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 demonstrate the integration of the framework within quantum hyperdensity functional theory and show that it generalizes naturally to nonequilibrium.

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 behaviour of the fundamental physical degrees of freedom, which are often taken to be fields. The gauge transformations can carry intricate mathematical structure, 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 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. 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. (19). The perseverance of this theoretical structure is remarkable, given the fundamental changes in the underlying microscopic description of the many-body physics.

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 $\hat{\rho}(\mathbf{r}) = \sum_i \delta(\mathbf{r} - \mathbf{r}_i)$, see e.g. Ref. [24], where the sum runs over all particles $i = 1, \ldots, N$, 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, $\partial \hat{A}(t)/\partial t = (-\mathrm{i}/\hbar)[\hat{A}(t), H(t)]$, where $[\,\cdot\,,\,\cdot\,]$ denotes the commutator, 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, $\hat{A} = \hat{\rho}(\mathbf{r})$, the generic Heisenberg equation of motion reduces to the continuity equation, $\partial \hat{\rho}(\mathbf{r}, t)/\partial t = -\nabla \cdot \hat{\mathbf{J}}(\mathbf{r}, t)$. 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 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 [24] by calculating explicitly the commutator $(-\mathrm{i}/\hbar)[m\hat{\mathbf{J}}(\mathbf{r}, t), H(t)] = \hat{\mathbf{F}}(\mathbf{r}, t)$. This formulation forms a perfectly valid starting point for developing the quantum statistical mechanics of N-body systems.

Here we first take a step back and lay out the canonical quantization according to Dirac's correspondence principle [25] by starting from a *classical* N-body system. The role of the commutator is then played by the (scaled) Poisson brackets and general classical observables $\hat{A}_{\mathrm{cl}}(\mathbf{r}^N, \mathbf{p}^N)$ are functions on the N-body phase space. We use shorthand notations for positions, $\mathbf{r}^N = \mathbf{r}_1, \ldots, \mathbf{r}_N$, and for momenta, $\mathbf{p}^N = \mathbf{p}_1, \ldots, \mathbf{p}_N$, with $\mathbf{p}_i$ denoting the momentum of the classical particle $i = 1, \ldots, N$. The Liouville equation for the time evolution of a classical observable is $\partial \hat{A}_{\mathrm{cl}}(t)/\partial t = \{\hat{A}_{\mathrm{cl}}(t), H(t)\}$, where the Hamiltonian is now a phase space function and $\{\,\cdot\,,\,\cdot\,\}$ indicates the Poisson brackets [26]. The time argument t indicates dynamical dependence according to the Heisenberg picture, which here is classical [26]. As the phase space variables are canonical, they satisfy $\{\mathbf{r}_i, \mathbf{r}_j\} = \{\mathbf{p}_i, \mathbf{p}_j\} = 0$ and $\{\mathbf{r}_i, \mathbf{p}_j\} = \delta_{ij}\mathbb{1}$, where δ_{ij} is the Kronecker symbol and $\mathbb{1}$ denotes the $d \times d$ unit matrix. Choosing the observable of interest as the classical one-body current, $\hat{A} = \hat{\mathbf{J}}_{\rm cl}(\mathbf{r})$, and applying the Liouville equation of motion yields the classical force density phase space function $\hat{\mathbf{F}}_{\rm cl}(\mathbf{r},t) = \{m\hat{\mathbf{J}}_{\rm cl}(\mathbf{r},t), H(t)\}$. The prior quantum description then follows identically by replacing Poisson brackets with (scaled) commutators, i.e., $\{\,\cdot\,,\,\cdot\,\} \to (-{\rm i}/\hbar)[\,\cdot\,,\,\cdot\,]$ and identifying classical phase space variables with their corresponding quantum operators.

The recent classical gauge theory is based on viewing the above Poisson brackets $\{m\hat{\mathbf{J}}_{\rm cl}(\mathbf{r},t), H(t)\}$ as an operator that acts on $H(t)$ [16]. Upon exchanging the order of arguments and multiplying by -1, this generates the following classical 'shifting' operators [12, 13, 16], which are given, in classical Schrödinger form [26], as:

$$\boldsymbol{\sigma}_{\rm cl}(\mathbf{r}) = \{\,\cdot\,, m\hat{\mathbf{J}}_{\rm cl}(\mathbf{r})\}, \tag{1}$$

and we refer to Ref. [16] for the explicit phase space form. The classical shifting operators (1) represent a canonical transformation [27] and they generate a specific gauge transformation on phase space [12, 13]. The shifting operators possess remarkable algebraic properties, such as being anti-self-adjoint on phase space and having nontrivial (Lie algebra) commutator structure. This differential operator structure has profound consequences when applied to classical statistical mechanical averages both in thermal equilibrium [12, 13] and in general nonequilibrium situations [16]. A range of exact sum rules follows and these have been shown to be computationally accessible using classical particle-based simulations [16, 18].

Here we formulate *quantum* shifting gauge invariance and start by applying Dirac's correspondence principle [25] to the Poisson bracket form (1) of the classial shifting operators $\boldsymbol{\sigma}_{\rm cl}(\mathbf{r})$. This leads one to postulate the following quantum 'shifting superoperator':

$$\boldsymbol{\sigma}(\mathbf{r}) = -\frac{i}{\hbar}[\,\cdot\,, m\hat{\mathbf{J}}(\mathbf{r})], \tag{2}$$

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

$$m\hat{\mathbf{J}}(\mathbf{r}) = \frac{1}{2}\sum_i [\hat{\mathbf{p}}_i \delta(\mathbf{r}-\mathbf{r}_i) + \delta(\mathbf{r}-\mathbf{r}_i)\hat{\mathbf{p}}_i], \tag{3}$$

with $\hat{\mathbf{p}}_i = -{\rm i}\hbar\nabla_i$ denoting the momentum operator of quantum particle i, where $\nabla_i = \partial/\partial\mathbf{r}_i$. Equation (2) 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 (2) is the appropriate quantum mechanical entity to encapsulate statistical mechanical gauge invariance by laying out several of its key properties.

