

Revisiting quantum notions of stress

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An important aspect of multi-scale modelling of materials is to link continuum concepts, such as fields, to the underlying discrete microscopic behaviour in a seamless manner. With the growing importance of atomistic calculations to understand material behaviour, reconciling continuum and discrete concepts is necessary to interpret molecular and quantum-mechanical simulations. In this work, we provide a quantum-mechanical framework to a distinctly continuum quantity: mechanical stress. While the concept of the *global* macroscopic stress tensor in quantum mechanics has been well established, there still exist open issues when it comes to a spatially varying local quantum stress tensor. We attempt to shed some light on this topic by establishing a general quantum-mechanical operator-based approach to continuity equations and from those, introduce a local quantum-mechanical stress tensor. Further, we elucidate the analogies that exist between the (classical) molecular-dynamics-based stress definition and the quantum stress. Our derivations appear to suggest that the local quantum-mechanical stress may not be an observable in quantum mechanics and therefore traces the non-uniqueness of the atomistic stress tensor to the gauge arbitrariness of the quantum-mechanical state function. Lastly, the virial stress theorem (of empirical molecular dynamics) is re-derived in a transparent manner that elucidates the analogy between quantum-mechanical global stresses.

Keywords: quantum stress; atomistic stress; virial stress; multi-scale modelling

1. Introduction and background

Several processes occur in nature wherein physical phenomena occur across multiple length and temporal scales. An oft-used example is that of protein folding: the time scale for the vibration of the covalent bonds is of the order of a few femtoseconds (10^{-15} s), while the folding of the proteins takes place of the order of a few seconds. The electromechanical behaviour of solids is another typical example that exhibits such a multi-scale characteristic. At the fundamental level, the properties of the solid can be attributed to the electronic structure, whereas atomic interactions and crystal structures can be described at the atomistic scale by using an atomic/molecular picture. Electrical and deformation behaviours in macroscopic samples, in contrast, are routinely described using continuum theories, wherein the notion of the underlying discrete

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atomic structure of matter is discounted in favour of the idea of a smeared-out continuum. Continuum theories introduce kinematic measures, such as displacement fields, and electrical measures, such as polarization fields, as opposed to discrete atomistic quantities, such as atomic coordinates and induced dipole moments. This process of zooming out from an electronic to an atomistic to a continuum picture is accompanied by an enormous decrease in the degrees of freedom, which serves to considerably simplify analysis. For several applications of practical interest in structural and electrical engineering, the accuracy and predictive power of continuum theories are known to be more than sufficient. Any minute improvement in the accuracy gained by applying atomistic methods in such situations is rendered superfluous owing to the enormous increase in the computational expenses that atomistic methods require.

The tremendous decrease in the degrees of freedom that continuum theories offer is often a result of certain simplifying assumptions based on which such continuum theories are constructed. When the discrete nature of matter becomes apparent, say in nanoscale phenomena, there is an expectation that classical continuum theories may fail to apply in some contexts and may need to be ‘informed’ of the insights obtained through atomistic considerations. Indeed, in recent years, novel size effects are being routinely observed in a variety of contexts such as plasticity, electromechanical response of nanosized dielectric thin films, quantum dots and nanocomposites among others.

Certain scenarios may present themselves wherein a substantial part of the system essentially behaves like a continuum, with the remaining part of the system exhibiting fully fledged atomistic behaviour that cannot be captured by a full continuum theory. Multi-scale modelling techniques aim to identify the multiple natural length and time scales in a phenomenon and to transfer information across them in a seamless fashion (see the following representative articles: Li *et al.* 1998; Miller & Tadmor 2002, 2007; Curtin & Miller 2003; Park & Liu 2004; Liu *et al.* 2006; Gavini *et al.* 2007; Silva *et al.* 2007; Kulkarni *et al.* 2008; and references therein). This often requires reconciling the atomistic notions that represent the true mechanistic underpinnings behind a process, with coarse-grained (including continuum) ideas that serve to capture the essential physics in a phenomenological manner. Even with the sustained interest in multi-scale modelling techniques over past years, a ‘seamless’ integration has proved to be challenging, especially when it comes to bridging temporal scales (see the following review article: Jun *et al.* 2009 and references therein).

In this paper, our focus is the concept of ‘mechanical stress’. Numerous works have appeared that have attempted the reconciliation of classical molecular-dynamics stress and the continuum definition of stress. The reader is referred to the following representative (non-exhaustive) list of papers and the references therein: Murdoch & Bedeaux (1994); Cormier *et al.* (2001); Murdoch (2003*a,b*, 2007); Zhou (2003); Zimmerman *et al.* (2004); Chen (2006); Silling & Lehoucq (2007); Webb *et al.* (2008), among others. In particular, we highlight the classic paper by Noll (2009) (originally published in 1955 in German), which was recently updated (and translated by Lehoucq and Lillienfeld-Toal). This paper (in addition to that of Irving & Kirkwood (1950)) provided interesting methodologies that were later used by Murdoch (2007) to perform coarse graining of discrete quantities and derived a rigorous expression for atomistic stress. In this paper,

we go a step further and attempt to establish the definition of *quantum* stress and elucidate its relation to both the classical molecular-dynamics-based stress and its continuum counterpart.

Investigations into the quantum-mechanical definition of stress were well preceded by early fundamental work on the concept of quantum-mechanical force (Ehrenfest 1927; Pauli 1933; Hellmann 1937; Feynman 1939) and pressure (Born *et al.* 1926; Finkelstein 1928; Hylleraas 1929; Fock 1930; Slater 1933, 1963, 1967). Ehrenfest's theorem (Ehrenfest 1927), which states that the net force on a particle is given by the expectation value of the negative of the gradient of the potential, is such an example. We will discuss Ehrenfest's theorem in more detail shortly. Pauli (1933), Hellmann (1937) and Feynman (1939) modified Ehrenfest's theorem to a form appropriate for application to forces between molecules. The consequences of the so-called Hellmann–Feynman theorem are significant. Previously, forces within molecules and associated problems involving the estimation of lattice constants, calculations of phase transitions, elastic properties, phonon dispersion, stiffness of valence bonds and others were addressed, invoking the energy formalism in an indirect manner. These usually involve calculations of energy for several neighbouring configurations of the molecule; the force is then obtained by determining the slope of the plot of energy versus position. The Hellmann–Feynman theorem offers a direct way to estimate the force for a given configuration, given that only the particular configuration of interest is known. The quantum-mechanical virial theorem, which states that the total pressure in a many-body quantum-mechanical system is defined by the kinetic energy and the virial of the potential (much like its classical counterpart), also attracted attention from authors including Born *et al.* (1926), Finkelstein (1928), Hylleraas (1929), Fock (1930), Slater (1933, 1963, 1967) and Ross (1969). Although several early works of varying levels of sophistication have considered the quantum-mechanical stress tensor (Schrödinger 1927; Pauli 1933; Feynman 1939; Martin & Schwinger 1959; Kugler 1967; McLellan 1974, 1984; Folland 1986), we mainly use the seminal work by Nielsen & Martin (1983, 1985) as a starting point.

