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Force balance in thermal quantum many-body systems from Noether's theorem

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Abstract

We address the consequences of invariance properties of the free energy of spatially inhomogeneous quantum many-body systems. We consider a specific position-dependent transformation of the system that consists of a spatial deformation and a corresponding locally resolved change of momenta. This operator transformation is canonical and hence equivalent to a unitary transformation on the underlying Hilbert space of the system. As a consequence, the free energy is an invariant under the transformation. Noether's theorem for invariant variations then allows to derive an exact sum rule, which we show to be the locally resolved equilibrium one-body force balance. For the special case of homogeneous shifting, the sum rule states that the average global external force vanishes in thermal equilibrium.

Keywords: force balance, quantum statistical mechanics, YBG equation, density functional theory, Noether's theorem

1. Introduction

When investigating global equilibrium properties such as the equation of state for a given many-body Hamiltonian, the strategies in classical and quantum statistical mechanical treatments differ markedly from each other. Obtaining the partition sum in the classical case requires, in principle, to carry out the high-dimensional phase space integral over the

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Boltzmann factor of the Hamiltonian [1]. The quantum mechanical analog thereof is the trace over the Boltzmann factor of the Hamiltonian, where the latter is viewed as an infinite-dimensional matrix expressed in a suitable basis of e.g. energy eigenfunctions [2]. In both cases, quantum and classical, the leap from the dynamics of the particle-based many-body description to the thermal average is both powerful and abstract. As a result physically meaningful quantities, such as the pressure, chemical and thermal susceptibilities etc become systematically available, at least in principle, through derivatives of the free energy, which are readily available from the partition sum. On a higher level of detail, locally resolved correlation functions are available as statistical averages and they characterize the microscopic structure of the system and allow to obtain global properties via suitable integration.

On the other hand the concept of forces, while being at the very heart of mechanics, often receives less attention in both statistical and quantal contexts. Nevertheless in the realm of quantum many-body systems several recent publications [3–5] addressed in detail the force balance relationship on the one-body level of correlation functions. Here the forces are resolved in position and also in time in the dynamic case. Tarantino and Ullrich [3] reformulated time-dependent Kohn–Sham density functional theory (DFT) in terms of the second time derivative of the density. In their approach forces feature prominently. They argue that the causal structure of their formulation is more transparent than that of the standard Kohn–Sham formalism of DFT. Tchenkoue *et al* [4] have addressed the force balance in several advanced approximations in DFT. They state that their approach avoids differentiability and causality issues and having to carry out the optimized-effective-potential procedure of orbital-dependent functionals.

Earlier than these advancements, Tokatly had already honed in on the force balance relationship in the framework of his time-dependent deformation functional theory [6]. The theory is based on considering a hydrodynamic Lagrangian view of quantum many-body dynamics [7, 8]. The force balance equation plays a role of a gauge condition that fixes the reference frame [7]. The approach yields formally exact equations of motion and conservation laws [7] and it provided the basis for a geometric formulation of time-dependent DFT [8]. Ullrich and Tokatly were then able to address important nonadiabatic effects in the electron dynamics in time-dependent density-functional theory [9].

Locally resolved force fields play a prominent role in the recent power functional framework for many-body dynamics [5]. Besides the time-dependent density profile, this variational approach includes the locally resolved current and acceleration distributions as its fundamental physical variables. The theory has been formulated for classical [10, 11] and quantum [12, 13] systems; a recent review [5] gives much background. The respective variational equation has the clear physical interpretation of a nonequilibrium force balance relationship and it allows to categorize flow and structural forces [5] and acceleration viscous forces [5], all of which go beyond the adiabatic forces that are captured by the dynamical classical DFT [14–18]. Standard DFT is recovered as the equilibrium limit of the power functional theory [5].

Furthermore, in the classical context, forces were recently put to the fore in methods to obtain statistically averaged quantities, such as the density profile of a spatially inhomogeneous system, via computer simulation of the many-body problem. In his recent review [19], Rotenberg gives a clear account of such force-sampling techniques; see e.g. [20–22] for original work. On the theoretical side, classical DFT [14–16] offers access to forces via building the gradient of the Euler–Lagrange minimization equation [5]. An alternative that applies to pairwise interparticle interactions is the force integral over the two-body density correlation function [23, 24]. The two-body density is explicitly available within state-of-the-art classical density functionals, such as fundamental measure theory, see e.g. [25]. Two-body density correlation functions are also central to the recently developed conditional probability DFT for quantum systems [26, 27].

In prior work we have applied Noether's theorem of invariant variations [28, 29] to the classical statistical mechanics of particle-based many-body systems [30–33]. Rather than starting with the invariance properties of an action functional, the approach is based on considering the symmetry properties of appropriate statistical functionals, such as the partition sum, in order to derive exact identities. These 'sum rules' carry clear physical interpretation as interrelations between forces when starting with spatial displacement, and between torques when starting with spatial rotations. Different types of identities result, depending on whether the elementary free energy is displaced (leading to external force sum rules), the excess free energy density functional (internal force identities) or the power functional (memory identities [30] that connect time direct correlation functions [5]).

We emphasize that Noether's original work [28] is not restricted to the action integral of a physical system. She rather deals with functionals of a general nature, formulating carefully necessary (and for our practical purposes very mild) assumptions of analyticity. Background from an entirely mathematical perspective can be found in [34]. Descriptions of the standard application to the action can be found in many sources, including [35] and on a more popular level [36]. For the classical case, the differences between the present use in thermal physics and the standard deterministic form are discussed in [31]. Briefly, within our present setting, we require to identify a functional $F[\boldsymbol{\epsilon}]$ of a position-dependent vector field $\boldsymbol{\epsilon}(\mathbf{r})$. On the one hand $\boldsymbol{\epsilon}(\mathbf{r})$ parametrizes the functional dependence on further fields (suppressed in the notation). Noether's theorem applies, when despite this apparent dependence, on the other hand the functional is invariant under changes of $\boldsymbol{\epsilon}(\mathbf{r})$. Hence trivially $\delta F[\boldsymbol{\epsilon}]/\delta\boldsymbol{\epsilon}(\mathbf{r}) = 0$. Quite remarkably this leads to a nontrivial identity, when taken as a concrete recipe for calculation of the left-hand side.

The invariant variational techniques have aided the development of a force-based approach to classical DFT [33]. Here the fundamental starting equation is the locally resolved equilibrium force balance relationship, which (for pairwise interparticle forces) is a classical result [1] that dates back to Yvon [23], and to Born and Green [24]. The derivation of this fundamental equation is performed by considering an inhomogeneous spatial displacement of the entire system, as described by a vector field $\boldsymbol{\epsilon}(\mathbf{r})$ in three-dimensional space. Together with a corresponding change of momenta (described in detail below) the change of variables constitutes a canonical transformation on classical phase space, and hence it preserves the phase space volume element [37]. The specific form of the transformation (in particular it being independent of time) also preserves the Hamiltonian. Hence the partition sum itself is unchanged under the transformation and so is the free energy. (The Hamiltonian, via its associated Boltzmann factor, and the phase space integral are the only nontrivial ingredients in the partition sum.) One is hence faced with an invariant variational problem, as addressed succinctly by Emmy Noether in her classical work [28]; see [29] for a historical account.

In the present contribution, we demonstrate that Noether's theorem is applicable to the equilibrium statistical properties of quantum many-body systems. We present a quantal shifting transformation of the position and momentum operators that reduces to the transformation of [33] in the classical case. Quantum mechanically, the transformation is canonical [38], i.e. it preserves the fundamental commutator relation between position and momentum. Such transformations represent unitary transformations on the Hilbert space of the considered system. The partition sum is hence invariant under the transformation, as it is given as the trace of the Hamiltonian's Boltzmann factor, with both the trace and the Hamiltonian being invariants, as is the case classically. The result, to first order in the displacement field, is the locally resolved equilibrium force balance relationship [3–5]. While one could expect on general grounds that the Noether line of thought would indeed apply to quantum systems, the details of the derivation differ markedly from the classical case, and we spell out the details in the following.

2. Thermal invariance theory

2.1. Quantum canonical transformation

We consider Hamiltonians of the form

$$H = \sum_i \frac{\mathbf{p}_i^2}{2m} + u(\mathbf{r}^N) + \sum_i V_{\text{ext}}(\mathbf{r}_i), \tag{1}$$

where the sums run over all particles $i = 1, \ldots, N$, with the total number of particles N. All particles possess identical mass m and each particle i is characterized by its position ($\mathbf{r}_i$) and momentum ($\mathbf{p}_i$) operator. The interparticle interaction potential $u(\mathbf{r}^N)$ depends on all particle positions and we use the compact notation $\mathbf{r}^N \equiv \mathbf{r}_1, \ldots, \mathbf{r}_N$. The system is under the influence of an external one-body potential $V_{\text{ext}}(\mathbf{r})$, where $\mathbf{r}$ is a generic position variable.