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

$$\boldsymbol{\sigma}(\mathbf{r})1 = 0, \tag{4}$$

which follows from the definition (2) 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,

$$\hat{\mathbf{F}}(\mathbf{r}) = -\boldsymbol{\sigma}(\mathbf{r})H, \tag{5}$$

which constitutes the Schrödinger form of $\hat{\mathbf{F}}(\mathbf{r},t)$ and is specified in more detail later. Equation (5) follows from the definition (2) and the Heisenberg equation of motion for the current density.

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

$$\hat{\mathbf{S}}_A(\mathbf{r}) = \boldsymbol{\sigma}(\mathbf{r})\hat{A}, \tag{6}$$

which is the quantum analog of the corresponding classical phase space function [12, 18] and is expressed as $\hat{\mathbf{S}}_A(\mathbf{r}) = (-{\rm i}/\hbar)[\hat{A}, m\hat{\mathbf{J}}(\mathbf{r})]$ according to the commutator form (2). 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 $[\boldsymbol{\sigma}(\mathbf{r})\hat{A}]^\dagger = \boldsymbol{\sigma}(\mathbf{r})\hat{A}$ for $\hat{A} = \hat{A}^\dagger$. This property can in turn be derived from

$$[\boldsymbol{\sigma}(\mathbf{r})\hat{A}]^\dagger = \boldsymbol{\sigma}(\mathbf{r})\hat{A}^\dagger, \tag{7}$$

where $\hat{A}$ can be general (not necessarily self-adjoint). Equation (7) is a consequence of the commutator structure (2) 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 [25, 28] 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 [29], the adjoint $\mathcal{O}^\dagger$ of a general superoperator $\mathcal{O}$ is defined as ${\rm Tr}\,\hat{A}^\dagger\mathcal{O}\hat{B} = {\rm Tr}\,(\mathcal{O}^\dagger\hat{A})^\dagger\hat{B}$, where $\hat{A}$ and $\hat{B}$ are general Hilbert space operators and ${\rm Tr}\,\cdot\, = \sum_n \langle n|\,\cdot\,|n\rangle$ indicates the trace over Hilbert space. This will be important for the statistical mechanics described later.

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

$$\boldsymbol{\sigma}^\dagger(\mathbf{r}) = -\boldsymbol{\sigma}(\mathbf{r}), \tag{8}$$

which follows from the quantum trace being invariant under cyclic permutations [29]. More specifically, ${\rm Tr}\,\hat{A}[\hat{B},\hat{C}] = {\rm Tr}\,[\hat{C},\hat{A}]\hat{B}$, where one chooses $\hat{C} = (-{\rm i}/\hbar)m\hat{\mathbf{J}}(\mathbf{r})$. Together with Eq. (2) this leads to

$${\rm Tr}\,\hat{A}[\boldsymbol{\sigma}(\mathbf{r})\hat{B}] = -{\rm Tr}\,[\boldsymbol{\sigma}(\mathbf{r})\hat{A}]\hat{B}, \tag{9}$$

where replacing $\hat{A}$ with $\hat{A}^\dagger$ and combining with Eq. (7) gives Eq. (8).

While the relationships (4)–(9) point towards the prowess of individual uses of the shifting superoperator, one needs to consider multiple instances of $\boldsymbol{\sigma}(\mathbf{r})$ 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:

$$[\boldsymbol{\sigma}(\mathbf{r}), \boldsymbol{\sigma}(\mathbf{r}')] = [\nabla\delta(\mathbf{r}-\mathbf{r}')]\boldsymbol{\sigma}(\mathbf{r}) + \boldsymbol{\sigma}(\mathbf{r}')[\nabla\delta(\mathbf{r}-\mathbf{r}')], \tag{10}$$

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 $\nabla\delta(\mathbf{r}-\mathbf{r}') = (\mathrm{i}/\hbar)[\hat{\mathbf{p}}, \delta(\mathbf{r}-\mathbf{r}')]$ upon introducing a generic momentum operator $\hat{\mathbf{p}} = -\mathrm{i}\hbar\nabla$ that satisfies the canonical commutator relationship $[\mathbf{r}, \hat{\mathbf{p}}] = \mathrm{i}\hbar\mathbb{1}$ 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 $\Sigma[\boldsymbol{\epsilon}] = \int d\mathbf{r}\boldsymbol{\epsilon}(\mathbf{r})\cdot\boldsymbol{\sigma}(\mathbf{r})$, where the brackets indicate functional dependence on the shifting field $\boldsymbol{\epsilon}(\mathbf{r})$. An explicit form of $\Sigma[\boldsymbol{\epsilon}]$ is obtained by expressing $\boldsymbol{\sigma}(\mathbf{r})$ via the commutator (2), using the scaled current (3), and carrying out the position integral, which yields:

$$\Sigma[\boldsymbol{\epsilon}] = -\frac{\mathrm{i}}{2\hbar}\sum_i [\,\cdot\,, \boldsymbol{\epsilon}(\mathbf{r}_i)\cdot\hat{\mathbf{p}}_i + \hat{\mathbf{p}}_i\cdot\boldsymbol{\epsilon}(\mathbf{r}_i)]. \tag{11}$$

As an illustration of Eq. (11) we consider the effect of $1+\Sigma[\boldsymbol{\epsilon}]$ acting on the fundamental position and momentum degrees of freedom. The result is $(1+\Sigma[\boldsymbol{\epsilon}])\mathbf{r}_j = \mathbf{r}_j + \boldsymbol{\epsilon}(\mathbf{r}_j)$ and $(1+\Sigma[\boldsymbol{\epsilon}])\hat{\mathbf{p}}_j = \hat{\mathbf{p}}_j - [(\nabla_j\boldsymbol{\epsilon}(\mathbf{r}_j))\cdot\hat{\mathbf{p}}_j + \hat{\mathbf{p}}_j\cdot(\nabla_j\boldsymbol{\epsilon}(\mathbf{r}_j))^{\mathsf{T}}]/2$, where the superscript T indicates transposition of a $d\times d$ matrix. Thus we recover the (linearized) quantum canonical shifting transformation of Ref. [19], where quantum canonical transformations [30] generalize their classical counterparts [27].