The outline of our paper is as follows. In §2, we introduce the concept of a global macroscopic stress in three different settings: continuum mechanics, classical (empirical) molecular dynamics and finally quantum mechanics. An attempt will be made to relate the well-known kinetic and potential contributions to the stress in continuum mechanics to analogous quantities in discrete settings such as molecular dynamics and quantum mechanics. In §3, we delve into the idea of stress as a locally varying field-theoretic quantity. While this idea is quite intuitive in continuum mechanics, there is still a lack of consensus about how best to represent a locally varying stress in a discrete setting. In this respect, we introduce Murdoch's (2007) formulation for a locally varying stress field from discrete atomistic quantities using the approach of weighting functions. In the same spirit, we also introduce a novel approach to a local spatially varying stress field in quantum mechanics by deriving the continuity equations for an arbitrary Hermitian operator. The concept of the virial pressure is closely tied with the ideas of stress, which are introduced in §§2 and 3. In §4, we outline an alternate derivation of the well-known Clausius virial theorem, which brings out some interesting physical insights and makes the comparison with quantum global stress quite transparent. We conclude in §5 with a summary of the physical

insights gained out of the previous sections, along with a brief discussion of our perspective on some open issues that remain in the area of quantum-mechanical description of stress.

2. Macroscopic stress

(a) Macroscopic stress in continuum mechanics

We first review the expression for macroscopic stress in continuum mechanics. Consider a continuum body occupying region Ω , the equation of motion can be written as

$$\operatorname{div} \boldsymbol{\sigma} + \rho \mathbf{b} = \rho \ddot{\mathbf{r}}, \quad (2.1)$$

where $\boldsymbol{\sigma}$ is the Cauchy stress, ρ is the mass density, \mathbf{b} is the body-force density and \mathbf{r} is taken to be the displacement with respect to a fixed point (assumed to be at the origin). The mean Cauchy stress $\bar{\boldsymbol{\sigma}}$ is given by

$$V_{\Omega} \bar{\boldsymbol{\sigma}} = \int_{\Omega} \boldsymbol{\sigma} dV = \int_{\Omega} \boldsymbol{\sigma} \operatorname{grad} \mathbf{r} dV. \quad (2.2)$$

By employing the divergence theorem and defining $\mathbf{t} = \boldsymbol{\sigma} \cdot \mathbf{n}$, it can be shown that

$$V_{\Omega} \bar{\boldsymbol{\sigma}} = \int_{\Omega} \rho \dot{\mathbf{r}} \otimes \dot{\mathbf{r}} dV - \frac{d}{dt} \int_{\Omega} \rho (\dot{\mathbf{r}} \otimes \dot{\mathbf{r}}) dV + \int_{\Omega} \rho \mathbf{b} \otimes \mathbf{r} dV + \int_{\partial\Omega} \mathbf{t} \otimes \mathbf{r} dA. \quad (2.3)$$

The trace of the first term on the r.h.s. can be seen to be twice the kinetic energy K_{Ω} for the body. Taking an average over ‘a very long time’¹ and assuming that the quantity $\int_{\Omega} \rho (\dot{\mathbf{r}} \otimes \dot{\mathbf{r}}) dV$ remains bounded in time, the space- and time-averaged macroscopic stress becomes

$$V_{\Omega} \langle \bar{\boldsymbol{\sigma}} \rangle = \left\langle \int_{\Omega} \rho \dot{\mathbf{r}} \otimes \dot{\mathbf{r}} dV + \int_{\Omega} \rho \mathbf{b} \otimes \mathbf{r} dV + \int_{\partial\Omega} \mathbf{t} \otimes \mathbf{r} dA \right\rangle, \quad (2.4)$$

where the symbol $\langle \rangle$ denotes the temporal average.

We note that the preceding derivation holds when the object is not in equilibrium. In equilibrium, we have

$$V_{\Omega} \langle \bar{\boldsymbol{\sigma}} \rangle = \left\langle \int_{\Omega} \rho \mathbf{b} \otimes \mathbf{r} dV + \int_{\partial\Omega} \mathbf{t} \otimes \mathbf{r} dA \right\rangle. \quad (2.5)$$

(b) Macroscopic stress in molecular dynamics

This section is partly based on Zimmerman *et al.* (2004) and Murdoch (2007). The aim here is to establish a link between the continuum global virial stress of a macroscopic body (discussed previously in this section) and its molecular content.

¹Here, we avoid the rigour needed to justify this statement. The reader may wish to consult lecture notes by Murdoch (2003a,b).

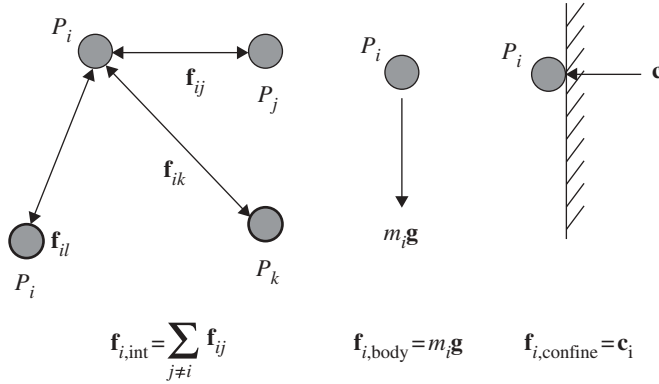


Figure 1. Different types of forces acting on a particle.

Accordingly, let us consider a set of interacting point masses P_i ($i = 1, 2, 3, \dots, N$). The motion of P_i in an inertial frame is governed by

$$\dot{\mathbf{p}}_i = \frac{d}{dt}(m_i \mathbf{v}_i) = \mathbf{f}_i, \quad (2.6)$$

where \mathbf{f}_i are the forces on the particles, while m_i and \mathbf{v}_i signify masses and velocities, respectively. A quantity \mathbf{G} is defined such that

$$\mathbf{G} := \sum_i \mathbf{p}_i \otimes \mathbf{r}_i, \quad (2.7)$$

where \mathbf{r}_i denotes the displacement of the point particles from a fixed point. Taking the time derivative of \mathbf{G} ,

$$\frac{d\mathbf{G}}{dt} = \sum_i m_i \mathbf{v}_i \otimes \mathbf{v}_i + \sum_i \mathbf{f}_i \otimes \mathbf{r}_i. \quad (2.8)$$

Taking a sufficiently long time average and assuming that the quantity \mathbf{G} remains bounded in time, we have

$$\left\langle \sum_i m_i \mathbf{v}_i \otimes \mathbf{v}_i \right\rangle + \left\langle \sum_i \mathbf{f}_i \otimes \mathbf{r}_i \right\rangle = 0. \quad (2.9)$$

The force \mathbf{f}_i on a particle can be written as a summation of an inter-particle force $\mathbf{f}_{i,\text{int}}$ (which the particle experiences owing to interaction with other particles in the system), a body force $\mathbf{f}_{i,\text{body}}$ and a confinement force $\mathbf{f}_{i,\text{confine}}$, which serves to confine a particle say enclosed within a vessel (figure 1).