Position and momentum satisfy the fundamental commutator relations

$$[\mathbf{r}_i, \mathbf{p}_j] = \mathrm{i}\hbar\delta_{ij}\mathbb{1}, \tag{2}$$

where i is the imaginary unit, $\hbar$ denotes the reduced Planck constant, δ_{ij} is the Kronecker symbol and $\mathbb{1}$ indicates the 3×3-unit matrix. The commutator of two vectors involves transposition according to $[\mathbf{r}_i, \mathbf{p}_j] = \mathbf{r}_i\mathbf{p}_j - \mathbf{p}_j\mathbf{r}_i^{\mathsf{T}}$, where the multiplication of two vectors is dyadic and the superscript T denotes the transpose of a 3×3-matrix. Hence in component notation $[r_i^\alpha, p_j^\gamma] = r_i^\alpha p_j^\gamma - p_j^\gamma r_i^\alpha$, where Greek superscripts α, γ denote Cartesian components of position and momentum. Equation (2) then reads as $[r_i^\alpha, p_j^\gamma] = \mathrm{i}\hbar\delta_{ij}\delta_{\alpha\gamma}$. We work in position representation, such that the momentum operator of particle i is given by $\mathbf{p}_i = -\mathrm{i}\hbar\nabla_i$, where ∇_i indicates the derivative with respect to $\mathbf{r}_i$.

We consider the following transformation of position and momenta

$$\mathbf{r}_i \to \mathbf{r}_i + \boldsymbol{\epsilon}(\mathbf{r}_i), \tag{3}$$

$$\mathbf{p}_i \to \left\{(\mathbb{1} + (\nabla_i\boldsymbol{\epsilon}_i))^{-1} \cdot \mathbf{p}_i + \mathbf{p}_i \cdot (\mathbb{1} + (\nabla_i\boldsymbol{\epsilon}_i)^{\mathsf{T}})^{-1}\right\}/2, \tag{4}$$

where $\boldsymbol{\epsilon}(\mathbf{r})$ is a given real-valued three-dimensional vector field with $\mathbf{r}$ indicating position, $\boldsymbol{\epsilon}_i = \boldsymbol{\epsilon}(\mathbf{r}_i)$ is a shorthand notation, and the superscript -1 indicates matrix inversion. In equation (4) the gradient operator ∇_i acts only on $\boldsymbol{\epsilon}_i$, as is indicated by the surrounding parentheses; hence in position representation each entry of the 3×3-matrix $(\nabla_i\boldsymbol{\epsilon}_i)$, which is obtained as a dyadic product of the vectors ∇_i and $\boldsymbol{\epsilon}_i$, acts only as a multiplication operator on the wave function. In our notation the dot product of a matrix A and a vector $\mathbf{x}$ is understood in the standard way as $(\mathsf{A} \cdot \mathbf{x})_\alpha = A_{\alpha\gamma}x_\gamma$, with summation being implied over the repeated index γ. For convenience we also define this product with the reversed order of factors as $(\mathbf{x} \cdot \mathsf{A})_\alpha = x_\gamma A_{\gamma\alpha}$. This appears in the second term in the sum in equation (4).

We assume throughout that the vector field $\boldsymbol{\epsilon}(\mathbf{r})$ is such that a bijection is established between old and new coordinates. Hence the transformations (3) and (4) need to be invertible. (A poignant counterexample is $\boldsymbol{\epsilon}(\mathbf{r}) = -\mathbf{r}$, which renders equation (3) to be $\mathbf{r}_i \to 0$ and the matrix inversion in the momentum transformation (4) becoming ill-defined.) The momentum transformation is the self-adjoint version of the classical phase space transformation considered in [33], which is in linear order, as given in [33], simply $\mathbf{p}_i \to \mathbf{p}_i - (\nabla_i\boldsymbol{\epsilon}_i) \cdot \mathbf{p}_i$. Here there is no need to pay attention to the ordering of terms, as the classical phase space variables commute with each other. The finite version thereof is $\mathbf{p}_i \to (\mathbb{1} + \nabla_i\boldsymbol{\epsilon}_i)^{-1} \cdot \mathbf{p}_i$, as can be shown via a generating function that via differentiation yields the transformation equations. Equation (4) is obtained as the arithmetic mean of this expression and its adjoint. Very briefly, the classical generator (see the appendix of [33]) is $\mathcal{G} = \sum_{i=1}^{N} \tilde{\mathbf{p}}_i \cdot (\mathbf{r}_i + \boldsymbol{\epsilon}(\mathbf{r}_i))$, and the transformation equations are obtained via the identities $\tilde{\mathbf{r}}_i = \partial\mathcal{G}/\partial\tilde{\mathbf{p}}_i$ and $\mathbf{p}_i = \partial\mathcal{G}/\partial\mathbf{r}_i$, where the tilde indicates the transformed variables.

We expand the inverse matrix in equation (4) to linear order in the gradient of the displacement field according to: $(\mathbb{1} + (\nabla_i\boldsymbol{\epsilon}_i))^{-1} = \mathbb{1} - (\nabla_i\boldsymbol{\epsilon}_i)$, where terms of the order $(\nabla_i\boldsymbol{\epsilon}_i)^2$ and higher have been omitted. Using this expansion, equation (4) in component notation is: $p_i^\alpha \to p_i^\alpha - \sum_\gamma \left\{(\nabla_i^\alpha \epsilon_i^\gamma) p_i^\gamma + p_i^\gamma(\nabla_i^\alpha \epsilon_i^\gamma)\right\}/2$, which when resorting back to vector notation is:

$$\mathbf{p}_i \to \mathbf{p}_i - \left\{(\nabla_i\boldsymbol{\epsilon}_i)\cdot\mathbf{p}_i + \mathbf{p}_i\cdot(\nabla_i\boldsymbol{\epsilon}_i)^{\mathsf{T}}\right\}/2. \tag{5}$$

We first ascertain that the new coordinates $\tilde{\mathbf{r}}_i$ and new momenta $\tilde{\mathbf{p}}_i$, as defined by the right-hand sides of the transformation (3) and (4), also satisfy canonical commutation relations. We start with the prominent case of position and momentum:

$$[\tilde{\mathbf{r}}_i, \tilde{\mathbf{p}}_j] = \left[\mathbf{r}_i + \boldsymbol{\epsilon}_i, \mathbf{p}_j - \left\{(\nabla_j\boldsymbol{\epsilon}_j)\cdot\mathbf{p}_j + \mathbf{p}_j\cdot(\nabla_j\boldsymbol{\epsilon}_j)^{\mathsf{T}}\right\}/2\right] \tag{6}$$

$$= [\mathbf{r}_i, \mathbf{p}_j] + [\boldsymbol{\epsilon}_i, \mathbf{p}_j] - [\mathbf{r}_i, (\nabla_j\boldsymbol{\epsilon}_j)\cdot\mathbf{p}_j]/2 - [\mathbf{r}_i, \mathbf{p}_j\cdot(\nabla_j\boldsymbol{\epsilon}_j)^{\mathsf{T}}]/2 \tag{7}$$

$$= \mathrm{i}\hbar\delta_{ij}\mathbb{1}, \tag{8}$$

where we have truncated in (7) at linear order in the displacement field and its gradient. As the left-hand side of (6) involves no coupling between different particles, it is straightforward to see that for distinct particles, $i \neq j$, the result vanishes, as is indeed the case in equation (8). For $i = j$ we use the explicit form of the momentum operator $\mathbf{p}_i = -\mathrm{i}\hbar\nabla_i$ to find that the second term in (7) is $[\boldsymbol{\epsilon}_i, \mathbf{p}_i] = \mathrm{i}\hbar(\nabla_i\boldsymbol{\epsilon}_i)$. This contribution is precisely cancelled by the sum of the third and the fourth term in (7), which can be shown to have the form $-[\mathbf{r}_i, (\nabla_i\boldsymbol{\epsilon}_i)\cdot\mathbf{p}_i] = -(\nabla_i\boldsymbol{\epsilon}_i)\cdot(\mathrm{i}\hbar\mathbb{1}) = -\mathrm{i}\hbar(\nabla_i\boldsymbol{\epsilon}_i)$. Hence the first term in (7) alone gives the result (8) upon using the fundamental commutator (2).