Working with the superoperator (2) 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 shifting fields $\boldsymbol{\epsilon}_1(\mathbf{r})$ and $\boldsymbol{\epsilon}_2(\mathbf{r})$ the corresponding integrated superoperators form a noncommutative Lie algebra,

$$[\Sigma[\boldsymbol{\epsilon}_1], \Sigma[\boldsymbol{\epsilon}_2]] = \Sigma[\boldsymbol{\epsilon}_\Delta]. \tag{12}$$

The explicit form of the difference shifting field is

$$\boldsymbol{\epsilon}_\Delta(\mathbf{r}) = \boldsymbol{\epsilon}_1(\mathbf{r})\cdot\nabla\boldsymbol{\epsilon}_2(\mathbf{r}) - \boldsymbol{\epsilon}_2(\mathbf{r})\cdot\nabla\boldsymbol{\epsilon}_1(\mathbf{r}), \tag{13}$$

which is identical to the standard Lie bracket of the two vector fields $\boldsymbol{\epsilon}_1(\mathbf{r})$ and $\boldsymbol{\epsilon}_2(\mathbf{r})$, as holds also classically [12, 13]. Using the generic momentum operator $\hat{\mathbf{p}}$ allows one to express Eq. (13) alternatively as $\boldsymbol{\epsilon}_\Delta(\mathbf{r}) = (\mathrm{i}/\hbar)\big(\boldsymbol{\epsilon}_1(\mathbf{r})\cdot[\hat{\mathbf{p}}, \boldsymbol{\epsilon}_2(\mathbf{r})] - \boldsymbol{\epsilon}_2(\mathbf{r})\cdot[\hat{\mathbf{p}}, \boldsymbol{\epsilon}_1(\mathbf{r})]\big)$. The derivation of Eq. (12) is based on resolving the nested commutators on the left hand side. The commutator relationship (10) between the localized superoperators $\boldsymbol{\sigma}(\mathbf{r})$ and $\boldsymbol{\sigma}(\mathbf{r}')$ then follows via building the mixed second functional derivative of Eq. (12), $\delta^2/[\delta\boldsymbol{\epsilon}_1(\mathbf{r})\delta\boldsymbol{\epsilon}_2(\mathbf{r}')]$, observing that $\delta\Sigma[\boldsymbol{\epsilon}]/\delta\boldsymbol{\epsilon}(\mathbf{r}) = \boldsymbol{\sigma}(\mathbf{r})$, 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

$$H = \sum_i \frac{\hat{\mathbf{p}}_i^2}{2m} + u(\mathbf{r}^N) + \sum_i V_{\mathrm{ext}}(\mathbf{r}_i), \tag{14}$$

where $u(\mathbf{r}^N)$ is the interparticle interaction potential and $V_{\mathrm{ext}}(\mathbf{r})$ is an external one-body potential. We first consider stationary Hamiltonians H_0, where the subscript 0 indicates the absence of explicit time dependence. The corresponding canonical quantum partition sum is $Z = \mathrm{Tr}\,\mathrm{e}^{-\beta H_0}$, 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 $\langle\,\cdot\,\rangle = \mathrm{Tr}\,\cdot\,\mathrm{e}^{-\beta H_0}/Z$.

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 (11) to a given observable $\hat{A}$ will in general have a nonvanishing effect on $\hat{A}$, such that $(1+\Sigma[\boldsymbol{\epsilon}])\hat{A} = \hat{A} + \Sigma[\boldsymbol{\epsilon}]\hat{A} \neq \hat{A}$, since $\Sigma[\boldsymbol{\epsilon}]\hat{A} \neq 0$. However, on average $\langle\Sigma[\boldsymbol{\epsilon}]\hat{A}\rangle = 0$, irrespective of the specific form of the gauge function $\boldsymbol{\epsilon}(\mathbf{r})$ and of the observable $\hat{A}$; we recall the thermal mean as $\langle\Sigma[\boldsymbol{\epsilon}]\hat{A}\rangle = \mathrm{Tr}\,\Sigma[\boldsymbol{\epsilon}]\hat{A}\mathrm{e}^{-\beta H_0}/Z$ with $\Sigma[\boldsymbol{\epsilon}]$ acting on the product $\hat{A}\mathrm{e}^{-\beta H_0}$. That the average vanishes can be seen by expressing $\Sigma[\boldsymbol{\epsilon}]$ in the form given above Eq. (11) to re-write $\langle\Sigma[\boldsymbol{\epsilon}]\hat{A}\rangle = \int d\mathbf{r}\boldsymbol{\epsilon}(\mathbf{r})\cdot\langle\boldsymbol{\sigma}(\mathbf{r})\hat{A}\rangle$, where $\langle\boldsymbol{\sigma}(\mathbf{r})\hat{A}\rangle = 0$ due to $\langle\boldsymbol{\sigma}(\mathbf{r})\hat{A}\rangle = \langle[\boldsymbol{\sigma}^\dagger(\mathbf{r})1]^\dagger\hat{A}\rangle = -\langle[\boldsymbol{\sigma}(\mathbf{r})1]^\dagger\hat{A}\rangle = 0$, as follows from the anti-self-adjointness (8) and Eq. (4).

