force density operator [36] by calculating explicitly the commutator $(-i/\hbar)[m\hat{\mathbf{J}}(\mathbf{r}, t), \hat{H}(t)] = \hat{\mathbf{F}}(\mathbf{r}, t)$. This formulation forms a perfectly valid starting point for developing the quantum statistical mechanics of N -body systems. A description of the relationship with classical statistical mechanics is given in Ref. [24].

Here we formulate *quantum* shifting gauge invariance. Inspired by the recent classical formulation of gauge shifting based on Poisson brackets [16] we introduce the following quantum “shifting superoperator”:

$$\sigma(\mathbf{r}) = -\frac{i}{\hbar}[\cdot, m\hat{\mathbf{J}}(\mathbf{r})], \quad (1)$$

where the (scaled) quantum one-body current (density) operator in Schrödinger form is

$$m\hat{\mathbf{J}}(\mathbf{r}) = \frac{1}{2} \sum_i [\hat{\mathbf{p}}_i \delta(\mathbf{r} - \mathbf{r}_i) + \delta(\mathbf{r} - \mathbf{r}_i) \hat{\mathbf{p}}_i], \quad (2)$$

with $\hat{\mathbf{p}}_i = -i\hbar\nabla_i$ denoting the momentum operator of quantum particle i , where $\nabla_i = \partial/\partial\mathbf{r}_i$. Equation (1) defines a quantum superoperator, as this applies to Hilbert space operators (first argument of the commutator) and it also returns a Hilbert space operator (the result of the scaled commutator). We demonstrate in the following that the shifting superoperator (1) is the appropriate quantum mechanical entity to encapsulate statistical mechanical gauge invariance by laying out several of its key properties.

As an aside, the relationship with classical phase space shifting [16], as based on Dirac's correspondence principle [37], is noteworthy. In the classical description of the many-body statistical mechanics, the shifting acts on phase space [12,13]. The differential operators that generate the transform can be expressed [16] based on Poisson brackets as $\sigma_{\text{cl}}(\mathbf{r}) = \{\cdot, m\hat{\mathbf{J}}_{\text{cl}}(\mathbf{r})\}$, with $\{\cdot, \cdot\}$ denoting the (classical) Poisson brackets and $\hat{\mathbf{J}}_{\text{cl}}(\mathbf{r})$ the classical phase space current observable. We note the analogy of $\sigma_{\text{cl}}(\mathbf{r})$ to the quantum shifting superoperator (1) and refer the reader to Ref. [24] for a detailed description of the (nontrivial) classical-quantum shifting correspondence.

As a seemingly trivial initial case, applying the quantum shifting superoperator (1) to the identity operator 1 yields

$$\sigma(\mathbf{r})1 = 0, \quad (3)$$

which follows from the definition (1) and the identity commuting with the current operator, $[1, m\hat{\mathbf{J}}(\mathbf{r})] = 0$. The application of the superoperator to the negative Hamiltonian yields the force density operator,

$$\hat{\mathbf{F}}(\mathbf{r}) = -\sigma(\mathbf{r})\hat{H}, \quad (4)$$

which constitutes the Schrödinger form of $\hat{\mathbf{F}}(\mathbf{r}, t)$ and is specified in more detail later. Equation (4) follows from the definition (1) and the Heisenberg equation of motion for the current operator.

When considering a general quantum observable $\hat{A}$ and applying $\sigma(\mathbf{r})$ we refer to the result as the *hyperforce* density operator

$$\hat{\mathbf{S}}_A(\mathbf{r}) = \sigma(\mathbf{r})\hat{A}, \quad (5)$$

which is the quantum analog of the corresponding classical phase space function [12,18] and is expressed as $\hat{\mathbf{S}}_A(\mathbf{r}) = (-i/\hbar)[\hat{A}, m\hat{\mathbf{J}}(\mathbf{r})]$ according to the commutator form (1). That $\hat{\mathbf{S}}_A(\mathbf{r})$ is indeed a quantum observable, $\hat{\mathbf{S}}_A^\dagger(\mathbf{r}) = \hat{\mathbf{S}}_A(\mathbf{r})$, follows from $[\sigma(\mathbf{r})\hat{A}]^\dagger = \sigma(\mathbf{r})\hat{A}^\dagger$ for $\hat{A} = \hat{A}^\dagger$. This property can in turn be derived from

$$[\sigma(\mathbf{r})\hat{A}]^\dagger = \sigma(\mathbf{r})\hat{A}^\dagger, \quad (6)$$

where $\hat{A}$ can be general (not necessarily self-adjoint). Equation (6) is a consequence of the commutator structure (1) and the self-adjointness of the current operator, $m\hat{\mathbf{J}}(\mathbf{r}) = m\hat{\mathbf{J}}^\dagger(\mathbf{r})$.

