Comment on "Microscopic stress tensors in quantum systems"

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We show that the expressions for microscopic stress fields derived previously by the present authors encompass those given in a recent paper by Folland and are correct, in contradiction to claims made by Folland.

I. INTRODUCTION

In a recent paper[1] Folland has derived expressions for the microscopic stress tensor field in quantum systems under the restrictions that (1) all particles interact via Coulomb forces; (2) the nuclei are classical particles at fixed positions; and (3) electronic exchange and correlation are treated within a one-electron, a local density, or a Hartree-Fock framework, respectively. The present authors have also considered the microscopic stress tensor field and have presented in a previous paper[2] (denoted here as NM) expressions valid for general many-body systems and general forms of the interactions. It is claimed by Folland in two places in Ref. 1 that the results of NM are incorrect. The purpose of this Comment is to present our response that (1) the expressions in NM are correct (except for minor corrections given in an erratum[3]) and there is no basis for the claims by Folland concerning our work, and (2) the expressions in NM are the same as those given by Folland when specialized to the above restrictions. Thus we find that the results of Folland are formally correct as far as we can ascertain, and that we agree with him except for points of interpretation discussed below. In the following we will refer to equations in the work of Folland[1] by F(Eq. no.) and similarly for equations in NM.

We first summarize the reasoning and expressions of NM, hopefully clarifying the results by collecting together central expressions from different sections of NM. We subsequently discuss the relation to Folland's work.

II. MICROSCOPIC STRESS FIELDS

The microscopic stress tensor field $\sigma_{\alpha\beta}(\mathbf{r})$ in a quantum system is defined by the condition that its divergence is the force field,[1,2] in correspondence with classical mechanics. While the force field, NM(11), is uniquely defined, the stress field is *not* unique because the curl of any dyadic field (i.e., a divergence-free field) can be added to the stress without affecting the forces.[5] The stress field can therefore be formulated using arbitrarily chosen "gauges" that give identical physically observable forces.

In order to derive formal expressions for stress valid in general cases, NM used a form (i.e., gauge) due to Kugler.[4] This form contains undesirable long-range terms discussed by NM (see especially Appendix A) and Folland, but it is to our knowledge the only form valid for general interactions. Because NM concluded that "for the important special case of Coulomb interactions . . . it is preferable to use the Maxwell form" of the stress field, they devoted Appendix B to that case and gave expressions which encompass Folland's results. We note that for the case of Coulomb interactions a lucid exposition was given almost 50 years ago in a thesis by Feynman.[5]

The expressions for stress fields given by both NM and Folland[2] (denoted F in the following) are sums of kinetic and potential terms. The explicit expression given by NM(14) is

$$\sigma_{\alpha\beta}(\mathbf{r})=-\sum_i \frac{1}{4m_i}\langle [p_{i\alpha},[p_{i\beta},\delta(\mathbf{r}-\mathbf{r}_i)]_+]_+\rangle + \frac{1}{4\pi}\sum_i \langle \nabla_i (V_{\rm int})_\alpha \nabla(|\mathbf{r}-\mathbf{r}_i|^{-1})_\beta\rangle, \quad (1)$$

where α and β are Cartesian coordinates, $p_{i\alpha}$ is the momentum operator of particle i with mass m_i, $V_{\rm int}$ is the interaction potential which in general is a function of all the coordinates, $[a,b]_+=ab+ba$ denotes the anticommutator and $\langle\ \rangle$ denotes the expectation value over the exact quantum ground state. [In Eq. NM(14) the expectation values were omitted by mistake.[3]] The kinetic terms are easily seen to be equivalent to the expectation value of Folland's Eqs. F(25) and F(21) which, when specialized to uncorrelated single particle wave functions, reduce to Eq. F(28b). In the above expression the potential terms are expressed in the Kugler form.[4] In order to give the Maxwell form of stress one must combine NM(14) with Eqs. NM(B1) and NM(B2) giving the full expression for the stress field in a Coulomb system,

$$\sigma_{\alpha\beta}(\mathbf{r})=-\sum_i \frac{1}{4m_i}\langle [p_{i\alpha},[p_{i\beta},\delta(\mathbf{r}-\mathbf{r}_i)]_+]_+\rangle + \frac{1}{4\pi}\langle E_\alpha(\mathbf{r})E_\beta(\mathbf{r})-\tfrac{1}{2}\delta_{\alpha\beta}E^2(\mathbf{r})\rangle, \quad (2)$$