Furthermore, identification can be made between the effect of discrete confinement forces \mathbf{c}_i with that of an applied traction field $\mathbf{t}(\mathbf{r})$ and between the discrete body forces on a particle \mathbf{b}_i on particles with that of a continuum body-force density $\mathbf{b}(\mathbf{r})$, as shown in figure 2.

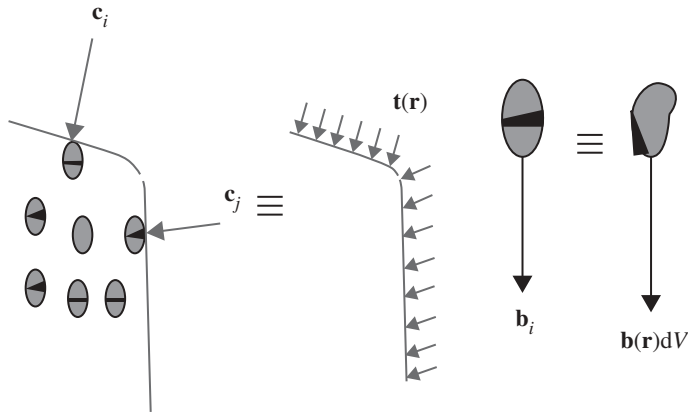


Figure 2. Identifying the discrete confinement forces with the continuum traction field and discrete body forces with continuum body-force density.

Therefore, we can write

$$\sum_i \mathbf{c}_i \otimes \mathbf{r}_i \equiv \int_{\partial R} \mathbf{t} \otimes \mathbf{r} \, ds \quad (2.10)$$

and

$$\sum_i \mathbf{b}_i \otimes \mathbf{r}_i \equiv \int_R \rho \mathbf{b} \otimes \mathbf{r} \, dV. \quad (2.11)$$

From equations (2.10), (2.11) and (2.8),

$$\frac{d\mathbf{G}}{dt} + \frac{1}{2} \sum_i \mathbf{f}_{ij} \otimes (\mathbf{r}_j - \mathbf{r}_i) - \sum_i m_i \mathbf{v}_i \otimes \mathbf{v}_i = \int_R ((\operatorname{div} \boldsymbol{\sigma} + \rho \mathbf{b}) \otimes \mathbf{r} + \boldsymbol{\sigma}) \, dV. \quad (2.12)$$

For macroscopic equilibrium in which \mathbf{G} remains bounded in time, an average over sufficiently long times yields the following expression for the macroscopic stress (Murdoch 2007):

$$\langle \bar{\boldsymbol{\sigma}} \rangle = \frac{1}{\Omega} \left(\left\langle \frac{1}{2} \sum_i \mathbf{f}_{ij} \otimes (\mathbf{r}_j - \mathbf{r}_i) \right\rangle - \left\langle \sum_i m_i \mathbf{v}_i \otimes \mathbf{v}_i \right\rangle \right). \quad (2.13)$$

(c) Macroscopic stress in quantum mechanics

The total stress of a stationary system can be obtained by applying a variational principle together with a scaling of the wave function. The derivation follows the same methodology as that given for the virial theorem by Fock (1930; see also Nielsen & Martin (1985) and our review article Maranganti *et al.* (2007)). First, we consider a many-body Hamiltonian of the form

$$H = \sum_i \frac{\mathbf{p}_i^2}{2m_i} + V_{\text{int}} + V_{\text{ext}}, \quad (2.14)$$

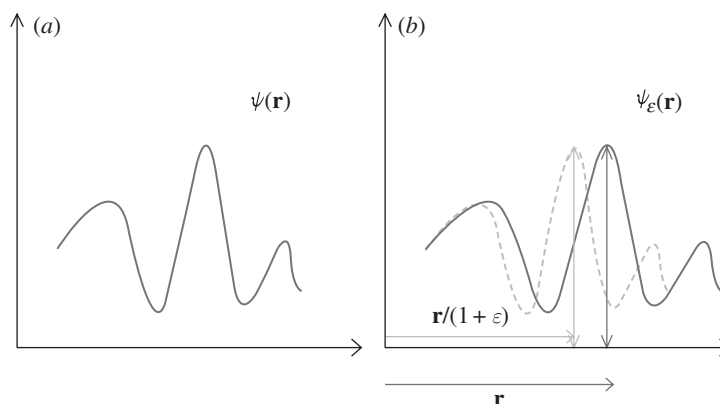


Figure 3. Rescaling of the wave function under a homogeneous ‘stretch’.

where $V := V_{\text{int}} + V_{\text{ext}}$ denotes the potential energy of the whole system; it is a function of the positions of all the particles. Note that both nuclei and electrons are regarded as particles. V_{int} is the intrinsic contribution consisting of inter-atomic potentials, whereas V_{ext} incorporates the potentials associated with external influences such as body forces. We will only consider potentials that are velocity-independent (i.e. potentials are only dependent on spatial coordinates of the particles). The many-body Schrödinger equation (2.15) can then be solved to obtain the many-body eigenstates ψ ,

$$H\psi = E\psi. \quad (2.15)$$

The quantum-mechanical variational principle requires that the ground state is the minimum of the energy E with respect to the allowed variations in ψ ,

$$E = \langle \psi | H | \psi \rangle. \quad (2.16)$$

It should be noted that, in the context of quantum mechanics, the symbol $\langle \rangle$ denotes expectation value. To derive the stress, a homogeneous scaling is applied to the ground state $\psi(\mathbf{r})$, where \mathbf{r} denotes a list of all particle coordinates. Consider a transformation on this coordinates of the form

$$r_{i\alpha} \rightarrow r_{i\alpha} + \sum_{\beta} \varepsilon_{\alpha\beta} r_{i\beta}. \quad (2.17)$$

Here, $\varepsilon_{\alpha\beta}$ is a symmetric strain tensor. The change in the wave function is given by

$$\psi_{\varepsilon}(\mathbf{r}) \rightarrow \det(1 + \varepsilon)^{-1/2} \psi((1 + \varepsilon)^{-1}\mathbf{r}). \quad (2.18)$$

The above scaling of the wave function can be explained diagrammatically as shown in figure 3.