For completeness, adjoining an operator $\hat{A}$ is indicated by the dagger, $\hat{A}^\dagger$, and defined throughout in the standard way [37,38] as $\langle n'|\hat{A}n\rangle = \langle \hat{A}^\dagger n'|n\rangle$ for all n and n' of a general N -body Hilbert space basis $|n\rangle$. By extension [39], the adjoint $\mathcal{O}^\dagger$ of a general superoperator $\mathcal{O}$ is defined as $\text{Tr} \hat{A}^\dagger \mathcal{O} \hat{B} = \text{Tr} (\mathcal{O}^\dagger \hat{A})^\dagger \hat{B}$, where $\hat{A}$ and $\hat{B}$ are general Hilbert space operators and $\text{Tr} \cdot = \sum_n \langle n| \cdot |n\rangle$ indicates the trace over Hilbert space. This will be important for the statistical mechanics described later.

In this extended sense, the shifting superoperator (1) is anti-self-adjoint,

$$\sigma^\dagger(\mathbf{r}) = -\sigma(\mathbf{r}), \quad (7)$$

which follows from the quantum trace being invariant under cyclic permutations [39]. More specifically, $\text{Tr} \hat{A}[\hat{B}, \hat{C}] = \text{Tr} [\hat{C}, \hat{A}]\hat{B}$, where one chooses $\hat{C} = (-i/\hbar)m\hat{\mathbf{J}}(\mathbf{r})$. Together with Eq. (1) this leads to

$$\text{Tr} \hat{A}[\sigma(\mathbf{r})\hat{B}] = -\text{Tr} [\sigma(\mathbf{r})\hat{A}]\hat{B}, \quad (8)$$

where replacing $\hat{A}$ with $\hat{A}^\dagger$ and combining with Eq. (6) gives Eq. (7).

While the relationships (3)–(8) point towards the prowess of individual uses of the shifting superoperator, one needs to consider multiple instances of $\sigma(\mathbf{r})$ to reveal the full mathematical structure. Before we demonstrate below the existence of a Lie superoperator algebra, we first address the commutator of two shifting superoperators:

$$[\sigma(\mathbf{r}), \sigma(\mathbf{r}')] = [\nabla\delta(\mathbf{r} - \mathbf{r}')]\sigma(\mathbf{r}) + \sigma(\mathbf{r}')[\nabla\delta(\mathbf{r} - \mathbf{r}')], \quad (9)$$

where $[\nabla\delta(\mathbf{r} - \mathbf{r}')] is the derivative of the Dirac distribution and the brackets limit the scope of ∇ . Analogously one can express $\nabla\delta(\mathbf{r} - \mathbf{r}') = (i/\hbar)[\hat{\mathbf{p}}, \delta(\mathbf{r} - \mathbf{r}')] upon introducing a generic momentum operator $\hat{\mathbf{p}} = -i\hbar\nabla$ that satisfies the canonical commutator relationship $[\mathbf{r}, \hat{\mathbf{p}}] = i\hbar\mathbb{1}$ with the generic position $\mathbf{r}$. The commutator of two superoperators $\mathcal{O}_1$ and $\mathcal{O}_2$ is defined as $[\mathcal{O}_1, \mathcal{O}_2]\hat{A} = \mathcal{O}_1(\mathcal{O}_2\hat{A}) - \mathcal{O}_2(\mathcal{O}_1\hat{A})$ for any general operator $\hat{A}$.$$

To connect to the quantum shifting transform [19] and to be able to identify the Lie superoperator algebra we consider the integrated shifting superoperators $\Sigma[\epsilon] = \int d\mathbf{r} \epsilon(\mathbf{r}) \cdot \sigma(\mathbf{r})$, where the square brackets indicate functional dependence on the (smooth) shifting field $\epsilon(\mathbf{r})$. An explicit form of $\Sigma[\epsilon]$ is obtained by expressing $\sigma(\mathbf{r})$ via the commutator (1), using

the scaled current (2), and carrying out the position integral, which yields

$$\Sigma[\epsilon] = -\frac{i}{2\hbar} \sum_i [\cdot, \epsilon(\mathbf{r}_i) \cdot \hat{\mathbf{p}}_i + \hat{\mathbf{p}}_i \cdot \epsilon(\mathbf{r}_i)]. \quad (10)$$