The localized shifting superoperator (2) 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:

$$\boldsymbol{\sigma}(\mathbf{r})\mathrm{e}^{-\beta H_0} = \int_0^\beta d\beta'\mathrm{e}^{-\beta' H_0}\hat{\mathbf{F}}_0(\mathbf{r})\mathrm{e}^{\beta' H_0}\mathrm{e}^{-\beta H_0}, \tag{15}$$

where the force density operator (5) is

$$\hat{\mathbf{F}}_0(\mathbf{r}) = -\boldsymbol{\sigma}(\mathbf{r})H_0. \tag{16}$$

Equation (15) follows from the commutator form (2) and the general property of exponentiated operators $[\hat{B}, \mathrm{e}^{-\beta\hat{C}}] = -\int_0^\beta d\beta'\mathrm{e}^{-\beta'\hat{C}}[\hat{B}, \hat{C}]\mathrm{e}^{\beta'\hat{C}}\mathrm{e}^{-\beta\hat{C}}$ by setting $\hat{B} = (\mathrm{i}/\hbar)m\hat{\mathbf{J}}(\mathbf{r})$ and $\hat{C} = H_0$. The additive structure of the Hamiltonian (14) induces the force density splitting [24] into $\hat{\mathbf{F}}_0(\mathbf{r}) = \nabla\cdot\hat{\boldsymbol{\tau}}_0(\mathbf{r}) + \hat{\mathbf{F}}_{\mathrm{int},0}(\mathbf{r}) - \hat{\rho}(\mathbf{r})\nabla V_{\mathrm{ext},0}(\mathbf{r})$, where $\hat{\boldsymbol{\tau}}_0(\mathbf{r})$ is the kinetic stress tensor [19, 24], $\hat{\mathbf{F}}_{\mathrm{int},0}(\mathbf{r}) = -\sum_i\delta(\mathbf{r}-\mathbf{r}_i)\nabla_i u_0(\mathbf{r}^N)$ is the interparticle force density, and $V_{\mathrm{ext},0}(\mathbf{r})$ 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. (4). This yields $0 = \langle 0 \rangle = \langle [\boldsymbol{\sigma}(\mathbf{r})1]^\dagger \rangle = \langle \boldsymbol{\sigma}^\dagger(\mathbf{r}) \rangle = -\langle \boldsymbol{\sigma}(\mathbf{r}) \rangle = -\mathrm{Tr}\, \boldsymbol{\sigma}(\mathbf{r}) \mathrm{e}^{-\beta H_0}/Z = -\langle \beta \hat{\mathbf{F}}_0(\mathbf{r}) \rangle$, which follows from Eq. (8), writing out the canonical average, using the Boltzmann operator identity (15) 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

$$\mathbf{F}_0(\mathbf{r}) = 0, \tag{17}$$

which is the equilibrium force density balance [19, 24].

To incorporate general observables $\hat{A}$ into the framework, we apply the averaging strategy to the adjoint of Eq. (6). 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 $\langle [\boldsymbol{\sigma}(\mathbf{r})\hat{A}]^\dagger \rangle = \langle \hat{A}^\dagger \boldsymbol{\sigma}^\dagger(\mathbf{r}) \rangle = -\langle \hat{A}^\dagger \boldsymbol{\sigma}(\mathbf{r}) \rangle = -\mathrm{Tr}\, \hat{A}^\dagger \boldsymbol{\sigma}(\mathbf{r}) \mathrm{e}^{-\beta H_0}/Z = -\big(\hat{A}|\beta \hat{\mathbf{F}}_0(\mathbf{r})\big)$, where we have first built the adjoint of the shifting superoperator, used its anti-self-adjointness (8), and then written out the thermal average. In the last step we have first applied Eq. (15) and in the notation used the Mori(-Kubo-Bogoliubov) product $(\,\cdot\,|\,\cdot\,)$ as a general means to describe response [29, 31, 32]. The Mori product constitutes a scalar product of two general operators $\hat{A}$ and $\hat{B}$ and it is defined as $(\hat{A}|\hat{B}) = \beta^{-1} \int_0^\beta d\beta' \mathrm{Tr}\, \hat{A}^\dagger \mathrm{e}^{-\beta' H_0} \hat{B} \mathrm{e}^{\beta' H_0} \mathrm{e}^{-\beta H_0}/Z$, 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 $t = \mathrm{i}\hbar\beta'$, see e.g. Ref. [33]. When applied to the present case we obtain:

$$\big(\hat{A}|\beta \hat{\mathbf{F}}_0(\mathbf{r})\big) = \int_0^\beta d\beta' \langle \hat{A}^\dagger \mathrm{e}^{-\beta' H_0} \hat{\mathbf{F}}_0(\mathbf{r}) \mathrm{e}^{\beta' H_0} \rangle, \tag{18}$$

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

We recall that Eq. (18) is the thermal average of the adjoint right hand side of Eq. (6), which equals $\mathbf{S}_A(\mathbf{r})$, see above. Restoring the equality and re-arranging one obtains the following equilibrium quantum hyperforce balance:

$$\mathbf{S}_A(\mathbf{r}) + \big(\hat{A}|\beta \hat{\mathbf{F}}_0(\mathbf{r})\big) = 0, \tag{19}$$

which is exact. Since $\hat{A} = \hat{A}^\dagger$ both terms in Eq. (19) are real-valued. Hence one can express the Mori product alternatively as $(\beta \hat{\mathbf{F}}_0(\mathbf{r})|\hat{A})$ or as the covariance $\mathrm{cov}\big(\hat{A}|\beta \hat{\mathbf{F}}_0(\mathbf{r})\big) = \big(\hat{A}|\beta \hat{\mathbf{F}}_0(\mathbf{r})\big) - \langle \hat{A}^\dagger \rangle \langle \beta \hat{\mathbf{F}}_0(\mathbf{r}) \rangle$, where the latter holds true due to the vanishing mean force density (17). The sum rule (19) can alternatively be obtained by considering the forces in an extended ensemble with modified Hamiltonian, see Appendix A.