For completeness, the new variables also satisfy $[\tilde{\mathbf{r}}_i, \tilde{\mathbf{r}}_j] = 0$ and $[\tilde{\mathbf{p}}_i, \tilde{\mathbf{p}}_j] = 0$. The former relationship is trivial, as in position representation only coordinates are involved according to the transformation (3). The momentum identity can be worked out straightforwardly, as we show in appendix A.1. Furthermore the new degrees of freedom are self-adjoint operators. For the positions this is trivial, as we we have $\tilde{\mathbf{r}}_i^\dagger = \mathbf{r}_i^\dagger + \boldsymbol{\epsilon}(\mathbf{r}_i)^\dagger = \mathbf{r}_i + \boldsymbol{\epsilon}(\mathbf{r}_i) \equiv \tilde{\mathbf{r}}_i$, because $\boldsymbol{\epsilon}(\mathbf{r})$ is real-valued. For the momenta: $\tilde{\mathbf{p}}_i^\dagger = \mathbf{p}_i^\dagger - \{(\nabla_i\boldsymbol{\epsilon}_i)\cdot\mathbf{p}_i + \mathbf{p}_i\cdot(\nabla_i\boldsymbol{\epsilon}_i)^{\mathsf{T}})\}^\dagger/2 = \mathbf{p}_i - \{\mathbf{p}_i\cdot(\nabla_i\boldsymbol{\epsilon}_i)^{\mathsf{T}} + (\nabla_i\boldsymbol{\epsilon}_i)\cdot\mathbf{p}_i\}/2 \equiv \tilde{\mathbf{p}}_i$. For completeness we demonstrate that the transformation is quantum canonical beyond linear order in appendix A.2.

2.2. *Functional derivatives by local shift*

Having ascertained that the new variables form a sound basis for the description of the quantum mechanics, we wish to illustrate the effect of the transformation on the system. The following considerations will be an essential ingredient in the thermal physics addressed further below. We wish to investigate the effect on the Hamiltonian $H[\boldsymbol{\epsilon}]$, which is obtained by applying the operator replacements (3) and (4) in the form (1) of the original Hamiltonian. We consider the functional derivative of the transformed Hamiltonian with respect to the displacement field:

$$\frac{\delta H[\boldsymbol{\epsilon}]}{\delta\boldsymbol{\epsilon}(\mathbf{r})} = \frac{\delta}{\delta\boldsymbol{\epsilon}(\mathbf{r})}\left(\sum_i \frac{\tilde{\mathbf{p}}_i^2}{2m} + u(\tilde{\mathbf{r}}^N) + \sum_i V_{\mathrm{ext}}(\tilde{\mathbf{r}}_i)\right). \tag{9}$$

To make progress, we first address the fundamental derivatives of the new position and new momentum with respect to the displacement field. These are easily obtained as follows:

$$\frac{\delta\tilde{\mathbf{r}}_i}{\delta\boldsymbol{\epsilon}(\mathbf{r})}\bigg|_{\boldsymbol{\epsilon}=0} = \delta(\mathbf{r}-\mathbf{r}_i)\mathbb{1}, \tag{10}$$

$$\frac{\delta\tilde{\mathbf{p}}_i}{\delta\boldsymbol{\epsilon}(\mathbf{r})}\bigg|_{\boldsymbol{\epsilon}=0} = \nabla\{\delta(\mathbf{r}-\mathbf{r}_i)\mathbf{p}_i + \mathbf{p}_i\delta(\mathbf{r}-\mathbf{r}_i)\}/2, \tag{11}$$

where $\delta(\cdot)$ denotes the (three-dimensional) Dirac distribution and the derivatives are taken at vanishing displacement field, $\boldsymbol{\epsilon}(\mathbf{r})=0$, as is indicated in the notation on both left-hand sides. The right-hand side of equation (10) constitutes the density operator of particle i times the unit matrix. The right-hand side of equation (11) is the spatial gradient of the momentum density operator of particle i. That both correctly localized operators appear naturally as functional derivatives is an initial indication that the considered transformation indeed can be used as a successful probe for the spatially resolved behaviour of the system.

For completeness, in index notation equation (11) reads as

$$\delta\tilde{p}_i^{\alpha}/\delta\epsilon^{\gamma} = \nabla^{\alpha}(\delta_i p_i^{\gamma} + p_i^{\gamma}\delta_i)/2, \tag{12}$$

where we have introduced the shorthand notations $\delta_i = \delta(\mathbf{r}-\mathbf{r}_i)$ and $\epsilon^{\gamma} = \epsilon^{\gamma}(\mathbf{r})$ and the derivative is again evaluated at vanishing displacement field (such that higher than linear powers in the displacement gradient, as they occur in the *finite* momentum transformation (4), vanish).

In order to obtain the functional derivative (9) of the Hamiltonian we proceed by first differentiating the kinetic energy. We defer the detailed calculations to appendix B, which contains both the simpler one-dimensional case, where matrix-vector complexities are absent (appendix B.1), as well as the present three-dimensional case (appendix B.2). The latter calculation, carried out in index notation in appendix B.2, gives the following result:

$$\frac{\delta}{\delta\boldsymbol{\epsilon}(\mathbf{r})}\sum_i\frac{\tilde{\mathbf{p}}_i^2}{2m}\bigg|_{\boldsymbol{\epsilon}=0} = \nabla\cdot\sum_i\frac{\mathbf{p}_i\delta_i\mathbf{p}_i + \mathbf{p}_i\delta_i\mathbf{p}_i^{\mathsf{T}}}{2m} - \frac{\hbar^2}{4m}\nabla\nabla^2\sum_i\delta(\mathbf{r}-\mathbf{r}_i). \tag{13}$$

We recall that the transpose (superscript T) acts on the entire 3×3-matrix $\mathbf{p}_i\delta_i\mathbf{p}_i$ and that the multiplication of vector and matrix, as is relevant for the divergence, contracts the vector index with the first matrix index; we recall our description thereof after equation (4). Equation (13) is also given in index notation in appendix B.2.

The first term on the right-hand side of equation (13) is directly analogous to the classical case [33], upon viewing the momentum operators as phase space variables. The second term on the right-hand side of equation (13) is genuinely quantum mechanical, as it is quadratic in $\hbar$ and hence vanishes in the classical limit $\hbar\to 0$. This contribution can be rewritten upon expressing the gradient of the Laplace operator as $\nabla\nabla^2 = \nabla^2\,\nabla = \nabla\cdot\nabla\nabla$. Then one can express the second term in equation (13) as $-\nabla\cdot\nabla\nabla\sum_i\delta(\mathbf{r}-\mathbf{r}_i)\hbar^2/(4m)$. Here the Hessian of the density operator, $\nabla\nabla\sum_i\delta(\mathbf{r}-\mathbf{r}_i)$, together with the factor $\hbar^2/(4m)$ forms the quantal kinetic stress contribution $\nabla\nabla\sum_i\delta(\mathbf{r}-\mathbf{r}_i)\hbar^2/(4m)$.

Together with the first term in equation (13), which already is of divergence form, we can define the position-resolved kinetic stress operator (see e.g. [5]) as

$$\hat{\boldsymbol{\tau}}(\mathbf{r}) = -\sum_i\frac{\mathbf{p}_i\delta_i\mathbf{p}_i + \mathbf{p}_i\delta_i\mathbf{p}_i^{\mathsf{T}}}{2m} + \frac{\hbar^2}{4m}\nabla\nabla\sum_i\delta_i. \tag{14}$$

We have hence adopted the convention to include the wave-like contribution $\hbar^2\nabla\nabla\hat{\rho}(\mathbf{r})/(4m)$ into the kinematic stress, where $\hat{\rho}(\mathbf{r}) = \sum_i\delta(\mathbf{r}-\mathbf{r}_i)$ is the standard form of the one-body density operator. The classical kinetic stress is recovered by letting $\hbar\to 0$, such that $\hat{\boldsymbol{\tau}}(\mathbf{r})$ reduces to $-\sum_i\delta(\mathbf{r}-\mathbf{r}_i)\mathbf{p}_i\mathbf{p}_i/m$, where here $\mathbf{p}_i$ denotes the classical phase space variable, which trivially commutes with the spatial delta distribution, and the transpose becomes irrelevant as for the phase space variable $\mathbf{p}_i\mathbf{p}_i = \mathbf{p}_i\mathbf{p}_i^{\mathsf{T}}$.