The additional factor of $\det(1 + \varepsilon)^{-1/2}$ is included so that the normalization of the wave function is preserved. The expectation value of H with respect to ψ involves an integral over all the coordinates, \mathbf{r} ,

$$\langle \psi_{\varepsilon} | H | \psi_{\varepsilon} \rangle = \int \psi_{\varepsilon}^*(\mathbf{r}) \left[\sum_i \frac{\mathbf{p}_i^2}{2m_i} + V_{\text{int}} + V_{\text{ext}} \right] \psi_{\varepsilon}(\mathbf{r}) \, \mathbf{r}. \quad (2.19)$$

By substituting $\mathbf{r} \rightarrow (1 + \boldsymbol{\varepsilon})\mathbf{r}$, we can rewrite the integral in equation (2.19) as

$$\langle \psi_\varepsilon | H | \psi_\varepsilon \rangle = \int \psi^*(\mathbf{r}) \left[\sum_i \frac{-1}{2m_i} \frac{d^2}{d((1 + \boldsymbol{\varepsilon})\mathbf{r}_i)^2} + V_{\text{int}}((1 + \boldsymbol{\varepsilon})\mathbf{r}) + V_{\text{ext}}((1 + \boldsymbol{\varepsilon})\mathbf{r}) \right] \psi(\mathbf{r}) \, d\mathbf{r}. \quad (2.20)$$

On further simplification, the integral in equation (2.20) can be rewritten as

$$\langle \psi_\varepsilon | H | \psi_\varepsilon \rangle = \int \psi^*(\mathbf{r}) \left[\sum_i \left(\frac{\mathbf{p}_i^2 - 2\varepsilon_{\alpha\beta} p_{i\alpha} p_{i\beta} + 3\varepsilon_{\alpha\beta} \varepsilon_{\alpha\gamma} p_{i\beta} p_{i\gamma} + \dots}{2m_i} \right) + V_{\text{int}}((1 + \boldsymbol{\varepsilon})\mathbf{r}) + V_{\text{ext}}((1 + \boldsymbol{\varepsilon})\mathbf{r}) \right] \psi(\mathbf{r}) \, d\mathbf{r}. \quad (2.21)$$

The variational principle requires that $\langle \psi_\varepsilon | H | \psi_\varepsilon \rangle$ varies from $\langle \psi | H | \psi \rangle$ only to second order in the strain; therefore,

$$\frac{\partial \langle \psi_\varepsilon | H | \psi_\varepsilon \rangle}{\partial \varepsilon_{\alpha\beta}} = 0 = \int \psi^*(\mathbf{r}) \left[\sum_i \left(\frac{p_{i\alpha} p_{i\beta}}{m_i} - r_{i\beta} \nabla_{i\alpha} (V_{\text{int}} + V_{\text{ext}}) \right) \right] \psi(\mathbf{r}) \, d\mathbf{r}. \quad (2.22)$$

The term involving V_{ext} in equation (2.22) represents the stress exerted by the external environment upon the solid. This stress is symmetric for a system in equilibrium in the absence of external torques,

$$T_{\alpha\beta} = - \left\langle \psi \left| \sum_i r_{i\beta} \nabla_{i\alpha} V_{\text{ext}} \right| \psi \right\rangle. \quad (2.23)$$

The net torque owing to external forces is given by

$$\tau_\alpha = \varepsilon_{\alpha\beta\gamma} \left\langle \psi \left| \sum_i r_{i\beta} f_{i\gamma} \right| \psi \right\rangle = - \varepsilon_{\alpha\beta\gamma} \left\langle \psi \left| \sum_i r_{i\gamma} f_{i\beta} \right| \psi \right\rangle. \quad (2.24)$$

Here, $\varepsilon_{\alpha\beta\gamma}$ is the Levi-Cevita symbol defined by

$$\varepsilon_{ijk} = \begin{cases} +1, & \text{if } (i, j, k) \text{ is an even permutation of } (1, 2, 3), \\ -1, & \text{if } (i, j, k) \text{ is an odd permutation of } (1, 2, 3), \\ 0, & \text{if any index is repeated.} \end{cases} \quad (2.25)$$

However, if the stress is symmetric, then

$$\left\langle \psi \left| \sum_i r_{i\gamma} f_{i\beta} \right| \psi \right\rangle = \left\langle \psi \left| \sum_i r_{i\beta} f_{i\gamma} \right| \psi \right\rangle. \quad (2.26)$$

From the properties of the Levi-Cevita operator, we arrive at the following:

$$\tau_\alpha = -\tau_\alpha. \quad (2.27)$$

Thus, from equation (2.27), we can infer that the net external torque vanishes if the stress is symmetric. The stress intrinsic to the system is then given by

$$T_{\alpha\beta} = -\left\langle \psi \left| \sum_i \left(\frac{p_{i\alpha} p_{i\beta}}{m_i} - r_{i\beta} \nabla_{i\alpha} (V_{\text{int}}) \right) \right| \psi \right\rangle. \quad (2.28)$$

Equation (2.28) is one form of the stress theorem that expresses the total macroscopic stress in terms of the expectation values of internal operators intrinsic to the system. It can be seen that the expression for the macroscopic stress in molecular dynamics (equation (2.13)) and the expression for the global virial stress in quantum mechanics (equation (2.28)) are closely parallel to each other.

We note that equation (2.28) provides the macroscopic stress, even for systems subjected to *inhomogeneous external stresses*. Is this statement justified? The answer is in the affirmative since the macroscopic stress is arrived at by applying a uniform strain to the ground state of the system and extracting its response. There is no restriction on the strain state of the ground state of the system. It may be, for example, subject to inhomogeneous residual stresses.