As a consistency check, choosing $\hat{A} = 1$ in Eq. (19) gives from Eq. (6) the result $\hat{\mathbf{S}}_{\hat{A}=1}(\mathbf{r}) = 0$, which from Eq. (19) equals $-\big(1|\beta \hat{\mathbf{F}}_0(\mathbf{r})\big) = -\beta \mathbf{F}_0(\mathbf{r})$, such that the hyperforce density balance (19) reduces to the equilibrium force density balance (17). As a specific example we choose the sum of positions, $\hat{A} = \sum_i \mathbf{r}_i$, which yields from Eq. (6) the hyperforce density operator as $\hat{\mathbf{S}}_A(\mathbf{r}) =$

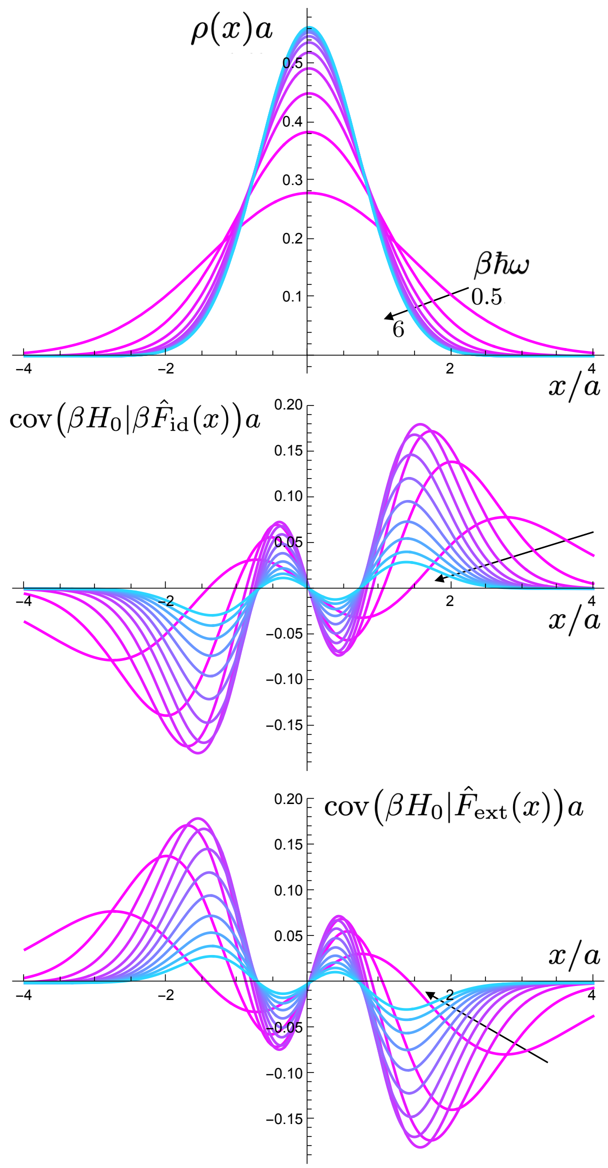

FIG. 1. Demonstration of the general sum rule (19) applied to the observable $\hat{A} = \beta H_0$ of a harmonic oscillator with frequency ω. The results are for different values of scaled inverse temperature $\beta\hbar\omega = 0.5, 1, \ldots, 6$ (from magenta to blue) and shown as a function of the scaled coordinate x/a with lengthscale $a = \hbar/(m\omega)$. Shown are thermal density profile $\rho(x)a$ (top panel), kinetic Mori term $\mathrm{cov}\big(\beta H_0|\beta \hat{F}_{\mathrm{id}}(x)\big)a$ (middle panel), and external force Mori term $\mathrm{cov}\big(\beta H_0|\hat{F}_{\mathrm{ext}}(x)\big)a$ (bottom panel). Both Mori covariances display pronouced spatial structuring. For each value of β the sum of the ideal and external covariances vanishes. In general the interparticle covariance term will contribute.

$(-\mathrm{i}/\hbar)[\sum_i \mathbf{r}_i, m\hat{\mathbf{J}}(\mathbf{r})] = \hat{\rho}(\mathbf{r})\mathbb{1}$, as follows from explicit calculation of the commutator. Then the sum rule (19) yields the density profile: $\rho(\mathbf{r})\mathbb{1} = -(\sum_i \mathbf{r}_i|\beta\hat{\mathbf{F}}_0(\mathbf{r}))$. For the choice $\hat{A} = \beta H_0$, due to Eq. (17) the sum rule (19) attains the form $\mathrm{cov}\big(\beta H_0|\beta\mathbf{F}_0(\mathbf{r})\big) = 0$. 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 Appendix B 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, $\mathrm{Tr}'\cdot = \sum_{N=0}^{\infty}\sum_n \langle n| \cdot |n\rangle e^{\beta\mu N}/N!$, 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. Despite its limitations [34] we found Dirac's correspondence principle to be highly useful for postulating the superoperator (2). All subsequent results follow rigorously within the quantum treatment, without invoking the classical physics again. 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.

Due to its applicabilty to general observables, the hyperforce sum rule (19) provides much potential for the integration within further theoretical approaches. As a demonstration of such uses, we present in Appendix C the quantum version of hyperdensity functional theory [35, 36], which provides a framework to represent the thermal equilibrium behaviour of general observables as density functionals [37]. Dynamical situations in which the initial thermal system with Hamiltonian H_0 is driven out of equilibrium by a general time-dependent Hamiltonian H are addressed in Appendix D. In this nonequilibrium setup the dynamical gauge invariance yields an exact 'hypercurrent' sum rule (36), which provides a nonequilibrium generalization of the thermal hyperforce balance (19) 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 [38–45] and with standard approaches, such as linear repsonse and the Green-Kubo theory [31, 46], and with quantum work relations [47] as well as with the recent gauge treatment of quantum thermodynamics [48, 49].