We have so far shown that the considered quantum canonical transformation the functional derivative of kinetic energy with respect to the displacement field creates the following fundamental result:

$$\left.\frac{\delta H_{\mathrm{kin}}[\boldsymbol{\epsilon}]}{\delta\boldsymbol{\epsilon}(\mathbf{r})}\right|_{\boldsymbol{\epsilon}=0} = -\nabla\cdot\hat{\boldsymbol{\tau}}(\mathbf{r}). \tag{15}$$

Here we have split the Hamiltonian (1) according to $H = H_{\mathrm{kin}} + H_{\mathrm{pot}}$, where the potential energy contains the interparticle and external contributions, $H_{\mathrm{pot}} = u(\mathbf{r}^N) + \sum_i V_{\mathrm{ext}}(\mathbf{r}_i)$. As already laid out above, the functional dependence on $\boldsymbol{\epsilon}(\mathbf{r})$ that is indicated on the left-hand side of (15) arises from expressing the original positions and momenta in the Hamiltonian (1) via the transformation (3) and (4). One could view the result (15) as being unexpectedly simple, despite the technical complexity of the kinematic stress operator $\hat{\boldsymbol{\tau}}(\mathbf{r})$. Recall that the kinematic stress occurs in the Heisenberg equation of motion for the one-body current density [5, 7, 8] and that it hence constitutes a meaningful physical object in its own right. That it is created here from the functional derivative of kinetic energy with respect to the shift field is a strong indicator that the thermal Noether invariance against the local shifting transformation given by equations (3) and (4) carries actual physical significance.

Treating the effects of the local displacement transformation on the potential energy is comparatively easier than the above kinetic energy consideration, as here only position coordinates are involved and hence the commutator structure is trivial. The calculation is very closely analogous to the classical case [31]. We obtain

$$\left.\frac{\delta H_{\mathrm{pot}}[\boldsymbol{\epsilon}]}{\delta\boldsymbol{\epsilon}(\mathbf{r})}\right|_{\boldsymbol{\epsilon}=0} = \left.\frac{\delta u(\tilde{\mathbf{r}}^N)}{\delta\boldsymbol{\epsilon}(\mathbf{r})}\right|_{\boldsymbol{\epsilon}=0} + \sum_i \left.\frac{\delta V_{\mathrm{ext}}(\tilde{\mathbf{r}}_i)}{\delta\boldsymbol{\epsilon}(\mathbf{r})}\right|_{\boldsymbol{\epsilon}=0} \tag{16}$$

$$= \sum_i \left(\nabla_i u(\mathbf{r}^N)\right)\delta_i + \sum_i \left(\nabla_i V_{\mathrm{ext}}(\mathbf{r}_i)\right)\delta_i \tag{17}$$

$$= -\hat{\mathbf{F}}_{\mathrm{int}}(\mathbf{r}) + \hat{\rho}(\mathbf{r})\nabla V_{\mathrm{ext}}(\mathbf{r}), \tag{18}$$

where we have defined the one-body interparticle force density operator $\hat{\mathbf{F}}_{\mathrm{int}}(\mathbf{r}) = -\sum_i(\nabla_i u(\mathbf{r}^N))\delta_i$. The rewriting that involves the external force field $-\nabla V_{\mathrm{ext}}(\mathbf{r})$ in (18) is possible as the derivatives ∇_i and ∇, as well as the positions $\mathbf{r}$ and $\mathbf{r}_i$, can be identified with each other due to the presence of the delta function. The negative external force field $\nabla V_{\mathrm{ext}}(\mathbf{r})$ can then be taken as a common factor outside of the second sum in equation (17) and the density operator remains.

Summing up the kinetic energy derivative (15) and the potential energy identity (18) we obtain

$$-\left.\frac{\delta H[\boldsymbol{\epsilon}]}{\delta\boldsymbol{\epsilon}(\mathbf{r})}\right|_{\boldsymbol{\epsilon}=0} = \nabla\cdot\hat{\boldsymbol{\tau}}(\mathbf{r}) + \hat{\mathbf{F}}_{\mathrm{int}}(\mathbf{r}) - \hat{\rho}(\mathbf{r})\nabla V_{\mathrm{ext}}(\mathbf{r}), \tag{19}$$

which makes explicit that the Hamiltonian generates, via its negative functional derivative with respect to the displacement field, the sum of all one-body force density distributions that act in the system.

That the transformation (3) and (4) has an effect on the Hamiltonian could have been expected from the outset, as the transformation has a nontrivial spatial structure via its dependence on the vector field $\boldsymbol{\epsilon}(\mathbf{r})$. Hence Noether's theorem seemingly does not apply, due to the absence of a direct corresponding invariance. In contrast to this standard application, here we proceed differently and search for an invariance that applies in thermal equilibrium. This requires an average to be an invariant rather than the corresponding operator itself being an invariant, as we lay out in the following.

2.3. Force balance from thermal Noether invariance

We hence turn to a statistical mechanical description which we base on the free energy in the canonical ensemble, expressed as

$$F = -k_{\mathrm{B}} T \ln Z, \tag{20}$$

$$Z = \mathrm{Tr}\, e^{-\beta H} \tag{21}$$

$$= \sum_n \langle n | e^{-\beta H} | n \rangle, \tag{22}$$

where k_{B} denotes the Boltzmann constant and T is absolute temperature. The trace in Hilbert space is denoted by Tr and it is made explicit in (22) with $|n\rangle$ denoting the complete set of orthonormal eigenstates of H labelled by index n. (Possibly degenerate energy eigenstates occur multiple times in the sum.) In more explicit notation, using position representation, $|n\rangle = \phi_n(\mathbf{r}^N)$ such that $\langle n| \cdot |n\rangle = \int d\mathbf{r}^N \phi_n^*(\mathbf{r}^N) \cdot \phi_n(\mathbf{r}^N)$, where the integral is over all position coordinates, $\int d\mathbf{r}^N \cdot = \int d\mathbf{r}_1 \int d\mathbf{r}_2 \ldots \int d\mathbf{r}_N \cdot$ and the asterisk denotes complex conjugation. Here and throughout, we assume that the partition sum (22) and hence the free energy (20) exists, see Giesbertz and Ruggenthaler's [39] account of the divergences that occur in even simple unbounded systems. In our case, we assume (as we do classically [31]) that the system is bounded via the influence of appropriate container walls, as modelled by a corresponding form of the external potential $V_{\mathrm{ext}}(\mathbf{r})$. We hence adopt a pragmatic stance to the existence of the free energy [40].

We expand the free energy (20) in the transformation parameter according to:

$$\left.\frac{\delta F[\boldsymbol{\epsilon}]}{\delta \boldsymbol{\epsilon}(\mathbf{r})}\right|_{\boldsymbol{\epsilon}=0} = -\frac{k_B T}{Z} \left.\frac{\delta Z[\boldsymbol{\epsilon}]}{\delta \boldsymbol{\epsilon}(\mathbf{r})}\right|_{\boldsymbol{\epsilon}=0} \tag{23}$$

$$= -\frac{k_B T}{Z} \mathrm{Tr} \left.\frac{\delta e^{-\beta H[\boldsymbol{\epsilon}]}}{\delta \boldsymbol{\epsilon}(\mathbf{r})}\right|_{\boldsymbol{\epsilon}=0} \tag{24}$$

$$= \sum_n \frac{e^{-\beta E_n}}{Z} \langle n | \left.\frac{\delta H[\boldsymbol{\epsilon}]}{\delta \boldsymbol{\epsilon}(\mathbf{r})}\right|_{\boldsymbol{\epsilon}=0} | n \rangle, \tag{25}$$

where in equation (23) we have used the definition (20) of the free energy via the partition sum $Z[\boldsymbol{\epsilon}]$ of the transformed system. In equation (24) we have used the form (21) of the partition sum and have exchanged the order of the functional derivative and building the trace. Equation (25) constitutes a thermal equilibrium average, where E_n denotes the energy eigenvalue corresponding to the energy eigenstate $|n\rangle$. We have hence obtained

$$\left.\frac{\delta F[\boldsymbol{\epsilon}]}{\delta \boldsymbol{\epsilon}(\mathbf{r})}\right|_{\boldsymbol{\epsilon}=0} = \left\langle \left.\frac{\delta H[\boldsymbol{\epsilon}]}{\delta \boldsymbol{\epsilon}(\mathbf{r})}\right|_{\boldsymbol{\epsilon}=0} \right\rangle_{\mathrm{eq}}, \tag{26}$$

where on the right-hand side we have used the notation $\langle \cdot \rangle_{\mathrm{eq}}$ to indicate the average over the canonical ensemble as it occurs in equation (25); explicitly this is $\langle \cdot \rangle_{\mathrm{eq}} = \sum_n Z^{-1} e^{-\beta E_n} \langle n| \cdot |n\rangle$. The identity (26) is remarkable as it indicates that the local transformation (3) and (4) to lowest order in the displacement field generates a well-defined and physically meaningful thermal average, that of the functional derivative of the Hamiltonian. This mathematical structure mirrors closely that of standard partial derivatives of the free energy with respect to thermodynamic variables, such as e.g. obtaining the entropy via $S = -\partial F / \partial T$.