where

$$E_\alpha(\mathbf{r})=\sum_i Z_i \frac{(\mathbf{r}-\mathbf{r}_i)_\alpha}{|\mathbf{r}-\mathbf{r}_i|^3} \tag{3}$$

is the operator giving the electric field due to particles (electrons as well as nuclei) with charge Z_i and position operators $\mathbf{r}_i$. This is still a full many-body form which involves expectation values of the bilinear combinations of the fields produced by pairs of particles which may be correlated. In order to derive Folland's expressions from the present Eq. (2), one must assume that the particles are uncorrelated. Within one-electron Hartree-like approximations, the potential term can be factorized in the form

$$\frac{1}{4\pi}[\langle E_\alpha(\mathbf{r})\rangle\langle E_\beta(\mathbf{r})\rangle-\tfrac{1}{2}\delta_{\alpha\beta}\langle \mathbf{E}(\mathbf{r})\rangle^2] \tag{4}$$

which is just the classical Maxwell stress[6] for the electrostatic field caused by the total charge density due to electrons and nuclei and is the same as in Folland's Eqs. F(38) and F(39). If the effects of exchange and correlation are approximated by an additional term in the total energy, e.g., in the local density approximation, there is a term which is a local function of the charge density. The full expression is given in NM(30a)–NM(30e) as integrals over all of space, and in microscopic form using the Maxwell stress in NM(14), NM(B1) and NM(B2) [see Eq. (2) above] plus the exchange-correlation term NM(29). These results are equivalent to Folland's microscopic equations F(28b) and F(37)–F(39). Folland also gives an explicit expression, F(43), for the Hartree-Fock case, where the potential term in Eq. (2) factorizes into direct and exchange terms.

Folland first criticizes (F Sec. III) the results of NM for microscopic stress fields integrated over surfaces, NM(17) and NM(18), and states that they are "not consistent [because] the divergence is nonzero." The so-called "planar stress" NM(17) is defined by NM as "the force in the α direction transmitted across P_β" (the infinite plane normal to the β direction), and its derivation and physical interpretation is discussed in detail by NM. The divergence of the planar stress is in general nonzero because NM considered general systems where the atoms are not necessarily at their equilibrium positions (whereas the electron system is in the ground state for the given atomic configuration). This property, which is illustrated in Fig. 1 of NM, allows the calculation of atomic forces from the divergence of planar stress. This is in fact one of the main results of the NM paper. Also, NM point out that "If the solid is in equilibrium [planar stress] is a constant tensor," which of course means that it has zero divergence, and that the macroscopic stress is found by integrating the planar stress. Thus, there is no basis whatsoever for Folland's claim of inconsistency in NM.

Folland's other criticism is stated more strongly: "their expression for the macroscopic pressure, N[M](35), is incorrect," supported only by the claim that the nonzero divergence discussed above will invalidate our expression. We have shown above that the nonzero divergence is allowed and is essential for general surface integrals. However, the surface integrals for stress, NM(33), and for pressure [which equals $-\mathrm{tr}(\mathrm{stress})/3$], NM(35), were derived with the explicit condition of zero forces on the atoms. As stated in NM before Eq. NM(31), "We will assume that all forces in the unit cell are zero, so that the planar stress is constant everywhere. Nonzero forces have to be dealt with by averaging over planes cutting the unit cell." Thus we have established that Folland's criticism does not apply and apparently is based upon a misreading of NM.

In fact, we can show that Folland's result, F(60), agrees exactly with that of NM(35). The Maxwell form needed to compare explicitly with Folland is not written out by NM, but it is stated in words clearly following NM(33): "In the case of Coulomb interactions the potential terms may alternatively be given by integrating the Maxwell stress on the face A_j [meaning each part of the surface] since this involves only the electric field on the face." For the pressure this is exactly what Folland has given in Eqs. F(60a) and F(60b), where the stress field is given by Eqs. F(37)–F(39). A slight generalization of Folland's equations gives the Maxwell form of the complete stress tensor, corresponding to NM(33). Thus the results of NM are the same as those of Folland for Coulomb interactions, and should not have been described as incorrect by Folland.