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END MATTER

A. Extended ensembles and force balance

To demonstrate consistency, we show that the hyperforce sum rule (19) can be alternatively derived from the force density balance in a suitably extended ensemble [29, 50]. We follow the lines of the classical hyperdensity functional theory [35, 36] and hence consider the quantum statistical mechanics for the modified Hamiltonian

$$H_A = H_0 - \lambda\hat{A}/\beta. \tag{20}$$

We restrict ourselves to (self-adjoint) forms of $\hat{A}$ that render H_A well-behaved. The correspondingly extended quantum force density operator is generated via the generic mechanism (5) as $\hat{\mathbf{F}}_A(\mathbf{r}) = -\boldsymbol{\sigma}(\mathbf{r})H_A = -\boldsymbol{\sigma}(\mathbf{r})H_0 + \boldsymbol{\sigma}(\mathbf{r})\lambda\hat{A}/\beta = \hat{\mathbf{F}}_0(\mathbf{r}) + \lambda\hat{\mathbf{S}}_A(\mathbf{r})/\beta$, where we have identified $\hat{\mathbf{F}}_0(\mathbf{r})$ via Eq. (16) and $\hat{\mathbf{S}}_A(\mathbf{r})$ via Eq. (6). As the extended system is in equilibrium, its mean force density vanishes, $\langle\hat{\mathbf{F}}_A(\mathbf{r})\rangle_A = 0$. Here $\langle\cdot\rangle_A = \mathrm{Tr}\,\cdot\,\mathrm{e}^{-\beta H_A}/Z_A$ denotes the thermal average in the extended ensemble with extended partition sum $Z_A = \mathrm{Tr}\, \mathrm{e}^{-\beta H_A}$. Expansion to linear order in λ yields $\langle \hat{\mathbf{F}}_A(\mathbf{r})\rangle_A = \langle \hat{\mathbf{F}}_0(\mathbf{r})\rangle + \lambda[\langle \hat{\mathbf{S}}_A(\mathbf{r})\rangle + \mathrm{cov}(\beta\hat{\mathbf{F}}_0(\mathbf{r})|\hat{A})]/\beta = 0$, where both orders in λ necessarily vanish separately. The zeroth order recovers the original force density balance (17) and the linear order gives the hyperforce sum rule (19).

B. Product and two-body hyperforce sum rules

The shifting superoperator (2) can be used in flexible ways. When e.g. applied to products of observables, one finds $\hat{\mathbf{S}}_{AB}(\mathbf{r}) = \boldsymbol{\sigma}(\mathbf{r})\hat{A}\hat{B} = \hat{\mathbf{S}}_A(\mathbf{r})\hat{B} + \hat{A}\hat{\mathbf{S}}_B(\mathbf{r})$, which leads via (19) to the hyperforce product sum rule

$$\langle \hat{\mathbf{S}}_A(\mathbf{r})\hat{B}\rangle + \langle \hat{A}\hat{\mathbf{S}}_B(\mathbf{r})\rangle + \big(\hat{A}\hat{B}|\beta\hat{\mathbf{F}}_0(\mathbf{r})\big) = 0. \tag{21}$$

Higher-body correlation functions follow via averaging superoperator products, such as $\boldsymbol{\sigma}(\mathbf{r}')\boldsymbol{\sigma}(\mathbf{r})1 = 0$. This yields a quantum analog of the '3g'-sum rule [20]:

$$\big(\beta\hat{\mathbf{F}}_0(\mathbf{r})|\beta\hat{\mathbf{F}}_0(\mathbf{r}')\big) + \langle \hat{\mathsf{K}}_0(\mathbf{r},\mathbf{r}'))\rangle = 0, \tag{22}$$

where the Hamiltonian 'curvature' operator is $\hat{\mathsf{K}}_0(\mathbf{r},\mathbf{r}') = -\boldsymbol{\sigma}(\mathbf{r})\boldsymbol{\sigma}(\mathbf{r}')\beta H_0$, which is equivalent to the force density gradient operator $\boldsymbol{\sigma}(\mathbf{r})\beta\hat{\mathbf{F}}_0(\mathbf{r}')$ via Eq. (16). Alternatively, Eq. (22) is obtained from the hyperforce sum rule (19) upon simply setting $\hat{A} = \beta\hat{\mathbf{F}}_0(\mathbf{r}')$ therein. Further multi-body sum rules follow from the Lie commutator structure (10) and will be presented elsewhere.

C. Quantum hyperdensity funtional theory

We formulate the quantum analog of the classical hyperdensity functional theory [35, 36]. We work in the grand ensemble with the primed trace $\mathrm{Tr}\,'\cdot$ and chemical potential μ and consider the extended Hamiltonian $H_A = H_0 - \lambda\hat{A}/\beta$, cf. Eq. (20). We first make the hyperforce sum rule (19) more explicit by inserting the decomposition of the force density operator $\hat{\mathbf{F}}_0(\mathbf{r})$ into kinetic, interparticle, and external contributions, as given below Eq. (16). This yields, upon using the Mori covariance,

$$\begin{aligned}\mathbf{S}_A(\mathbf{r}) + \nabla\cdot\mathrm{cov}\big(\hat{A}|\beta\hat{\boldsymbol{\tau}}_0(\mathbf{r})\big) + \mathrm{cov}\big(\hat{A}|\beta\hat{\mathbf{F}}_{\mathrm{int},0}(\mathbf{r})\big)\\ - \chi_A(\mathbf{r})\nabla\beta V_{\mathrm{ext},0}(\mathbf{r}) = 0,\end{aligned} \tag{23}$$

where $\chi_A(\mathbf{r})$ is the hyperfluctuation profile,

$$\chi_A(\mathbf{r}) = \mathrm{cov}\big(\hat{A}|\hat{\rho}(\mathbf{r})\big), \tag{24}$$

which will provide the link to density functional theory.

For the extended system, the grand potential density functional is

$$\Omega[\rho] = F[\rho] + \int d\mathbf{r}\rho(\mathbf{r})[V_{\mathrm{ext},0}(\mathbf{r}) - \mu], \tag{25}$$

where $F[\rho]$ is the intrinsic free energy functional, which contains kinetic, Hartree, exchange, correlation, and entropic contributions, generated by the extended interparticle potential $u_A(\mathbf{r}^N) = u_0(\mathbf{r}^N) - \lambda\hat{A}/\beta$.