As an illustration of Eq. (10) we consider the effect of $1 + \Sigma[\epsilon]$ acting on the fundamental position and momentum degrees of freedom. The result is $(1 + \Sigma[\epsilon])\mathbf{r}_j = \mathbf{r}_j + \epsilon(\mathbf{r}_j)$ and $(1 + \Sigma[\epsilon])\hat{\mathbf{p}}_j = \hat{\mathbf{p}}_j - \{[\nabla_j \epsilon(\mathbf{r}_j)] \cdot \hat{\mathbf{p}}_j + \hat{\mathbf{p}}_j \cdot [\nabla_j \epsilon(\mathbf{r}_j)]^\top\}/2$, where the superscript $\top$ indicates transposition of a $d \times d$ matrix. Thus we recover the (linearized) quantum canonical shifting transformation of Ref. [19], where quantum canonical transformations [40] generalize their classical counterparts [41].

Working with the superoperator (1) allows one to make significant progress over the results obtained via the explicit quantum canonical transformation [19], as we demonstrate in the following. Given two smooth shifting fields $\epsilon_1(\mathbf{r})$ and $\epsilon_2(\mathbf{r})$ the corresponding integrated superoperators form a non-commutative Lie algebra:

$$[\Sigma[\epsilon_1], \Sigma[\epsilon_2]] = \Sigma[\epsilon_\Delta]. \quad (11)$$

The explicit form of the difference shifting field is

$$\epsilon_\Delta(\mathbf{r}) = \epsilon_1(\mathbf{r}) \cdot \nabla \epsilon_2(\mathbf{r}) - \epsilon_2(\mathbf{r}) \cdot \nabla \epsilon_1(\mathbf{r}), \quad (12)$$

which is identical to the standard Lie bracket of the two vector fields $\epsilon_1(\mathbf{r})$ and $\epsilon_2(\mathbf{r})$, as holds also classically [12,13]. Using the generic momentum operator $\hat{\mathbf{p}}$ allows one to express Eq. (12) alternatively as $\epsilon_\Delta(\mathbf{r}) = (i/\hbar)(\epsilon_1(\mathbf{r}) \cdot [\hat{\mathbf{p}}, \epsilon_2(\mathbf{r})] - \epsilon_2(\mathbf{r}) \cdot [\hat{\mathbf{p}}, \epsilon_1(\mathbf{r})])$. The derivation of Eq. (11) is based on resolving the nested commutators on the left-hand side. The commutator relationship (9) between the localized superoperators $\sigma(\mathbf{r})$ and $\sigma(\mathbf{r}')$ then follows via building the mixed second functional derivative of Eq. (11), $\delta^2/[\delta\epsilon_1(\mathbf{r})\delta\epsilon_2(\mathbf{r}')]$, observing that $\delta\Sigma[\epsilon]/\delta\epsilon(\mathbf{r}) = \sigma(\mathbf{r})$, and simplifying.

Having laid out the geometrical structure of the quantum mechanical shifting, we turn to its statistical mechanical consequences. We consider the following generic many-body Hamiltonian

$$\hat{H} = \sum_i \frac{\hat{\mathbf{p}}_i^2}{2m} + u(\mathbf{r}^N) + \sum_i V_{\text{ext}}(\mathbf{r}_i), \quad (13)$$

where $u(\mathbf{r}^N)$ is the interparticle interaction potential and $V_{\text{ext}}(\mathbf{r})$ is an external one-body potential. We consider stationary Hamiltonians $\hat{H}_0$, where the subscript 0 indicates the absence of explicit time dependence. The corresponding canonical quantum partition sum is $Z = \text{Tr} e^{-\beta\hat{H}_0}$, where $\beta = 1/(k_B T)$ with Boltzmann constant k_B and absolute temperature T . The canonical free energy is $F = -k_B T \ln Z$ and thermal equilibrium averages of general quantum observables are given by $\langle \cdot \rangle = \text{Tr} \cdot e^{-\beta\hat{H}_0}/Z$. This formulation encompasses both bosonic and fermionic systems. The respective exchange symmetry characterizes the Hilbert space basis $|n\rangle$, such that $|n\rangle$ acquires a factor $+1$ (bosons) or -1 (fermions) upon particle exchange; details are provided in Ref. [24].