The stress theorem is applicable to general quantum-mechanical systems with interactions that are differentiable functions of the particle coordinates. The potentials can be non-local in nature, i.e. functions of the coordinate of a given particle at more than one point in space. The non-local nature of potentials is especially relevant for the case of pseudo-potentials, which are extensively used in numerical quantum-mechanical-based computational schemes. In order to define the stress of equation (2.28) in an unambiguous manner, we have to express the stress in terms of relative coordinates of the interacting particles. In the case of particles acting through two-body potentials,

$$V_{\text{int}} = \frac{1}{2} \sum_{\substack{i,j \\ (j \neq i)}} V_{ij}(|\mathbf{r}_i - \mathbf{r}_j|). \quad (2.29)$$

Then, the stress theorem of equation (2.28) becomes

$$T_{\alpha\beta} = -\sum_i \left\langle \frac{p_{i\alpha} p_{i\beta}}{m_i} \right\rangle - \frac{1}{2} \sum_{\substack{i,j \\ (j \neq i)}} \left\langle \frac{(\mathbf{r}_i - \mathbf{r}_j)_\alpha (\mathbf{r}_i - \mathbf{r}_j)_\beta}{|\mathbf{r}_i - \mathbf{r}_j|} V'_{ij}(|\mathbf{r}_i - \mathbf{r}_j|) \right\rangle. \quad (2.30)$$

This form of the stress is symmetric (torque-free) and dependent only on the relative distances between the particles. In macroscopic systems in which the volume is well defined, the average stress density can be defined as

$$\sigma_{\alpha\beta} = \frac{T_{\alpha\beta}}{\Omega}. \quad (2.31)$$

For a periodic structure, the volume can be chosen to be a unit cell, and a stress density per unit cell volume may be defined. The quantum-mechanical

form of the virial theorem can be obtained by taking the negative of the trace of equation (2.30)

$$3P\Omega = 2 \sum_i \left\langle \frac{\mathbf{p}_i^2}{2m_i} \right\rangle - \frac{1}{2} \sum_{\substack{i,j \\ (j \neq i)}} \langle |\mathbf{r}_i - \mathbf{r}_j| V'_{ij}(|\mathbf{r}_i - \mathbf{r}_j|) \rangle, \quad (2.32)$$

where P denotes the pressure. Furthermore, if the interactions are of the form $V(r) = 1/r^n$, the virial theorem can be written in terms of the potential and kinetic energies. For the case of the Coulomb potential, the virial theorem takes the form

$$3P\Omega = 2E_{\text{kin}} + E_{\text{pot}}. \quad (2.33)$$

In most cases, it is advantageous to carry out calculations without introducing an explicit V_{ext} . Instead, often calculations are performed using $H = T_{\text{kin}} + V_{\text{int}}$ with the system being subject to constraints corresponding to V_{ext} . In this case, the wave function satisfies a restricted variational principle.

3. Stress as a microscopic field

Thus far we have considered the average macroscopic or the *global* virial stress of a system of particles both in the molecular dynamical and in the quantum-mechanical context. However, these treatments do not bring about the field nature of stress and force. In other words, the point-to-point spatial variation of the stress and force fields is (obviously) lost in the process of averaging over a macroscopic volume. If one, however, knows the spatially varying stress field, the ramifications can be important. Spatial variations in the planar stress can provide an insight into the forces operating in systems that are not in equilibrium (Nielsen & Martin 1985). Filippetti & Fiorentini (1999, 2000) envision using the microscopic stress as what they refer to as a stress microscope to examine the stress's role in explaining the physics of certain surface and interface phenomena. Ramer *et al.* (1998) applied the microscopic stress field to study piezoelectric effects in perovskites. While the local force field is uniquely specified in terms of kinetic and potential operators (Pauli 1933), the stress field, in contrast, can only be specified to an arbitrary gauge term (explained shortly) (Feynman 1939). Traditionally, the stress field is defined as any two-tensor field whose divergence yields the force field of the system,

$$\mathbf{f}(\mathbf{r}) = \text{div } \boldsymbol{\sigma}(\mathbf{r}). \quad (3.1)$$

To this stress field, one can add a term of the form

$$\frac{\partial A_{ijk}(\mathbf{r})}{\partial r_k}, \quad (3.2)$$

where $A_{ijk}(\mathbf{r})$ is an arbitrary tensor field antisymmetric in j and k and recover the same force field of equation (3.1). Thus, the stress field is undetermined to an arbitrary gauge term if one chooses to define it via equation (3.1). This is the

gauge arbitrariness associated with the microscopic stress field. We now examine a route to arrive at a microscopic stress field in discrete molecular dynamics by local spatial averaging.

(a) *Stress as a local spatial average: how to link continuum field values with microscopic behaviour at any length scale?*

In an empirical molecular-dynamics setting, Murdoch (2007) has outlined the following approach to arrive at a spatially varying stress field by means of local spatial averaging. Once again, consider a set of interacting point masses P_i ($i = 1, 2, 3, \dots, N$). The mass and momentum density fields are defined as

$$\left. \begin{aligned} \rho_w(\mathbf{r}, t) &:= \sum_i m_i w(\mathbf{r}_i(t) - \mathbf{r}) \\ \text{and} \quad \mathbf{p}_w(\mathbf{r}, t) &:= \sum_i m_i \mathbf{v}_i(t) w(\mathbf{r}_i(t) - \mathbf{r}). \end{aligned} \right\} \quad (3.3)$$

Here, the sums are taken over all particles, and $\mathbf{r}_i(t) - \mathbf{r}$ denotes the displacement of P_i from the geometrical point \mathbf{r} at time t . In accordance with the continuum notion of mass density, the weighting function w should be chosen such as to assign greater contributions to point masses near to r than far from there, have physical dimension L^3 and be continuously differentiable on the space of displacements in Euclidean space. To ensure that the integral of ρ_w over all space yields the total mass of the body, it is necessary and sufficient that

$$\int_V w(\mathbf{u}) \, d\mathbf{u} = 1. \quad (3.4)$$

Now holding \mathbf{r} fixed

$$\begin{aligned} \frac{\partial \rho_w}{\partial t} &= \sum_i m_i \nabla w \cdot \mathbf{v}_i = - \sum_i m_i \nabla_{\mathbf{r}} w \cdot \mathbf{v}_i \\ &= - \sum_i m_i \operatorname{div}(\mathbf{v}_i w) = - \operatorname{div} \mathbf{p}_w. \end{aligned} \quad (3.5)$$

Whenever $\rho_w \neq 0$, the corresponding velocity field can be written as

$$\mathbf{v}_w = \frac{\mathbf{p}_w}{\rho_w}. \quad (3.6)$$

From expression (3.6), the mass balance equation can be written as

$$\frac{\partial \rho_w}{\partial t} + \operatorname{div} \mathbf{p}_w = 0. \quad (3.7)$$

Similarly, a momentum balance equation can be arrived at as

$$\operatorname{div} \mathbf{T}_w + \mathbf{b}_w = \rho_w \mathbf{a}_w. \quad (3.8)$$

Here, the following definitions hold (the reader is referred to Murdoch's (2007) work for details):

$$\mathbf{T}_w = \mathbf{T}_w^- - \mathbf{D}_w, \quad (3.9)$$

$$\mathbf{b}_w(\mathbf{r}, t) := \sum_i b_i(t) w(\mathbf{r}_i(t) - \mathbf{r}), \quad (3.10)$$

$$\mathbf{a}_w := \frac{\partial \mathbf{v}_w}{\partial t} + (\nabla \mathbf{v}_w) \mathbf{v}_w, \quad (3.11)$$

$$\operatorname{div} \mathbf{T}_w^- = \mathbf{f}_w, \quad (3.12)$$

$$\mathbf{f}_w(\mathbf{r}, t) := \sum_i \sum_{j \neq i} \mathbf{f}_{ij}(t) w(\mathbf{r}_i(t) - \mathbf{r}) \quad (3.13)$$

and
$$\mathbf{D}_w(\mathbf{r}, t) := \sum_i m_i \mathbf{v}_i \otimes \mathbf{v}_i w(\mathbf{r}_i(t) - \mathbf{r}). \quad (3.14)$$