Mermin's minimization principle [37] ascertains that $\Omega[\rho]$ is minimized by the equilibrium density profile $\rho_0(\mathbf{r})$ and that the value of the density functional at the minimum is the true grand potential, $\Omega[\rho_0] = \Omega_0 = -\beta^{-1}\ln \mathrm{Tr}\,'\mathrm{e}^{-\beta(H_A-\mu N)}$. At the minimum the functional derivative vanishes, $\delta\Omega[\rho]/\delta\rho(\mathbf{r})|_{\rho=\rho_0} = 0$. Calculating the functional derivative yields the Euler-Lagrange equation,

$$C_1(\mathbf{r};[\rho]) - \beta V_{\mathrm{ext},0}(\mathbf{r}) + \beta\mu = 0, \tag{26}$$

where we have dropped the subscript 0 of the equilibrium density profile and have defined the full one-body direct correlation functional $C_1(\mathbf{r};[\rho]) = -\delta\beta F[\rho]/\delta\rho(\mathbf{r})$, which in particular includes the kinetic contributions.

Differentiating the Euler-Lagrange equation (26) with respect to λ yields

$$C_A(\mathbf{r};[\rho]) + \int d\mathbf{r}' C_2(\mathbf{r},\mathbf{r}';[\rho])\chi_A(\mathbf{r}') = 0, \tag{27}$$

where the hyperdirect correlation functional is given by $C_A(\mathbf{r};[\rho]) = \partial C_1(\mathbf{r};[\rho])/\partial\lambda|_\rho$ and the full two-body direct correlation functional is defined as $C_2(\mathbf{r},\mathbf{r}';[\rho]) = \delta C_1(\mathbf{r})/\delta\rho(\mathbf{r}')$. The hyperfluctuation profile (24) emerges in Eq. (27) due to

$$\chi_A(\mathbf{r}) = \frac{\partial\rho(\mathbf{r})}{\partial\lambda}, \tag{28}$$

as can be verified explicitly on the basis of the explicit average $\rho(\mathbf{r}) = \langle\hat{\rho}(\mathbf{r})\rangle_A$, taken in the extended grand ensemble (see Appendix A). Furthermore, parametric differentiation yields the mean of the considered observable $\hat{A}$,

$$A = -\frac{\partial\beta\Omega_0}{\partial\lambda}. \tag{29}$$

Functional relationships are as follows:

$$C_A(\mathbf{r};[\rho]) = \frac{\delta A[\rho]}{\delta\rho(\mathbf{r})}, \tag{30}$$

$$A[\rho] = \int \mathcal{D}[\rho] C_A(\mathbf{r};[\rho]), \tag{31}$$

where the functional line integral [51] in Eq. (31) is the inverse of Eq. (30). Briefly, one can derive Eq. (30) by recognizing that $A[\rho] = -\partial\beta\Omega[\rho]/\partial\lambda = -\partial\beta F[\rho]/\partial\lambda|_\rho$, where the latter identity follows from $\partial\Omega[\rho]/\partial\lambda = \partial F[\rho]/\partial\lambda|_\rho + \int d\mathbf{r}\chi_A(\mathbf{r})\delta\Omega[\rho]/\delta\rho(\mathbf{r})|_\lambda$ and the minimization condition $\delta\Omega[\rho]/\delta\rho(\mathbf{r}) = 0$. Exchanging the order of differentiation in $\partial\big(\delta F[\rho]/\delta\rho(\mathbf{r})\big)/\partial\lambda|_\rho = \delta\big(\partial F[\rho]/\partial\lambda|_\rho\big)/\delta\rho(\mathbf{r})$ yields Eq. (30), in analogy to the classical case [35, 36].

Taking the limit $\lambda\to 0$ restores the original ensemble with Hamiltonian H_0.

D. Dynamical gauge invariance

We take the thermal equilibrium physics, generated by H_0, as the initial state at time $t = 0$ and consider the dynamics for $t \geq 0$ as induced by an, in general, explicitly time-dependent Hamiltonian (14). The mass m, the interparticle potential $u(\mathbf{r}^N)$, and the external potential $V_{\rm ext}(\mathbf{r})$ can all depend on time and we suppress such mere parametric time dependence in the notation. The quantum propagator $\mathcal{U}(t,0)$ performs the time evolution, which is unitary such that $\mathcal{U}^\dagger(t,0)\mathcal{U}(t,0) = \mathcal{U}(t,0)\mathcal{U}^\dagger(t,0) = 1$ and $\mathcal{U}(0,0) = 1$. Heisenberg operators are then given in the standard way as $\hat{A}(t) = \mathcal{U}^\dagger(t,0)\hat{A}\,\mathcal{U}(t,0)$. The nonequilibrium physics is then described by time-dependent averages that are built over the ensemble of initial states, $A(t) = \langle \hat{A}(t)\rangle$.