One defining feature of any gauge transformation is that its application leaves measurable quantities invariant, which in the present case are quantum statistical mechanical averages. Applying the integrated shifting superoperator (10)

to a given observable $\hat{A}$ will in general have a nonvanishing effect on $\hat{A}$, such that $(1 + \Sigma[\epsilon])\hat{A} = \hat{A} + \Sigma[\epsilon]\hat{A} \neq \hat{A}$, since $\Sigma[\epsilon]\hat{A} \neq 0$. However, on average $\langle \Sigma[\epsilon]\hat{A} \rangle = 0$, irrespective of the specific form of the gauge function $\epsilon(\mathbf{r})$ and of the observable $\hat{A}$; we recall the thermal mean as $\langle \Sigma[\epsilon]\hat{A} \rangle = \text{Tr} \Sigma[\epsilon]\hat{A}e^{-\beta\hat{H}_0}/Z$ with $\Sigma[\epsilon]$ acting on the product $\hat{A}e^{-\beta\hat{H}_0}$. That the average vanishes can be seen by expressing $\Sigma[\epsilon]$ in the form given in the text above Eq. (10) to rewrite $\langle \Sigma[\epsilon]\hat{A} \rangle = \int d\mathbf{r} \epsilon(\mathbf{r}) \cdot \langle \sigma(\mathbf{r})\hat{A} \rangle$, where $\langle \sigma(\mathbf{r})\hat{A} \rangle = 0$ due to $\langle \sigma(\mathbf{r})\hat{A} \rangle = \langle [\sigma^\dagger(\mathbf{r})1]^\dagger \hat{A} \rangle = -\langle [\sigma(\mathbf{r})1]^\dagger \hat{A} \rangle = 0$, as follows from the anti-self-adjointness (7) and Eq. (3).

The localized shifting superoperator (1) has no dependence on the gauge function, and hence it forms a very efficient starting point for the derivation of sum rules. As a prerequisite, we consider applying the shifting superoperator to the Boltzmann factor:

$$\sigma(\mathbf{r})e^{-\beta\hat{H}_0} = \int_0^\beta d\beta' e^{-\beta'\hat{H}_0} \hat{\mathbf{F}}_0(\mathbf{r}) e^{\beta'\hat{H}_0} e^{-\beta\hat{H}_0}, \quad (14)$$

where the force density operator (4) is

$$\hat{\mathbf{F}}_0(\mathbf{r}) = -\sigma(\mathbf{r})\hat{H}_0. \quad (15)$$

Equation (14) follows from the commutator form (1) and the general property of exponentiated operators $[\hat{B}, e^{-\beta\hat{C}}] = -\int_0^\beta d\beta' e^{-\beta'\hat{C}} [\hat{B}, \hat{C}] e^{\beta'\hat{C}} e^{-\beta\hat{C}}$ by setting $\hat{B} = (i/\hbar)m\hat{\mathbf{J}}(\mathbf{r})$ and $\hat{C} = \hat{H}_0$. The additive structure of the Hamiltonian (13) induces the force density splitting [36] into $\hat{\mathbf{F}}_0(\mathbf{r}) = \nabla \cdot \hat{\boldsymbol{\tau}}_0(\mathbf{r}) + \hat{\mathbf{F}}_{\text{int},0}(\mathbf{r}) - \hat{n}(\mathbf{r})\nabla V_{\text{ext},0}(\mathbf{r})$, where $\hat{\boldsymbol{\tau}}_0(\mathbf{r})$ is the kinetic stress tensor [19,36], $\hat{\mathbf{F}}_{\text{int},0}(\mathbf{r}) = -\sum_i \delta(\mathbf{r} - \mathbf{r}_i) [\nabla_i u_0(\mathbf{r}^N)]$ is the interparticle force density, and $V_{\text{ext},0}(\mathbf{r})$ is the external potential, all for the equilibrium system.