\mathbf{D}_w represents the kinetic contribution to the stress, whereas \mathbf{T}_w^- represents the contribution owing to inter-particle interaction and can be uniquely specified only up to a divergence-free tensor. Therefore, this non-uniqueness can be exploited to arrive at many forms of the interaction stress tensor. Two forms, the Hardy stress and the Noll stress, have been discussed in the literature (Murdoch 2007),

$$\mathbf{T}_w^- = \sum_{i \neq j} \sum \mathbf{f}_{ij} \otimes \mathbf{b}_{ij}. \quad (3.15)$$

Hardy's choice is

$$\mathbf{b}_{ij} := \int_0^1 w(\lambda(\mathbf{r}_j - \mathbf{r}_i) + (\mathbf{r}_i - \mathbf{r}))(\mathbf{r}_j - \mathbf{r}_i) d\lambda, \quad (3.16)$$

and Noll's choice is

$$\mathbf{b}_{ij} := -\frac{1}{2} \int_V \int_0^1 \mathbf{u} w(\mathbf{r}_i - \mathbf{r} - \alpha \mathbf{u}) w(\mathbf{r}_j - \mathbf{r} + (1 - \alpha) \mathbf{u}) d\alpha d\mathbf{u}. \quad (3.17)$$

(b) *A local stress field in quantum mechanics: general formalism*

In this section, we develop a general quantum-mechanical operator-based approach to continuity equations for densities of Hermitian operators. Consider a Hermitian operator B corresponding to some physical observable. Then, one can define a corresponding spatially varying Hermitian density operator $A(\mathbf{r})$ as an anti-commutator of the form

$$A(\mathbf{r}) = \frac{1}{2} \{B, \delta(\hat{\mathbf{R}} - \mathbf{r})\} = \frac{B\delta(\hat{\mathbf{R}} - \mathbf{r}) + \delta(\hat{\mathbf{R}} - \mathbf{r})B}{2}. \quad (3.18)$$

Note that $\hat{\mathbf{R}}$ is the position operator, whereas \mathbf{r} is the spatial location of interest. As an example, the single-particle mass-density operator $\rho(\mathbf{r})$ is then

$$\rho(\mathbf{r}) = \frac{1}{2} \{m_i, \delta(\hat{\mathbf{R}}_i - \mathbf{r})\} = m_i \delta(\hat{\mathbf{R}}_i - \mathbf{r}). \quad (3.19)$$

Consider a cluster of a finite number of nuclei and electrons. The nuclei being massive, we will consider them as classical particles. Thus, the mass density owing to the nuclei becomes

$$\rho_n(\mathbf{r}) = \sum_i m_{n,i} \delta(\hat{\mathbf{R}}_{n,i} - \mathbf{r}), \quad (3.20)$$

where $m_{n,i}$ is the mass of the i th nucleus and $\mathbf{R}_{n,i}$ corresponds to its physical position. However, the mass-density operator corresponding to the electrons is

$$\rho_e(\mathbf{r}) = \sum_i m_{e,i} \delta(\hat{\mathbf{R}}_{e,i} - \mathbf{r}). \quad (3.21)$$

Here, $m_{e,i}$ is the mass of the electron. For an electronic wave function of the form $\Phi(\mathbf{r}; \mathbf{r}_2; \dots; \mathbf{r}_N)$, the expectation value of the electron mass density is

$$\langle \rho_e(\mathbf{r}) \rangle = Nm_e \int d\mathbf{r}_2, \dots, d\mathbf{r}_N \Phi^*(\mathbf{r}; \mathbf{r}_2; \dots; \mathbf{r}_N) \Phi(\mathbf{r}; \mathbf{r}_2; \dots; \mathbf{r}_N). \quad (3.22)$$

For a single particle, the expectation value becomes

$$\rho(\mathbf{r}) = m_e |\Phi(\mathbf{r})|^2. \quad (3.23)$$

From elementary quantum mechanics, we note the interpretation of the modulus of the wave function squared as the probability density distribution for the particle.

What kind of continuity equation will such density operators follow? We consider again a general Hermitian density operator of the form

$$A(\mathbf{r}) = \frac{1}{2} \{A, \delta(\hat{\mathbf{R}} - \mathbf{r})\}. \quad (3.24)$$

In order to find its time evolution, we write Heisenberg's equation of motion for this density operator, resulting in

$$\frac{\partial A(\mathbf{r})}{\partial t} = \frac{1}{i\hbar} [A(\mathbf{r}), H], \quad (3.25)$$

where H is the Hamiltonian operator. Expanding the commutator and the anti-commutator, we have

$$\frac{\partial A(\mathbf{r})}{\partial t} = \frac{i}{2\hbar} (\{[H, A], \delta(\hat{\mathbf{R}} - \mathbf{r})\} + \{A, [H, \delta(\hat{\mathbf{R}} - \mathbf{r})\}). \quad (3.26)$$

It is interesting to draw an analogy between equation (3.26) and the generalized continuity equation from classical mechanics

$$\frac{dp_i}{dt} + \frac{\partial}{\partial x_j} \Pi_{ij} = S_i. \quad (3.27)$$

Note that if H and A commute, then the first term on the r.h.s. of equation (3.26) vanishes. That is why we can identify this term to correspond to the source

term S_i in its classical counterpart. After some manipulation, equation (3.26) can be rewritten as

$$\frac{\partial}{\partial t}A(\mathbf{r}) + \frac{1}{4}\nabla_{r,i}\left\{A, \left\{\frac{p_i}{m}, \delta(\hat{\mathbf{R}} - \mathbf{r})\right\}\right\} = \frac{1}{2}\left\{\frac{\partial}{\partial t}A, \delta(\hat{\mathbf{R}} - \mathbf{r})\right\}. \quad (3.28)$$

From equation (3.28), the flux-density operator corresponding to operator A can be written as

$$T_i^A(\mathbf{r}) = \frac{1}{4}\left\{A, \left\{\frac{p_i}{m}, \delta(\hat{\mathbf{R}} - \mathbf{r})\right\}\right\}. \quad (3.29)$$