Before exploiting the specific form of the right-hand side of equation (26) further, we first proceed with the general invariance argument. We expand the free energy of the transformed system to linear order in the displacement field according to:

$$F[\boldsymbol{\epsilon}] = F + \int d\mathbf{r} \frac{\delta F[\boldsymbol{\epsilon}]}{\delta \boldsymbol{\epsilon}(\mathbf{r})}\bigg|_{\boldsymbol{\epsilon}=0} \cdot \boldsymbol{\epsilon}(\mathbf{r}) \tag{27}$$

$$= F + \int d\mathbf{r} \left\langle \frac{\delta H[\boldsymbol{\epsilon}]}{\delta \boldsymbol{\epsilon}(\mathbf{r})}\bigg|_{\boldsymbol{\epsilon}=0} \right\rangle_{\text{eq}} \cdot \boldsymbol{\epsilon}(\mathbf{r}), \tag{28}$$

where equation (27) is the functional Taylor expansion to linear order and the form (28) follows from using equation (26).

On the other hand, the free energy is an invariant under the quantum canonical transformation, and hence:

$$F[\boldsymbol{\epsilon}] = F, \tag{29}$$

where F is the free energy (20) of the original representation of the system. Equation (29) holds due to the fact that canonical transformations are analogous to unitary transformations on the underlying Hilbert space of the considered system; see e.g. the account given by Anderson [38]. We will return to this point below.

From comparison of the Taylor expansion (28) with the free energy invariance (29) we can conclude that the linear term in the expansions vanishes identically and it has to do so irrespective of the form of $\boldsymbol{\epsilon}(\mathbf{r})$. This can only hold provided that the prefactor vansishes:

$$\left\langle \frac{\delta H[\boldsymbol{\epsilon}]}{\delta \boldsymbol{\epsilon}(\mathbf{r})}\bigg|_{\boldsymbol{\epsilon}=0} \right\rangle_{\text{eq}} = 0. \tag{30}$$

Equation (30) is a bare consequence of the invariance of the free energy under the displacement operation, and it is obtained immediately from $\delta F[\boldsymbol{\epsilon}]/\delta\boldsymbol{\epsilon}(\mathbf{r})|_{\boldsymbol{\epsilon}=0} = 0$, as mentioned in the introduction, upon skipping the Taylor expansion argument expressed in equations (27) and (28). The identity (30) holds irrespective of the precise form of the interparticle interaction potential $u(\mathbf{r}^N)$ and of the external potential $V_{\text{ext}}(\mathbf{r})$ as they appear in the Hamiltonian (1).

In order to reveal the physical significance of the Noether sum rule (30) we proceed by inserting the explicit force form of the functional derivative of the Hamiltonian given by equation (19), which yields

$$\nabla \cdot \boldsymbol{\tau}(\mathbf{r}) + \mathbf{F}_{\text{int}}(\mathbf{r}) - \rho(\mathbf{r})\nabla V_{\text{ext}}(\mathbf{r}) = 0. \tag{31}$$

Here we have introduced the equilibrium averages for the locally resolved kinetic stress: $\boldsymbol{\tau}(\mathbf{r}) = \langle \hat{\boldsymbol{\tau}}(\mathbf{r})\rangle_{\text{eq}}$, for the interparticle force density: $\mathbf{F}_{\text{int}}(\mathbf{r}) = \langle \hat{\mathbf{F}}_{\text{int}}(\mathbf{r})\rangle_{\text{eq}}$, and for the one-body density distribution: $\rho(\mathbf{r}) = \langle \hat{\rho}(\mathbf{r})\rangle_{\text{eq}}$. The force density balance relationship (31) is a known exact equilibrium sum rule, see e.g. [3–5]. Our derivation demonstrates its origin in the invariance of the free energy under the quantum canonical transformation (3) and (4).

As a special case we consider a uniform displacement such that $\boldsymbol{\epsilon}(\mathbf{r}) = \boldsymbol{\epsilon}_0 = \text{const}$. For classical systems the invariance of the free energy under such homogeneous displacement leads to the sum rule of vanishing global external force in thermal equilibrium [30, 31]. This result readily translates to the quantum case as follows.

First we obtain the global identity by starting with the locally resolved force balance relationship (31) and integrating over all positions. Two of the resulting integrals vanish, $\int d\mathbf{r}\nabla\cdot\boldsymbol{\tau}(\mathbf{r}) = 0$ and $\int d\mathbf{r}\mathbf{F}_{\text{int}}(\mathbf{r}) = 0$, where the former identity can be shown via integration by parts and the latter identity is a consequence of the translational invariance of the interparticle interaction potential: $\int d\mathbf{r}\mathbf{F}_{\text{int}}(\mathbf{r}) = \int d\mathbf{r}\langle\hat{\mathbf{F}}_{\text{int}}(\mathbf{r})\rangle_{\text{eq}} = \langle\int d\mathbf{r}\hat{\mathbf{F}}_{\text{int}}(\mathbf{r})\rangle_{\text{eq}} = \langle\hat{\mathbf{F}}^{\text{o}}_{\text{int}}\rangle_{\text{eq}} = 0$. This holds due to the global force operator vanishing identically: $\hat{\mathbf{F}}^{\text{o}}_{\text{int}} = -\sum_i(\nabla_i u(\mathbf{r}^N)) \equiv 0$, which can be seen straightforwardly by displacing all positions arguments in $u(\mathbf{r}^N)$ and observing that this leaves its value invariant. Explicitly the invariance is $u(\mathbf{r}_1,\ldots,\mathbf{r}_N) = u(\mathbf{r}_1+\boldsymbol{\epsilon}_0,\ldots,\mathbf{r}_N+\boldsymbol{\epsilon}_0)$, as the global shift leaves all distance vectors $\mathbf{r}_i-\mathbf{r}_j$ unchanged. The Taylor expansion of the right-hand side is to first order $u(\mathbf{r}_1,\ldots,\mathbf{r}_N)+\boldsymbol{\epsilon}_0\;\cdot\partial u(\mathbf{r}_1+\boldsymbol{\epsilon}_0,\ldots,\mathbf{r}_N+\boldsymbol{\epsilon}_0)/\partial\boldsymbol{\epsilon}_0|_{\boldsymbol{\epsilon}_0=0}$. The linear term can be rewritten as $\boldsymbol{\epsilon}_0\cdot\sum_i\nabla_i u(\mathbf{r}^N)$. As this vanishes for any $\boldsymbol{\epsilon}_0$, the prefactor vanishes identically which provides the anticipated vanishing of the global interparticle force.

This reasoning is analogous to Newton's third law, actio equals reactio, which holds due to the interparticle forces being conservative. The standard derivation does not require (nor identify) the translational invariance. Typically one addresses the special but important case of pairwise interparticle interactions, with given pair potential $\phi(r)$ as a function of interparticle distance r. Then the global interparticle potential energy is $u(\mathbf{r}^N)=\sum_{k,l}'\phi(|\mathbf{r}_k-\mathbf{r}_l|)/2$, where the primed sum indicates that the case $k=l$ has been omitted and the factor 1/2 corrects for double counting. The global interparticle force is then the (negative) sum of all gradients, $\hat{\mathbf{F}}_{\mathrm{int}}^{\mathrm{o}}=-\sum_i\sum_{k,l}'\nabla_i\phi(|\mathbf{r}_k-\mathbf{r}_l|)/2$. Via re-organizing the nested sums one obtains $\hat{\mathbf{F}}_{\mathrm{int}}^{\mathrm{o}}=\sum_{i,k}'[\nabla_i\phi(|\mathbf{r}_i-\mathbf{r}_k|)-\nabla_i\phi(|\mathbf{r}_i-\mathbf{r}_k|)]/2=0$, identical to the above result based on invariance.

The only term that remains of equation (31) after carrying out the position integral is the external force contribution, which reads as:

$$-\int d\mathbf{r}\rho(\mathbf{r})\nabla V_{\mathrm{ext}}(\mathbf{r})=0. \tag{32}$$

Equation (32) expresses the vanishing of the average global external force in thermal equilibrium.

Briefly, in our second route to equation (32) we start from the free energy (20) and directly perform the transformation for the special case of a homogeneous displacement $\boldsymbol{\epsilon}_0$. In this case the momenta are unchanged, as the gradient of the (constant) displacement field vanishes identically. Hence kinetic energy is trivially invariant. As laid out above, the coordinate change does not affect the interparticle potential energy, as the difference vectors are unaffected. Hence the only change in the Hamiltonian occurs in the external contribution and we obtain, following the same argumentation as in the case of position-dependent shifting, the result

$$-\left\langle\sum_i\nabla_i V_{\mathrm{ext}}(\mathbf{r}_i)\right\rangle_{\mathrm{eq}}=0, \tag{33}$$

which is analogous to the previous form (32) upon prepending $1=\int d\mathbf{r}\delta(\mathbf{r}-\mathbf{r}_i)$ to equation (33), moving the delta function into the thermal average, and identifying the density profile $\rho(\mathbf{r})=\langle\sum_i\delta(\mathbf{r}-\mathbf{r}_i)\rangle_{\mathrm{eq}}$.