To start the sum rule construction, we first build the equilibrium average of the trivial Eq. (3). This yields $0 = \langle 0 \rangle = \langle [\sigma(\mathbf{r})1]^\dagger \rangle = \langle \sigma^\dagger(\mathbf{r}) \rangle = -\langle \sigma(\mathbf{r}) \rangle = -\text{Tr} \sigma(\mathbf{r})e^{-\beta\hat{H}_0}/Z = -\langle \beta\hat{\mathbf{F}}_0(\mathbf{r}) \rangle$, which follows from Eq. (7), writing out the canonical average, using the Boltzmann operator identity (14), using the invariance of the trace under cyclic permutations, and identifying the thermal average. Defining the mean force density as $\mathbf{F}_0(\mathbf{r}) = \langle \hat{\mathbf{F}}_0(\mathbf{r}) \rangle$ leads to

$$\mathbf{F}_0(\mathbf{r}) = 0, \quad (16)$$

which is the equilibrium force density balance [19,36].

To incorporate general observables $\hat{A}$ into the framework, we apply the averaging strategy to the adjoint of Eq. (5). On the left-hand side this yields $\langle \hat{\mathbf{S}}_A^\dagger(\mathbf{r}) \rangle = \langle \hat{\mathbf{S}}_A(\mathbf{r}) \rangle = \mathbf{S}_A(\mathbf{r})$, where we have used the self-adjointness of the hyperforce density operator and then have defined the mean hyperforce density $\mathbf{S}_A(\mathbf{r})$. On the right-hand side one obtains $\langle [\sigma(\mathbf{r})\hat{A}]^\dagger \rangle = \langle \hat{A}^\dagger \sigma^\dagger(\mathbf{r}) \rangle = -\langle \hat{A}^\dagger \sigma(\mathbf{r}) \rangle = -\text{Tr} \hat{A}^\dagger \sigma(\mathbf{r})e^{-\beta\hat{H}_0}/Z = -\langle \hat{A} | \beta\hat{\mathbf{F}}_0(\mathbf{r}) \rangle$, where we have first built the adjoint of the shifting superoperator, used its anti-self-adjointness (7), and then written out the thermal average. In the last step we have first applied Eq. (14) and in the notation used the Mori(-Kubo-Bogoliubov) product $(\cdot | \cdot)$ as a general means to describe response [39,42,43]. The Mori product constitutes a scalar product of two general operators $\hat{A}$ and $\hat{B}$, and it is defined as $(\hat{A} | \hat{B}) = \beta^{-1} \int_0^\beta d\beta' \text{Tr} \hat{A}^\dagger e^{-\beta'\hat{H}_0} \hat{B} e^{\beta'\hat{H}_0} e^{-\beta\hat{H}_0}/Z$, where here

$\hat{B} = \beta \hat{\mathbf{F}}_0(\mathbf{r})$. An alternative and equivalent form is $(\hat{A}|\hat{B}) = \beta^{-1} \int_0^\beta d\beta' \langle \hat{A}^\dagger \hat{B}(i\hbar\beta') \rangle$, with $\hat{B}(i\hbar\beta')$ denoting the Heisenberg operator evaluated at imaginary time $t = i\hbar\beta'$; see, e.g., Ref. [44]. When applied to the present case we obtain

$$(\hat{A}|\beta \hat{\mathbf{F}}_0(\mathbf{r})) = \int_0^\beta d\beta' \langle \hat{A}^\dagger e^{-\beta' \hat{H}_0} \hat{\mathbf{F}}_0(\mathbf{r}) e^{\beta' \hat{H}_0} \rangle, \quad (17)$$

where we have identified the thermal average $\langle \cdot \rangle$ on the right-hand side.

We recall that Eq. (17) is the thermal average of the adjoint right-hand side of Eq. (5), which equals $\mathbf{S}_A(\mathbf{r})$, see above. Rearranging the equality one obtains the following equilibrium quantum hyperforce balance:

$$\mathbf{S}_A(\mathbf{r}) + (\hat{A}|\beta \hat{\mathbf{F}}_0(\mathbf{r})) = 0, \quad (18)$$

which is exact. Since $\hat{A} = \hat{A}^\dagger$ both terms in Eq. (18) are real-valued. Hence one can express the Mori product alternatively as $(\beta \hat{\mathbf{F}}_0(\mathbf{r})|\hat{A})$ or as the Mori covariance $\text{cov}(\hat{A}|\beta \hat{\mathbf{F}}_0(\mathbf{r})) = (\hat{A}|\beta \hat{\mathbf{F}}_0(\mathbf{r})) - \langle \hat{A}^\dagger \rangle \langle \beta \hat{\mathbf{F}}_0(\mathbf{r}) \rangle$, where the latter holds true due to the vanishing mean force density (16). The sum rule (18) can alternatively be obtained by considering the forces in an extended ensemble with modified Hamiltonian; see Ref. [24] for the derivation.