We introduce temporal dependence in the quantum gauge theory by following the lines of construction of the classical dynamical formulation [16]. Generalizing Eq. (2) allows one to define the following *dynamical* shifting superoperator:

$$\boldsymbol{\sigma}(\mathbf{r},t) = -\frac{\mathrm{i}}{\hbar}[\,\cdot\,, m\hat{\mathbf{J}}(\mathbf{r},t)] \tag{32}$$

where the (scaled) Heisenberg current operator is $m\hat{\mathbf{J}}(\mathbf{r},t) = \mathcal{U}^\dagger(t,0)m\hat{\mathbf{J}}(\mathbf{r})\mathcal{U}(t,0)$. Several basic properties of $\boldsymbol{\sigma}(\mathbf{r},t)$ follow analogously to those of the static counterpart $\boldsymbol{\sigma}(\mathbf{r})$, cf. Eqs. (4)–(9). Specifically one obtains: the trivial identity $\boldsymbol{\sigma}(\mathbf{r},t)1 = 0$, the force density operator $\hat{\mathbf{F}}(\mathbf{r},t) = -\boldsymbol{\sigma}(\mathbf{r},t)H(t)$, and the dynamical hyperforce density operator

$$\hat{\mathbf{S}}_A(\mathbf{r},t) = \boldsymbol{\sigma}(\mathbf{r},t)\hat{A}(t), \tag{33}$$

where spelling out the right hand side yields the standard Heisenberg form $\hat{\mathbf{S}}_A(\mathbf{r},t) = \mathcal{U}^\dagger(t,0)\hat{\mathbf{S}}_A(\mathbf{r})\mathcal{U}(t,0)$ with $\hat{\mathbf{S}}_A(\mathbf{r})$ given by Eq. (6). Furthermore anti-self-adjointness holds, $\boldsymbol{\sigma}^\dagger(\mathbf{r},t) = -\boldsymbol{\sigma}(\mathbf{r},t)$, and the dynamical trace identity is $\mathrm{Tr}\,\hat{A}[\boldsymbol{\sigma}(\mathbf{r},t)\hat{B}] = -\mathrm{Tr}\,[\boldsymbol{\sigma}(\mathbf{r},t)\hat{A}]\hat{B}$.

The implications of the dynamical gauge invariance reach beyond the above generic Heisenberg time dependence. To reveal this structure, in generalization of the initial state force density operator (16), one applies $\boldsymbol{\sigma}(\mathbf{r},t)$ to the *initial state* Hamiltonian H_0. Hence we define the quantum 'shift current operator' as

$$\hat{\mathbf{C}}(\mathbf{r},t) = -\boldsymbol{\sigma}(\mathbf{r},t)\beta H_0, \tag{34}$$

which is identical to the commutator form $\hat{\mathbf{C}}(\mathbf{r},t) = (\mathrm{i}/\hbar)[\beta H_0, m\hat{\mathbf{J}}(\mathbf{r},t)]$, as is obtained from application of the dynamical shifting superoperator (32). The shift current operator (34) is a quantum observable, $\hat{\mathbf{C}}(\mathbf{r},t) = \hat{\mathbf{C}}^\dagger(\mathbf{r},t)$, as is inherited from $m\hat{\mathbf{J}}(\mathbf{r},t) = m\hat{\mathbf{J}}^\dagger(\mathbf{r},t)$ and preserved by the definition (32). Equation (34) is the quantum analog of the classical hypercurrent observable, which constitutes an initial state time derivative that is accessible in trajectory-based simulations [12].

The mean shift current, $\mathbf{C}(\mathbf{r},t) = \langle\hat{\mathbf{C}}(\mathbf{r},t)\rangle$, satisfies the following exact shift current sum rule:

$$\mathbf{C}(\mathbf{r},t) = 0, \tag{35}$$

where the left hand side consists of a sum of kinetic, interparticle, and external contributions, as follows from the corresponding splitting of H_0 in Eq. (34). Briefly, Eq. (35) follows from averaging $\boldsymbol{\sigma}(\mathbf{r},t)1 = 0$, such that $0 = \langle\boldsymbol{\sigma}(\mathbf{r},t)\rangle = \mathrm{Tr}\,\boldsymbol{\sigma}(\mathbf{r},t)\mathrm{e}^{-\beta H_0}/Z = (1|\hat{\mathbf{C}}(\mathbf{r},t))$ and recognizing the resulting Mori product as $\langle\hat{\mathbf{C}}(\mathbf{r},t)\rangle$. At the initial time, the shift current operator (34) reduces to the (scaled) equilibrium force density operator (16), such that $\hat{\mathbf{C}}(\mathbf{r},0) = \beta\hat{\mathbf{F}}_0(\mathbf{r})$, and hence the shift current identity (34) becomes the force density balance (17).

The behaviour of general dynamical observables $\hat{A}(t)$ follows from generalizations of the derivations of Eqs. (15) and (18). The dynamical shifting operator being anti-self-adjoint leads to $\langle[\boldsymbol{\sigma}(\mathbf{r},t)\hat{A}(t)]^\dagger\rangle = -\langle\hat{A}^\dagger(t)\boldsymbol{\sigma}(\mathbf{r},t)\rangle = -(\hat{A}(t)|\hat{\mathbf{C}}(\mathbf{r},t))$. Identifying the left hand side as the dynamical hyperforce density $\mathbf{S}_A(\mathbf{r},t) = \langle\hat{\mathbf{S}}_A(\mathbf{r},t)\rangle = \langle\hat{\mathbf{S}}_A^\dagger(\mathbf{r},t)\rangle$ and re-arranging yields the following hypercurrent sum rule:

$$\mathbf{S}_A(\mathbf{r},t) + \big(\hat{A}(t)|\hat{\mathbf{C}}(\mathbf{r},t)\big) = 0, \tag{36}$$

where $\hat{\mathbf{C}}(\mathbf{r},t)$ is given via Eq. (34). The second term in Eq. (36) measures via the Mori product the correlation between the dynamical observable $\hat{A}(t)$ and the shift current $\hat{\mathbf{C}}(\mathbf{r},t)$. In general this average will be nonzero, despite the mean hypercurrent $\mathbf{C}(\mathbf{r},t)$ vanishing at all times, cf. Eq. (35). As a specific example, choosing $\hat{A} = \sum_i \mathbf{r}_i$ in Eq. (36) yields $\hat{\mathbf{S}}_A(\mathbf{r},t) = \hat{\rho}(\mathbf{r},t)\mathbb{1}$. Thus the dynamical density profile satisfies $\rho(\mathbf{r},t)\mathbb{1} = -\big(\sum_i \mathbf{r}_i(t)|\hat{\mathbf{C}}(\mathbf{r},t)\big)$.