It may be useful to point out that the actual expressions given by NM [Eqs. NM(33) and NM(35)] are given in a form where the potential terms are expressed as the total force crossing a surface. To our knowledge, for general interactions there is no way to find the force crossing a surface strictly from information evaluated on the surface itself. This is fortunately possible for the Maxwell stress, where the total force is given in terms of the electric field evaluated on the surface.

We wish to point out that our results differ from Folland's in one respect, namely concerning expressions for macroscopic pressure. Equation F(57) states that for finite systems the pressure is given by kinetic terms only, with no contribution from potential interactions. This result, based upon "Slater manipulations,"[7] is referred to as "Liberman's identity,"[8] which should be contrasted with the result F(60) for periodic boundary conditions which include potential interactions as well. We find that in general both kinetic and potential terms are *always present,* in accordance with Sham[9] and Kleinman[10], and with the "Pettifor-Andersen force theorem."[11] Furthermore, Andersen *et al.*[12] have recently arrived at the same conclusion using a scaling method and the variational principle. Lehmann and Ziesche[13] also found that potential terms are required. The "Liberman identity" F(57) is valid only in cases where the potential terms are manifestly zero, such as for a single particle interacting with a fixed potential.[7] Other examples include the special case of a monatomic solid with the Wigner-Seitz cell approximated as a neutral sphere, as discussed by Liberman, and selected one-body problems in which interactions are not included. We believe that it is *incorrect and misleading* to identify the surface integrals of the kinetic terms alone as a macroscopic pressure, as Folland does in Eq. F(57). The reason is that the identification with the macroscopic pressure is valid only if the surface encloses a periodic

cell or completely encloses a finite system: if it encloses a finite system the integral is trivially zero and if it encloses a periodic cell, it is in general not correct to omit the potential terms.

Finally, after Eq. F(40) Folland imposes conditions upon the forms that stress fields can take, and in Appendix A criticizes the Kugler form of stress[4] since it violates his conditions. However, as stated above no alternative form is known for general interactions. While we sympathize with the desire for mathematically well-behaved forms, we reemphasize that the stress field is *not* unique and can be subjected to arbitrary "gauge transformations" (see above and Ref. 5). This property is shared by the classical stress fields as well. In fact, the stress field is not necessarily an observable object in the quantum theory, in contrast to the statement by Folland. For example, the arbitrary gauge field may be chosen to contain an anti-Hermitian part giving imaginary components to the spectrum of the stress operator, which consequently is nonobservable. The physically observable forces are independent of any gauge transformations and therefore of the form of the stress field.

III. CONCLUSIONS

In conclusion, we hope that the properties of stress fields in quantum systems, as derived in NM (Ref. 2), have been clarified by the interpretations and discussions given in Folland's paper and in the present Comment. We regret that Folland has made erroneous claims concerning the work of NM seemingly based upon misunderstandings. Except for these problems and more minor points of interpretation, we find that the results of Folland agree with those given by NM when specialized to the cases considered by Folland.

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[1]N. O. Folland, Phys. Rev. B **34**, 8296 (1986).

[2]O. H. Nielsen and R. M. Martin, Phys. Rev. B **32**, 3780 (1985) (denoted here as NM); see also an earlier report in Phys. Rev. Lett. **50**, 697 (1983), and an Erratum (Ref. 3).

[3]O. H. Nielsen and R. M. Martin, Phys. Rev. B **35**, 9308(E) (1987).

[4]A. Kugler, Z. Phys. **198**, 236 (1967).

[5]R. P. Feynman, Bachelor's thesis, Massachusetts Institute of Technology, 1939.

[6]J. D. Jackson, *Classical Electrodynamics* (Wiley, New York, 1962).

[7]J. C. Slater, J. Chem. Phys. **1**, 687 (1933).

[8]D. A. Liberman, Phys. Rev. B **2**, 244 (1970); **3**, 2081 (1971).

[9]L. J. Sham, Phys. Rev. B **6**, 2509 (1972).

[10]L. Kleinman, Phys. Rev. B **3**, 3083 (1971).

[11]V. Heine, in *Solid State Physics,* edited by D. Turnbull, F. Seitz and H. Ehrenreich (Academic, New York, 1980), Vol. 35, p. 1.

[12]O. K. Andersen, R. M. Martin and O. H. Nielsen (unpublished).

[13]D. Lehmann and P. Ziesche, Phys. Status Solidi B **133**, K115 (1986); Wiss. Z. Tech. Univ. Dresden **35**, 7 (1986).