As a consistency check, choosing $\hat{A} = 1$ in Eq. (18) gives from Eq. (5) the result $\hat{\mathbf{S}}_{\hat{A}=1}(\mathbf{r}) = 0$, which from Eq. (18) equals $-(1|\beta \hat{\mathbf{F}}_0(\mathbf{r})) = -\beta \mathbf{F}_0(\mathbf{r})$, such that the hyperforce density balance (18) reduces to the equilibrium force density balance (16). As a specific example we choose the sum of positions, $\hat{A} = \sum_i \mathbf{r}_i$, which yields from Eq. (5) the hyperforce density operator as $\hat{\mathbf{S}}_A(\mathbf{r}) = (-i/\hbar)[\sum_i \mathbf{r}_i, m\hat{\mathbf{J}}(\mathbf{r})] = \hat{n}(\mathbf{r})\mathbb{1}$, as follows from explicit calculation of the commutator. Then the sum rule (18) yields the density profile: $n[\mathbf{r}]\mathbb{1} = -(\sum_i \mathbf{r}_i|\beta \hat{\mathbf{F}}_0(\mathbf{r}))$. For the choice $\hat{A} = \beta \hat{H}_0$, due to Eq. (16) the sum rule (18) attains the form $\text{cov}(\beta \hat{H}_0|\beta \hat{\mathbf{F}}_0(\mathbf{r})) = 0$. The harmonic oscillator, as a toy model, is used to exemplify the validity in Fig. 1.

The shifting superoperator can be used in flexible ways and we present in Ref. [24] the derivation of general two-body and product sum rules. While we have worked with fixed number of particles, all our considerations and resulting sum rules remain valid in the grand ensemble. One merely needs to replace the canonical trace with the grand canonical analog, $\text{Tr}' \cdot = \sum_{N=0}^\infty \sum_n \langle n| \cdot |n \rangle e^{\beta \mu N} / N!$, where μ denotes the chemical potential. The gauge theory applies to both fermions and bosons, as the exchange symmetry is encoded solely in the nature of the Hilbert space basis $|n\rangle$.

In conclusion, we have addressed the consequences of invariance against shifting in quantum many-body systems. That the formal structure of the resulting quantum gauge theory mirrors closely that of the classical version [12–16] is remarkable, given the stark differences between the mathematical objects that are involved. The quantum sum rules become formally analogous to their classical counterparts [12,13] upon identifying the quantum operators $\hat{\mathbf{S}}_A(\mathbf{r})$ and $\hat{A}$ with the respective classical phase space functions and reducing the Mori product to the thermal average of the classical phase space product. We provide further details and a description of how the analogy relates to Dirac's correspondence principle [37] in Ref. [24].