For completeness and as a final step, we make explicit that the quantum canonical transformation corresponds indeed to a unitary transformation on Hilbert space, as is relevant for the invariance (29) of the free energy under the transformation. For the present transformation, to linear order in $\boldsymbol{\epsilon}(\mathbf{r})$, the transformed Hamiltonian is obtained via functional Taylor expansion in the following form:

$$H[\boldsymbol{\epsilon}]=H+\int d\mathbf{r}\frac{\delta H[\boldsymbol{\epsilon}]}{\delta\boldsymbol{\epsilon}(\mathbf{r})}\bigg|_{\boldsymbol{\epsilon}=0}\cdot\boldsymbol{\epsilon}(\mathbf{r}), \tag{34}$$

and we recall the explicit one-body force density form (19) of the functional derivative of the Hamiltonian. We treat the second term in equation (34) as a perturbation to the original Hamiltonian H. (We recall that the thermal average over the functional derivative $\delta H[\boldsymbol{\epsilon}]/\delta\boldsymbol{\epsilon}(\mathbf{r})$

directly leads to the static force density balance relationship (31).) Then the transformed (perturbed) energy eigenstates $|\tilde{n}\rangle$ are given by

$$|\tilde{n}\rangle = \sum_k U_{nk}|k\rangle, \tag{35}$$

$$U_{nk} = \delta_{nk} + \frac{1-\delta_{nk}}{E_k - E_n}\int d\mathbf{r}\langle n|\frac{\delta H[\boldsymbol{\epsilon}]}{\delta\boldsymbol{\epsilon}(\mathbf{r})}\bigg|_{\boldsymbol{\epsilon}=0}|k\rangle\cdot\boldsymbol{\epsilon}(\mathbf{r}). \tag{36}$$

The form (36) of the matrix that performs the change of basis follows from applying time-independent first order perturbation theory, as is appropriate to capture the effects to linear order in $\boldsymbol{\epsilon}(\mathbf{r})$ that we consider. (We imply that the prefactor of the integral in equation (36) vanishes for $k = n$.) The matrix elements of the Hermitian conjugate to equation (36) can be obtained via exchanging indices n and k as

$$U^\dagger_{nk} = \delta_{kn} + \frac{1-\delta_{kn}}{E_n - E_k}\int d\mathbf{r}\langle k|\frac{\delta H[\boldsymbol{\epsilon}]}{\delta\boldsymbol{\epsilon}(\mathbf{r})}\bigg|^\dagger_{\boldsymbol{\epsilon}=0}|n\rangle\cdot\boldsymbol{\epsilon}(\mathbf{r}) \tag{37}$$

$$= \delta_{nk} - \frac{1-\delta_{nk}}{E_k - E_n}\int d\mathbf{r}\langle n|\frac{\delta H[\boldsymbol{\epsilon}]}{\delta\boldsymbol{\epsilon}(\mathbf{r})}\bigg|_{\boldsymbol{\epsilon}=0}|k\rangle\cdot\boldsymbol{\epsilon}(\mathbf{r}), \tag{38}$$

where to obtain the matrix elements (38) we have exploited that the functional derivative of the Hamiltonian is self-adjoint. We observe that the sole difference between equations (36) and (38) is the minus sign. Hence we can see explicitly that unitarity holds, $\sum_k U^\dagger_{nk}U_{km} = \delta_{nm}$ to linear order in $\boldsymbol{\epsilon}(\mathbf{r})$, as was expected on general grounds [38].

3. Outlook and conclusions

In conclusion we have investigated the consequences of a specific local displacement operation for the free energy of a quantum mechanical many-body system. The transformation consists of position-dependent shifting, as parameterized by a real-valued displacement (or 'shift') field, and a corresponding transformation of the quantum mechanical momentum operator of each particle. The entirety of the transformation can be viewed as the self-adjoint version of the corresponding local shifting transformation of the classical phase space variables [33]. We have explicitly shown that the new position and momentum operators are self-adjoint and that they satisfy the fundamental commutator relations and hence form a valid and complete set of degrees of freedom of the considered system. The transformation can be viewed as a basis change of the underlying Hilbert space of the quantal system and we have spelled out explicitly the corresponding unitary transformation between the original and the new basis.

The resulting invariance of the free energy under changes in the displacement field then leads, following Noether's theorem for invariant variations, to an exact local identity ('sum rule') which we have shown to be the thermal equilibrium force balance. The present derivation of this known and fundamental result from Noether's theorem sheds new light on the very nature of the identity. Existing derivations are based e.g. on the second time derivative of the one-body density profile [3] or, equivalently, on the first time derivative of the one-body current distribution [5] and then taking the equilibrium limit.

Our results hold for the ground state of the quantum system, as it is obtained in the limit $T \to 0$ of the free energy of the thermal system. We have used the canonical ensemble throughout as it captures the essence of the required thermal physics. We expect the reasoning to carry over straightforwardly to the grand ensemble with fluctuating particle number, as the classical canonical [31] and grand canonical cases lead to analogous results upon identifying the respective statistical averages.

Future work could be addressed at investigating how functional differentiation can be used to obtain quantum sum rules for higher-body correlation functions, as previously shown for classical systems [30]. It would be interesting to address the effects beyond linear order in the displacement field; classically the variance of the global external force was shown to be constrained by the external potential energy curvature [32]. Last but not least it would be worthwhile to find possible relationships of our displacement field and the strain field that is central to elasticity theory, see e.g. [41, 42] for recent work again in classical systems.

Identifying connections with Tokatly's work [6–9] would be highly interesting. His approach is more general than what we cover here, as it allows for the treatment of the dynamical and nonlinear cases. Clearly, attempting to generalize our approach to the dynamics of statistical quantum systems is an exciting and demanding research task. (We re-iterate that we have here only considered systems in static thermal equilibrium.)

The Noether argument itself is not restricted to linear transformations. The second order was shown, for the case of a global invariance, to relate the variance of fluctuations with the mean potential energy curvature [32]. Carrying through this concept for the quantum case is a further very worthwhile research task.

Data availability statement

No new data were created or analysed in this study.

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Appendix A. Momentum and position commutators

A.1. Momentum-momentum commutator

To derive the commutator of the new momenta, $[\tilde{\mathbf{p}}_i, \tilde{\mathbf{p}}_j]$, we insert the definition of the transformation (5) and consider terms up to linear order in the displacement gradient. In index notation this reads as follows:

$$\begin{aligned}2[\tilde{p}_i^\alpha, \tilde{p}_j^\gamma] = 2[p_i^\alpha, p_j^\gamma] - [p_i^\alpha, (\nabla_j^\gamma \epsilon_j^\delta) p_j^\delta] - [p_i^\alpha, p_j^\delta (\nabla_j^\gamma \epsilon_j^\delta)] \\ - [(\nabla_i^\alpha \epsilon_i^\delta) p_i^\delta, p_j^\gamma] - [p_i^\delta (\nabla_i^\alpha \epsilon_i^\delta), p_j^\gamma]. \qquad \text{(A1)}\end{aligned}$$

The correlator of the original momenta, as it appears in the first term on the right-hand side, vanishes trivially, $[p_i^\alpha, p_j^\gamma] = 0$. This identity also allows to take the operators p_i^δ and p_j^δ out of the commutator in the remaining terms on the right-hand side of equation (A1). We obtain

$$2[\tilde{p}_i^\alpha, \tilde{p}_j^\gamma] = -[p_i^\alpha, (\nabla_j^\gamma \epsilon_j^\delta)]p_j^\delta - p_j^\delta [p_i^\alpha, (\nabla_j^\gamma \epsilon_j^\delta)] + [p_j^\gamma, (\nabla_i^\alpha \epsilon_i^\delta)]p_i^\delta \\ + p_i^\delta [p_j^\gamma, (\nabla_i^\alpha \epsilon_i^\delta)], \tag{A2}$$

where we have exploited the anti-symmetry of the commutator, $[A, B] = -[B, A]$, for rewriting the third and the fourth term on the right-hand side of equation (A2).