For example, in order to find the flux density of particles, we can substitute the identity operator in place of A to obtain

$$T_i^{(N)}(\mathbf{r}) = \frac{\hbar}{m}\text{Im}(\psi^*\nabla_i\psi). \quad (3.30)$$

Equation (3.29) is recognizable as the expression for the well-known particle current density from quantum mechanics. Now, in order to find the kinetic contribution of stress, we substitute the momentum operator in place of A in equation (3.29) to obtain

$$\langle T_{ij}^{\text{kin}}(\mathbf{r}) \rangle = \frac{\hbar^2}{4m}\left[\frac{\partial\psi^*}{\partial r_i}\frac{\partial\psi}{\partial r_j} + \frac{\partial\psi^*}{\partial r_j}\frac{\partial\psi}{\partial r_i} - \frac{\partial^2\psi^*}{\partial r_i\partial r_j}\psi - \psi^*\frac{\partial^2\psi}{\partial r_i\partial r_j}\right]. \quad (3.31)$$

To find the interaction contribution to the stress, we have to focus on the source term in equation (3.28). Simple inspection shows that a form of stress due to Kugler (1967) satisfies equation (3.28), in the sense that its divergence yields the source term in equation (3.28). Kugler's stress definition, however, contains some objectionable features. Even if the interactions defined by V are short-ranged, the curl-free nature of the potential term renders the Kugler stress inherently long ranged and thus non-local. In particular, the long-range character of the Kugler stress derives from the term

$$T_{\alpha\beta}^{\text{pot}}(\mathbf{r}) = \frac{1}{4\pi}\nabla_{i\alpha}(V)\frac{(\mathbf{r} - \hat{\mathbf{R}})_\beta}{|\mathbf{r} - \hat{\mathbf{R}}|^3}. \quad (3.32)$$

The Kugler stress corresponding to the interaction between two particles A and B can be visualized as a radial flow of momentum from A to infinity, superimposed on a radial flow from infinity to B. This makes it possible to assign a distribution of sources at infinity, which need not bear any relation to the actual physical sources. The issue of the long-ranged character of the Kugler stress may be partially circumvented by computing stress by summing over pairs of interacting particles, thereby resulting in a dipole-like long-range distance dependence of the form. However, this form of stress field is still long ranged, albeit of a somewhat weaker form than the original one. When the interaction is Coulombic, Kugler's form of stress results in severe anomalies, and a different form of the stress tensor called the Maxwell form (Feynman 1939; Jackson 1999) is employed. The latter

is applicable for particles interacting via Coulombic forces. In the static limit (in the absence of magnetic effects), Maxwell's stress field is given as

$$\left. \begin{aligned} T_{\alpha\beta}^{\text{Max}}(\mathbf{r}) &= \frac{1}{4\pi} \left\langle E_{\alpha}(\mathbf{r})E_{\beta}(\mathbf{r}) - \frac{1}{2}\delta_{\alpha\beta}\mathbf{E}^2(\mathbf{r}) \right\rangle \\ \text{and} \\ E_{\alpha}(\mathbf{r}) &= \sum_i Z_i \frac{(\mathbf{r} - \hat{\mathbf{R}}_i)}{|\mathbf{r} - \hat{\mathbf{R}}_i|^3}. \end{aligned} \right\} \quad (3.33)$$

However, if the potential is a pair potential of the form V , then a Hardy stress-like operator can be derived for the potential part of the stress as

$$T_{\alpha\beta}^{\text{pot}}(\mathbf{r}) = -\frac{1}{2} \sum_{i,j} \int_0^1 d\lambda \delta[\mathbf{r} - \hat{\mathbf{R}}_i - \lambda(\hat{\mathbf{R}}_i - \hat{\mathbf{R}}_j)] (\hat{R}_{i,\alpha} - \hat{R}_{j,\alpha}) \frac{\partial w}{\partial \hat{R}_{i,\beta}}. \quad (3.34)$$

Similarly, a Noll-like stress can also be derived. Both the forms do not possess the long-ranged character of Kugler's potential and are more generally applicable than the Maxwell stress.

4. Revisiting the virial stress

The original virial theorem owing to Clausius provides a relation connecting the time-averaged translational kinetic energy of a stationary dynamical system of particles to the time average of the so-called virial of the forces acting on the particles. It can be extended to statistical mechanics by replacing the time averages by ensemble averages. We discussed a scaling-type approach to prove the virial theorem in the quantum-mechanical case in the previous section. It is intriguing to see whether a similar scaling approach will work for the classical/statistical mechanical case—arguably making the analogy to quantum-mechanical global stress more transparent.

In a canonical ensemble, we have

$$F(T, V) = -K_{\text{B}} T \ln Z(T, V), \quad (4.1)$$

where F is the Helmholtz free energy and Z is the partition function. From thermodynamics, we can express the pressure P as

$$P = - \left(\frac{\partial F}{\partial V} \right)_T. \quad (4.2)$$

Simplifying, we have

$$\begin{aligned} P &= K_{\text{B}} T \left(\frac{\partial \ln Z(T, V)}{\partial V} \right)_T = K_{\text{B}} T \left(\frac{1}{Z} \frac{\partial Z}{\partial V} \right)_T \\ &= - \frac{(\int (\partial H / \partial V) e^{-H/K_{\text{B}}T} d\tau)}{\int e^{-H/K_{\text{B}}T} d\tau} = - \left\langle \frac{\partial H}{\partial V} \right\rangle. \end{aligned} \quad (4.3)$$

Consider a set of particles with coordinates $\{\mathbf{r}_i\}$ and conjugate momenta $\{\mathbf{p}_i\}$ enclosed within a container in thermal equilibrium at temperature T . Consider the container to be a cubical box of volume V with rigid walls such that the potential owing to the wall is of the form

$$\begin{aligned} U'(\mathbf{r}_i) &= 0, \text{ all } \mathbf{r}_i \text{ inside box,} \\ &= \infty, \text{ any } \mathbf{r}_i \text{ outside box.} \end{aligned} \quad (4.4)$$

The pressure in statistical mechanics is written as

$$P = - \left\langle \frac{\partial H}{\partial V} \right\rangle. \quad (4.5)$$

Here, the brackets denote an ensemble average.

In order to evaluate this quantity, we assume a form for our Hamiltonian as

$$H = \sum_{i=1}^N \frac{p_i^2}{2m_i} + U(\mathbf{r}_1, \dots, \mathbf{r}_N). \quad (4.6)$$

We now scale the Hamiltonian using a simple canonical transformation of the form

$$\mathbf{r}'_i = L\mathbf{r}_i \quad \text{and} \quad \mathbf{p}'_i = L^{-1}\mathbf{p}_i, \quad (4.7)$$

where $L = V^{1/3}$. Therefore, the scaled cube is a cube of unit dimensions.