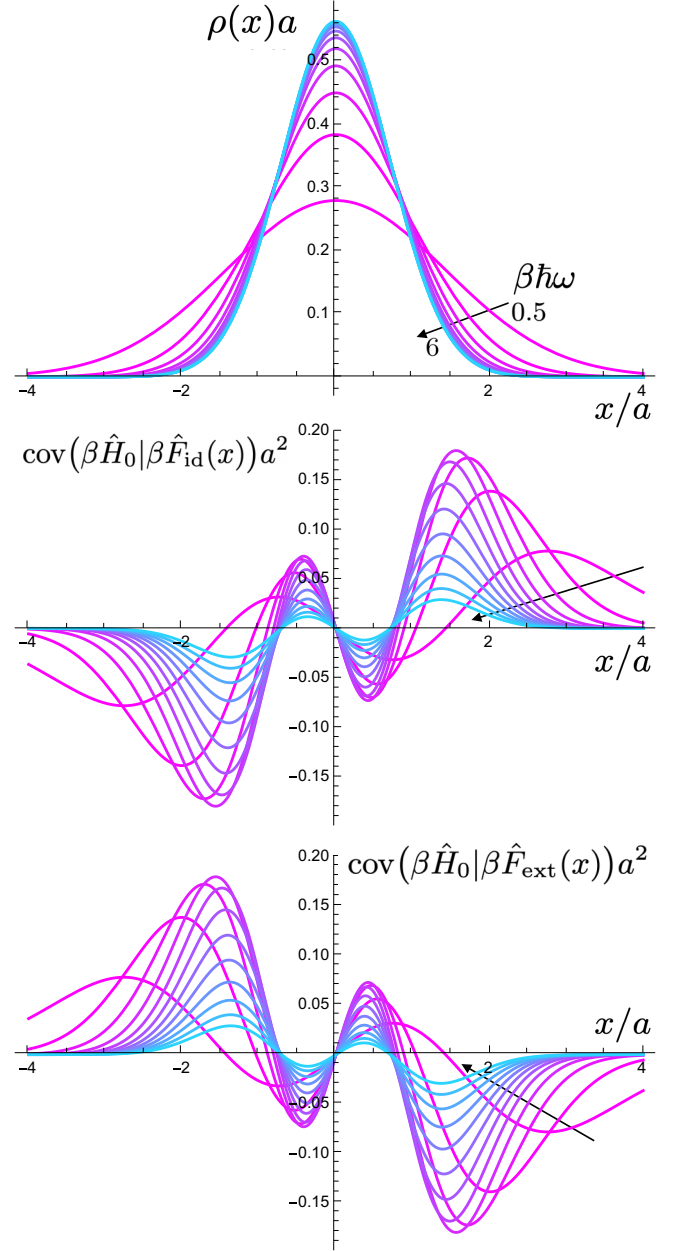


FIG. 1. Demonstration of the general sum rule (18) applied to the observable $\hat{A} = \beta \hat{H}_0$ of a harmonic oscillator with frequency ω . The results are for different values of scaled inverse temperature $\beta \hbar \omega = 0.5, 1, \dots, 6$ (from magenta to blue) and shown as a function of the scaled coordinate x/a with length scale $a = \sqrt{\hbar/(m\omega)}$. Shown are thermal density profile $n(x)a$ (top panel), kinetic Mori term $\text{cov}(\beta \hat{H}_0|\beta \hat{F}_{\text{id}}(x))a^2$ (middle panel), and external force Mori term $\text{cov}(\beta \hat{H}_0|\beta \hat{F}_{\text{ext}}(x))a^2$ (bottom panel). Both Mori covariances display pronounced spatial structuring. For each value of β the sum of the ideal and external covariances vanishes. In general the interparticle covariance term will contribute. Here the general force density operator [36] has the ideal contribution $\hat{F}_{\text{id}}(x) = \partial \hat{\tau}(x)/\partial x$, with one-dimensional kinetic stress operator $\hat{\tau}(x) = \hbar^2/(4m)\partial^2 \hat{n}(x)/\partial x^2 - \sum_i \hat{p}_i \delta(x - x_i) \hat{p}_i/m$, density operator $\hat{n}(x) = \sum_i \delta(x - x_i)$, external contribution $\hat{F}_{\text{ext}}(x) = -m\omega^2 x \hat{n}(x)$, and fundamental degrees of freedom $x_i, \hat{p}_i = -i\hbar \partial/\partial x_i$ with $N = 1$ in the present case.

Due to its applicability to general observables, the hyperforce sum rule (18) provides much potential for the integration within further theoretical approaches. As a demonstration of such uses, we present in Ref. [24] the quantum version of hyperdensity functional theory [45,46], which provides a framework to represent the thermal equilibrium behavior of general observables as density functionals [47]. Dynamical situations in which the initial thermal system with Hamiltonian $\hat{H}_0$ is driven out of equilibrium by a general time-dependent Hamiltonian $\hat{H}$ are also addressed in Ref. [24]. In this nonequilibrium setup the dynamical gauge invariance yields an exact “hypercurrent” sum rule [24], which provides a nonequilibrium generalization of the thermal hyperforce balance (18) and is the quantum analog of the corresponding classical result [16].

In future work, it would be interesting to further explore connections with modern developments in density functional theory [33–35,48–54] and with standard

approaches, such as linear response and the Green-Kubo theory [42,55] and quantum work relations [56]. Much inspiration could come from the recent gauge investigations of quantum thermodynamics [57,58], from the treatment of orientational degrees of freedom in classical anisotropic fluids [59], from the relationship with standard symmetries as recently investigated classically [60], as well as from distributional formulations within rigorous functional analysis [61]. We also refer the reader to Pham-Van’s deep very recent investigations into quantum statistical gauge geometry [62,63].

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Data availability. The data that support the findings of this article are openly available [64].

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