Writing out explicitly the commutator in the first contribution in equation (A2) yields $[p_i^\alpha, (\nabla_j^\gamma \epsilon_j^\delta)] = p_i^\alpha (\nabla_j^\gamma \epsilon_j^\delta) - (\nabla_j^\gamma \epsilon_j^\delta) p_i^\alpha$. Hence the momentum operator only acts on the gradient of the displacement field, $(p_i^\alpha \nabla_j^\gamma \epsilon_j^\delta) = -\mathrm{i}\hbar (\nabla_i^\alpha \nabla_j^\gamma \epsilon_j^\delta)$, where as before the parentheses indicate that the derivative(s) only act on the displacement field and we have expressed the momentum operator in position representation. Analog manipulation of all remaining commutators in equation (A2) then yields

$$\frac{2\mathrm{i}}{\hbar}[\tilde{p}_i^\alpha, \tilde{p}_j^\gamma] = -(\nabla_i^\alpha \nabla_j^\gamma \epsilon_j^\delta) p_j^\delta - p_j^\delta (\nabla_i^\alpha \nabla_j^\gamma \epsilon_j^\delta) + (\nabla_j^\gamma \nabla_i^\alpha \epsilon_i^\delta) p_i^\delta \\ + p_i^\delta (\nabla_j^\gamma \nabla_i^\alpha \epsilon_i^\delta). \tag{A3}$$

For $i \neq j$ it is now straightforward to see that each term on the right-hand side of equation (A3) vanishes individually: As the displacement field $\boldsymbol{\epsilon}_i$ only depends on positions $\mathbf{r}_i$, derivatives with respect to $\mathbf{r}_j$ vanish for $i \neq j$. For $i = j$ the first and the third term, as well as the second and the fourth term, on the right-hand side of equation (A3) cancel each other pairwise, as the derivatives ∇_i^α and ∇_j^γ commute. Collecting the cases $i = j$ and $i \neq j$ the commutator of the new momentum operators hence vanishes,

$$[\tilde{p}_i^\alpha, \tilde{p}_j^\gamma] = 0, \tag{A4}$$

which ascertains that the position-dependent momentum transformation does not generate any spurious terms.

A.2. Momentum-position commutator for finite transformations

The transformations (3) and (4) are canonical not only in linear order of $\nabla \boldsymbol{\epsilon}(\mathbf{r})$ and $\boldsymbol{\epsilon}(\mathbf{r})$, but also for finite values thereof. To demonstrate this property we show that the canonical commutation relations are satisfied given the finite transformations (3) and (4). The position-position commutator $[\tilde{\mathbf{r}}_i, \tilde{\mathbf{r}}_j]$ is unchanged compared to the derivation in linear order. This is due to the transformed position operator $\tilde{\mathbf{r}}_i$ (3) containing no higher than linear terms in $\boldsymbol{\epsilon}_i$.

In contrast, the transformed momenta $\tilde{\mathbf{p}}_i$ do contain higher contributions. We express the transformed momentum $\tilde{\mathbf{p}}_i$ given by equation (4) as an infinite Taylor series in matrix powers of $(\nabla_i \boldsymbol{\epsilon}_i)$ as

$$\tilde{\mathbf{p}}_i = \mathbf{p}_i + \frac{1}{2} \sum_{n=1}^{\infty} \left((-\nabla_i \boldsymbol{\epsilon}_i)^n \cdot \mathbf{p}_i + \mathbf{p}_i \cdot (-\nabla_i \boldsymbol{\epsilon}_i)^{\mathsf{T}n} \right). \tag{A5}$$

Note that here the order of transposing and raising the power can be interchanged, i.e. $(\nabla_i \boldsymbol{\epsilon}_i)^{\mathsf{T}n} = (\nabla_i \boldsymbol{\epsilon}_i)^{n\mathsf{T}}$.

We consider the commutator of position and momentum $[\tilde{\mathbf{r}}_i, \tilde{\mathbf{p}}_j]$. Only the case $i = j$ needs to be considered, since otherwise the commutator vanishes trivially. Insertion of the transformations (3) and (A5) and exploiting the linearity of the commutator gives

$$2[\tilde{\mathbf{r}}_i,\tilde{\mathbf{p}}_i] = 2[\mathbf{r}_i,\mathbf{p}_i] + \sum_{n=1}^{\infty}\Big([\mathbf{r}_i,(-\nabla_i\boldsymbol{\epsilon}_i)^n\cdot\mathbf{p}_i] + [\mathbf{r}_i,\mathbf{p}_i\cdot(-\nabla_i\boldsymbol{\epsilon}_i)^{\mathsf{T}n}]\Big)$$
$$+\sum_{n=0}^{\infty}\Big([\boldsymbol{\epsilon}_i,(-\nabla_i\boldsymbol{\epsilon}_i)^n\cdot\mathbf{p}_i] + [\boldsymbol{\epsilon}_i,\mathbf{p}_i\cdot(-\nabla_i\boldsymbol{\epsilon}_i)^{\mathsf{T}n}]\Big), \tag{A6}$$

where the contribution $2[\boldsymbol{\epsilon}_i,\mathbf{p}_i]$ is included as the $n=0$ term of the second series in equation (A6).

We rewrite the first term in the first series of equation (A6) using index notation:

$$[r_i^\alpha,(-\nabla_i\boldsymbol{\epsilon}_i)^n_{\beta\gamma}p_i^\gamma] = (-\nabla_i\boldsymbol{\epsilon}_i)^n_{\beta\gamma}[r_i^\alpha,p_i^\gamma] \tag{A7}$$

$$= (-\nabla_i\boldsymbol{\epsilon}_i)^n_{\beta\gamma}\mathrm{i}\hbar\delta_{\alpha\gamma} \tag{A8}$$

$$= \mathrm{i}\hbar(-\nabla_i\boldsymbol{\epsilon}_i)^n_{\beta\alpha}. \tag{A9}$$

Here for readability the indices indicating the Cartesian components of the matrix $(-\nabla_i\boldsymbol{\epsilon}_i)^n$ are written as subscripts. The factor $(-\nabla_i\boldsymbol{\epsilon}_i)^n_{\beta\gamma}$ is local and hence commutes with position, $[r_i^\alpha,(-\nabla_i\boldsymbol{\epsilon}_i)^n_{\beta\gamma}]=0$. Therefore this term can be taken outside of the commutator in equation (A7). We have inserted the usual position-momentum commutator in equation (A8) and evaluated the Kronecker delta in equation (A9).

Similarly we express the first term of the second series in equation (A6) as

$$[\epsilon_i^\alpha,(-\nabla_i\boldsymbol{\epsilon}_i)^n_{\beta\gamma}p_i^\gamma] = (-\nabla_i\boldsymbol{\epsilon}_i)^n_{\beta\gamma}[\epsilon_i^\alpha,p_i^\gamma] \tag{A10}$$

$$= (-\nabla_i\boldsymbol{\epsilon}_i)^n_{\beta\gamma}\mathrm{i}\hbar(\nabla_i\boldsymbol{\epsilon}_i)_{\gamma\alpha} \tag{A11}$$

$$= -\mathrm{i}\hbar(-\nabla_i\boldsymbol{\epsilon}_i)^{n+1}_{\beta\alpha}, \tag{A12}$$

where again the fact that $\boldsymbol{\epsilon}_i$ and $\nabla_i\boldsymbol{\epsilon}_i$ commute allows to take $(-\nabla_i\boldsymbol{\epsilon}_i)^n_{\beta\gamma}$ out of the commutator in equation (A10). In equation (A11) we have inserted the commutator $[\boldsymbol{\epsilon}_i,\mathbf{p}_i]=\mathrm{i}\hbar(\nabla_i\boldsymbol{\epsilon}_i)$.

Recall that both expressions (A9) and (A12) are part of a sum in equation (A6). It becomes apparent that the $(n+1)$th term of the first sum cancels with the nth contribution of the second sum. (This amounts to renaming the summation index in the first sum of equation (A6) as $n\to n+1$. Then the first part of both occurring sums become identical up to a minus sign.) The only remaining terms are both second contributions to the sums of equation (A6). These corresponding transposed terms also cancel each other following an analogous argumentation. Thus no contribution to the sums in equation (A6) remains and we determine the canonical commutator as

$$[\tilde{\mathbf{r}}_i,\tilde{\mathbf{p}}_j] = [\mathbf{r}_i,\mathbf{p}_j] = \mathrm{i}\hbar\delta_{ij}\mathbb{1}. \tag{A13}$$

The above considerations generalize equations (6)–(8) from linear order to the general case.

Showing explicitly that the momentum self commutator vanishes, $[\tilde{\mathbf{p}}_i,\tilde{\mathbf{p}}_j]=0$ can be done similarly to the treatment of the position-momentum commutator by explicitly using the transformation (A5). The corresponding calculation is straightforward though tedious, and we omit it here.