From equations (4.5) and (4.6), we have

$$P = - \left\langle \frac{\partial H}{\partial V} \right\rangle = - \frac{1}{N!h^{3N}} \frac{\int \exp[-\beta H_L] (\partial H_L / \partial V) d\mathbf{p}_1 \dots d\mathbf{p}_N d\mathbf{r}_1 \dots d\mathbf{r}_N}{Z_L}. \quad (4.8)$$

We now assess how the partition function Z scales under the canonical transformation given by equation (4.7).

The partition function Z for a system of N classical particles can be written as

$$Z = \frac{1}{N!h^{3N}} \int \exp[-\beta H(\mathbf{p}_1 \dots \mathbf{p}_N; \mathbf{r}_1 \dots \mathbf{r}_N)] d\mathbf{p}_1 \dots d\mathbf{p}_N d\mathbf{r}_1 \dots d\mathbf{r}_N. \quad (4.9)$$

The rescaled Hamiltonian becomes

$$H_L = H(\mathbf{p}_1/L, \dots, \mathbf{p}_N/L, L\mathbf{x}_1, \dots, L\mathbf{x}_N). \quad (4.10)$$

The rescaled partition function $Z[H_L]$ becomes

$$Z[H_L] = \frac{1}{N!h^{3N}} \int \exp[-\beta H_L] d\mathbf{p}_1 \dots d\mathbf{p}_N d\mathbf{r}_1 \dots d\mathbf{r}_N. \quad (4.11)$$

By substituting $\mathbf{p}_i \rightarrow L\mathbf{p}_i$ and $\mathbf{r}_i \rightarrow L^{-1}\mathbf{r}_i$ in the above equation, we have

$$Z[H_L] = \frac{1}{N!h^{3N}} \int \exp[-\beta H] L d\mathbf{p}_1 \dots L d\mathbf{p}_N L^{-1} d\mathbf{r}_1 \dots L^{-1} d\mathbf{r}_N = Z[H]. \quad (4.12)$$

Therefore, the partition function Z remains invariant under the canonical scaling.

Now consider

$$P = - \left\langle \frac{\partial H}{\partial V} \right\rangle = - \frac{1}{N! h^{3N}} \frac{\int \exp[-\beta H_L] (\partial H_L / \partial V) d\mathbf{p}_1 \dots d\mathbf{p}_N d\mathbf{r}_1 \dots d\mathbf{r}_N}{Z_L}. \quad (4.13)$$

Further,

$$\left. \begin{aligned} \frac{\partial H}{\partial V} &= \frac{2}{3} L^{-5} \sum_i \frac{p_i'^2}{2m_i} - \frac{1}{3} L^{-2} \sum_i \mathbf{x}_i' \cdot \nabla_i U \\ &= \frac{2}{3V} \sum_i \frac{p_i^2}{2m_i} - \frac{1}{3V} \sum_i \mathbf{x}_i \cdot \nabla_i U. \end{aligned} \right\} \quad (4.14)$$

So, from equations (4.13) and (4.14) and the invariance of the partition function, we have

$$3PV = \left\langle 2 \sum_i \frac{p_i^2}{2m_i} \right\rangle - \left\langle \sum_i \mathbf{x}_i \cdot \nabla_i U \right\rangle. \quad (4.15)$$

Equation (4.15) is the Clausius form of the virial theorem. If the particles are bound under the influence of their own internal interactions (say there is no box enclosing the particles), then the pressure P goes to zero.

The tensor form of the virial theorem can be obtained in an analogous manner by scaling the Hamiltonian using transformation of the form

$$r'_{i,\alpha} = h_{\alpha\beta} r_{i,\beta} \quad \text{and} \quad p'_{i,\alpha} = h_{\alpha\beta}^{-1} p_{i,\beta}. \quad (4.16)$$

Here, the tensor \mathbf{h} is represented as a matrix consisting of the vectors that make the sides of the box enclosing the N -particle system. The volume of this box is given by $\det(\mathbf{h})$.

A uniform strain applied to the whole box can be thought of as a rescaling of the metric tensor \mathbf{h} . The macroscopic stress is then simply given as

$$\sigma_{\alpha\beta} = - \left\langle \frac{\partial H}{\partial h_{\alpha\beta}} \right\rangle = - \frac{1}{N! h^{3N}} \frac{\int \exp[-\beta H'] (\partial H' / \partial h_{\alpha\beta}) d\mathbf{p}_1 \dots d\mathbf{p}_N d\mathbf{r}_1 \dots d\mathbf{r}_N}{Z'}. \quad (4.17)$$

From this, the tensor form of the virial theorem is easily recovered.

5. Discussion

The present paper provides a unified setting that connects continuum, empirical molecular-dynamics and quantum-mechanical stress concepts. The essential tool is provided by Murdoch's (2007) formalism of arriving at a spatially varying stress field in a discrete setting. Analogous to molecular dynamics, Hardy stress- and Noll stress-like operators can represent the microscopic stress measures in quantum mechanics. The major challenge that remains is to cast our formalism in a computationally favourable framework like density functional theory (DFT) and observe how well the various microscopic stress measures compare with Maxwell's stress that is the gauge of choice for Columbic systems. Our formalism is not restricted to Columbic potentials, so non-Coulomb-like potentials that often occur in pseudo-potentials used in DFT calculations can be included as well.

The issue of the uniqueness of the quantum-mechanical stress is still open to debate. The reader is referred to Maranganti *et al.* (2007) and references therein for further discussion. It remains to be seen whether the non-uniqueness of the quantum-mechanical stress is of any physical consequence. One viewpoint that can be taken is that the force is the physical quantity that is transmitted across scales, and since all stress measures when integrated over a surface yield the same force, the choice of the quantum-stress definition (whether it is Noll's, Hardy's or some other) is a matter of convenience. In fact, the form of quantum stress derived by us (which does not solely depend on the charge density) does not appear to be an observable in quantum mechanics. An arbitrary divergence-free non-Hermitian operator may be added to any permissible quantum-mechanical stress operator that will still satisfy the continuity equations. Accordingly, our belief is that, in the quantum-mechanical context, the spatially varying stress is non-observable. This strengthens the viewpoint that, in multi-scale modelling, passing information about the forces across multiple length scales may be more physical than stress. A counterpoint is that gauge dependence of the stress tensor does not necessarily imply non-existence of 'preferred' local stress. A suitable additional criterion would 'fix' this. At the moment, however, it is not clear what such a criterion should be. While quantum measurement theory may suggest a strategy, physical reasonableness may also be a way to make such a judgement. One way to motivate a 'preferred' definition may be to carry out simulations on some test problems and compare how different gauge choices perform. The criterion to decide the best choice will ultimately have to rest on how physically close any given quantum-stress definition comes to providing the correct insights.

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