Appendix B. Local shift derivative of kinetic energy

B.1. One dimension

As a preparation for the general three-dimensional case shown below, we first consider the simpler case of systems in one spatial dimension, with position x_i and momentum $p_i = -\mathrm{i}\hbar\partial/\partial x_i$ of particle $i = 1, \ldots, N$. We consider a one-dimensional displacement $\epsilon(x)$ of the position coordinate x, such that $x_i \to x_i + \epsilon(x_i)$, in analog to the three-dimensional case of equation (3). The one-dimensional momentum transformation [corresponding to equation (5)] is $p_i \to p_i - \{\epsilon'(x_i)p_i + p_i\epsilon'(x_i)\}/2 \equiv \tilde{p}_i$, where the prime denotes the derivative by the argument.

We wish to derive the one-dimensional analogue of equation (15), which reads as

$$\frac{\delta}{\delta\epsilon(x)}\sum_i \frac{\tilde{p}_i^2}{2m} = \frac{\partial}{\partial x}\sum_i \frac{p_i\delta_i p_i}{m} - \frac{\hbar^2}{4m}\frac{\partial^3}{\partial x^3}\sum_i \delta_i. \tag{B1}$$

Here the density operator of particle i is defined as $\delta_i = \delta(x_i - x)$ and the identity holds at $\epsilon(x) = 0$. The functional derivative on the left-hand side of equation (B1) can be moved inside of the sum over all particles and we hence need to consider

$$\frac{\delta\tilde{p}_i^2}{\delta\epsilon(x)} = p_i\frac{\delta\tilde{p}_i}{\delta\epsilon(x)} + \frac{\delta\tilde{p}_i}{\delta\epsilon(x)}p_i. \tag{B2}$$

This equality holds to first order in $\epsilon(x)$, as we have replaced $\tilde{p}_i$ by p_i on the right-hand side.

The first term on the right-hand side of equation (B2) becomes

$$p_i\frac{\delta\tilde{p}_i}{\delta\epsilon(x)} = \partial_x(p_i\delta_i p_i + p_i p_i\delta_i)/2 \tag{B3}$$

$$= \partial_x\{p_i\delta_i p_i + p_i(p_i\delta_i) + p_i\delta_i p_i\}/2, \tag{B4}$$

where $\partial_x = \partial/\partial x$ is a shortcut notation. We have used $\delta p_i/\delta\epsilon(x) = \partial_x(\delta_i p_i + p_i\delta_i)/2$, i.e. the one-dimensional analogue of equation (12), in the first equality and the product rule of differentiation for p_i in the second equality. The remaining second term in equation (B2) is

$$\frac{\delta\tilde{p}_i}{\delta\epsilon(x)}p_i = \partial_x(\delta_i p_i p_i + p_i\delta_i p_i)/2 \tag{B5}$$

$$= \partial_x\{p_i\delta_i p_i - (p_i\delta_i)p_i + p_i\delta_i p_i\}/2. \tag{B6}$$

The minus sign in equation (B6) allows to simplify the sum of the respective second terms:

$$p_i(p_i\delta_i) - (p_i\delta_i)p_i = (p_i p_i\delta_i) \tag{B7}$$

$$= -\hbar^2\left(\frac{\partial^2}{\partial x_i^2}\delta_i\right) \tag{B8}$$

$$= -\hbar^2\,\partial_x^2\,\delta_i, \tag{B9}$$

where in the second equality we have expressed the effect of the momentum operator on the delta function by the (negative) position gradient, i.e.

$$(p_i\delta_i) = -\mathrm{i}\hbar\frac{\partial\delta(x - x_i)}{\partial x_i} = \mathrm{i}\hbar\frac{\partial\delta(x - x_i)}{\partial x}. \tag{B10}$$

Collecting all terms yields

$$\frac{\delta\tilde{p}_i^2}{\delta\epsilon(x)} = \frac{\partial}{\partial x}2p_i\delta_i p_i - \frac{\hbar^2}{2}\frac{\partial^3}{\partial x^3}\delta_i, \tag{B11}$$

and summation over i and division by $2\,m$ then yields equation (B1), as desired.

The three-dimensional case covered below is closely related, with the additional complexity of the matrix and tensor indices interfering very little with the operator structure.

B.2. Three dimensions

We wish to derive equation (13), which we reproduce for convenience:

$$\frac{\delta}{\delta\boldsymbol{\epsilon}(\mathbf{r})}\sum_i \frac{\tilde{\mathbf{p}}_i^2}{2m}\bigg|_{\boldsymbol{\epsilon}=0} = \nabla\cdot\sum_i \frac{\mathbf{p}_i\delta_i\mathbf{p}_i + \mathbf{p}_i\delta_i\mathbf{p}_i^{\mathsf{T}}}{2m} - \frac{\hbar^2}{4m}\nabla\nabla^2\sum_i \delta(\mathbf{r}-\mathbf{r}_i). \tag{B12}$$

We use Einstein summation convention over pairs of Greek indices and after taking the functional derivative set $\boldsymbol{\epsilon}(\mathbf{r}) = 0$ throughout. We consider the γth component of the left-hand side of equation (B12) for particle i only, which yields

$$\frac{\delta}{\delta\epsilon^\gamma}\tilde{p}_i^\alpha\tilde{p}_i^\alpha = p_i^\alpha\frac{\delta\tilde{p}_i^\alpha}{\delta\epsilon^\gamma} + \frac{\delta\tilde{p}_i^\alpha}{\delta\epsilon^\gamma}p_i^\alpha, \tag{B13}$$

where the sum over α (repeated index) generates the square of momentum, as it occurs in the kinetic energy. The first term on the right-hand side, using the explicit form of the transformed momentum (5), becomes

$$p_i^\alpha\frac{\delta\tilde{p}_i^\alpha}{\delta\epsilon^\gamma} = \nabla^\alpha(p_i^\alpha\delta_i p_i^\gamma + p_i^\alpha p_i^\gamma\delta_i)/2 \tag{B14}$$

$$= \nabla^\alpha\{p_i^\alpha\delta_i p_i^\gamma + p_i^\alpha(p_i^\gamma\delta_i) + p_i^\alpha\delta_i p_i^\gamma\}/2, \tag{B15}$$

where we have used equation (12) in the first equality and the product rule of differentiation for the application of p_i^γ in the second equality. The remaining second term in equation (B13) is

$$\frac{\delta\tilde{p}_i^\alpha}{\delta\epsilon^\gamma}p_i^\alpha = \nabla^\alpha(\delta_i p_i^\gamma p_i^\alpha + p_i^\gamma\delta_i p_i^\alpha)/2 \tag{B16}$$

$$= \nabla^\alpha\{p_i^\gamma\delta_i p_i^\alpha - (p_i^\gamma\delta_i)p_i^\alpha + p_i^\gamma\delta_i p_i^\alpha\}/2. \tag{B17}$$

The appearance of the minus sign in equation (B17) allows to carry out the following cancellation of the respective 'middle' terms:

$$p_i^\alpha(p_i^\gamma\delta_i) - (p_i^\gamma\delta_i)p_i^\alpha = (p_i^\alpha p_i^\gamma\delta_i) \tag{B18}$$

$$= -\hbar^2(\nabla_i^\alpha\nabla_i^\gamma\delta_i) \tag{B19}$$

$$= -\hbar^2\,\nabla^\alpha\nabla^\gamma\delta_i, \tag{B20}$$

where in the second step we have rewritten the effect of the momentum operator on the delta function by the (negative) position gradient, i.e.

$$(p_i^\gamma\delta_i) = -\mathrm{i}\hbar(\nabla_i^\gamma\delta_i) = \mathrm{i}\hbar(\nabla^\gamma\delta_i). \tag{B21}$$

Collecting all terms we obtain the overall result for the shift derivative of kinetic energy,

$$\frac{\delta}{\delta\epsilon^\gamma}\sum_i\frac{\tilde{p}_i^\alpha\tilde{p}_i^\alpha}{2m}\bigg|_{\epsilon=0} = \nabla^\alpha\Big\{\sum_i\frac{p_i^\alpha\delta_i p_i^\gamma + p_i^\gamma\delta_i p_i^\alpha}{2m} - \frac{\hbar^2}{4m}\nabla^\gamma\nabla^\alpha\sum_i\delta_i\Big\} \tag{B22}$$

$$= -\nabla^\alpha\hat{\tau}^{\alpha\gamma}. \tag{B23}$$

As desired, equation (B22) is the γth Cartesian component of equation (13) [reproduced above as equation (B12)] and equation (B23) is analogous to equation (15), with tensor contractions and matrix transpositions expressed in index notation, and the definition of the kinetic stress operator as given by equation (14).

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