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Comment on Density and Physical Current Density Functional Theory

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In our paper [1] we claimed to prove that for a nondegenerate ground state of a system of electrons in an external electrostatic and magnetostatic field, there is a bijective relationship between the properties of the density $\rho(\mathbf{r})$ and physical current density $\mathbf{j}(\mathbf{r})$, and the external scalar $v(\mathbf{r})$ and vector $\mathbf{A}(\mathbf{r})$ potentials :

$$\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\} \longleftrightarrow \{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}. \tag{1}$$

As such the basic variables [2] of quantum mechanics are $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$. By basic variables we mean a gauge invariant property or properties whose knowledge determines the system wave functions. Since knowledge of the nondegenerate ground state $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$ uniquely determines $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$ (to within a constant and the gradient of a scalar function), the Hamiltonian $\hat{H}$ is known, since the kinetic $\hat{T}$ and electron-interaction $\hat{U}$ operators are assumed known. Then solution of the Schrödinger equation $\hat{H}\psi = E\psi$ leads to the ground and excited state wave functions of the system. It has been pointed out to us [3] that our proof of bijectivity when the ground state wave function ψ is complex is incorrect. The proof, however, remains valid for ψ real. There exists several examples for which the nondegenerate ground state wave function is real. One example [4] is the ground state of the Hooke's atom in a magnetic field $\mathbf{B}(\mathbf{r}) = \boldsymbol{\nabla} \times \mathbf{A}(\mathbf{r})$. In this case there exist an infinite number of nondegenerate ground state wave functions that are real. Another example of a real ground state wave function in the presence of a magnetic field is that of the Fock-Darwin model [5]. Yet another example is the case of two electrons in one-dimensional nanorings [6, 7]. Thus, there exists a domain for which the ground state wave function ψ is real. Hence, the proof of bijectivity for ψ real, and of the consequent conclusion that the basic variables of quantum mechanics are $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$, is of significance. It is also for this reason that the map from such an interacting electronic system to one of noninteracting fermions with the same $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$ is possible [8]. We note that the only other such proof of bijectivity is that between $\rho(\mathbf{r})$ and $v(\mathbf{r})$ due to Hohenberg and Kohn [9] for the case of $\mathbf{B}(\mathbf{r}) = \mathbf{0}$. Although at present there exists no bijectivity-type proof, there appears no reason why $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$ should not constitute the basic variables for the more general case of ψ complex.

The details of the proof for ψ real were not provided in our original work [1]. Hence, in this Comment we provide the proof of bijectivity for this case. We note that the proof explicitly accounts for the many-to-one relationship between $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$ and ψ. We then show where our proof for the general case is in error [3].

In units such that $e = \hbar = m = c = 1$ (for atomic units replace $\mathbf{A}(\mathbf{r})$ by $\mathbf{A}(\mathbf{r})/c$), the Hamiltonian $\hat{H}$ is

$$\hat{H} = \hat{T} + \hat{U} + \hat{V} + \int \hat{\mathbf{j}}(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r}) d\mathbf{r} - \frac{1}{2} \int \hat{\rho}(\mathbf{r}) A^2(\mathbf{r}) d\mathbf{r}, \tag{2}$$

where the physical current density operator

$$\hat{\mathbf{j}}(\mathbf{r}) = \hat{\mathbf{j}}_p(\mathbf{r}) + \hat{\rho}(\mathbf{r})\mathbf{A}(\mathbf{r}), \tag{3}$$

with the paramagnetic current $\hat{\mathbf{j}}_p(\mathbf{r})$ and density $\hat{\rho}(\mathbf{r})$ operators defined in [1]. Thus, the physical current density

$$\mathbf{j}(\mathbf{r}) = \; <\psi|\hat{\mathbf{j}}(\mathbf{r})|\psi> \; = \mathbf{j}_p(\mathbf{r}) + \rho(\mathbf{r})\mathbf{A}(\mathbf{r}), \tag{4}$$

with ψ the solution to the Schrödinger equation $\hat{H}\psi = E\psi$. For ψ real,

$$\mathbf{j}_p(\mathbf{r}) = 0, \tag{5}$$

so that from Eq. (3)

$$\mathbf{j}(\mathbf{r}) = \rho(\mathbf{r})\mathbf{A}(\mathbf{r}). \tag{6}$$

Thus, knowledge of $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$ uniquely determines $\mathbf{A}(\mathbf{r})$.

Suppose there exists a $[\{v, \mathbf{A}\}; \psi]$ and a $[\{v', \mathbf{A}'\}; \psi']$ with $[\{v, \mathbf{A}\}; \psi] \neq [\{v', \mathbf{A}'\}; \psi']$, that lead to the same $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$. We wish to prove that for ψ real this cannot be the case. (We exclude the possibility of $\{v, \mathbf{A}; \psi\}$ with ψ complex that lead to the same nondegenerate ground state $\{\rho, \mathbf{j}\}$.)

The physical current density operator for the primed system is defined as

$$\hat{\mathbf{j}}'(\mathbf{r}) = \hat{\mathbf{j}}_p(\mathbf{r}) + \hat{\rho}(\mathbf{r})\mathbf{A}'(\mathbf{r}). \tag{7}$$

Therefore

$$\mathbf{j}'(\mathbf{r}) = \; <\psi'|\hat{\mathbf{j}}'(\mathbf{r})|\psi'> \; = \mathbf{j}'_p(\mathbf{r}) + \rho'(\mathbf{r})\mathbf{A}'(\mathbf{r}). \tag{8}$$

For ψ' real

$$\mathbf{j}'_p(\mathbf{r}) = 0, \tag{9}$$

so that

$$\mathbf{j}'(\mathbf{r}) = \rho'(\mathbf{r})\mathbf{A}'(\mathbf{r}) = \rho(\mathbf{r})\mathbf{A}'(\mathbf{r}), \tag{10}$$

where in the last step we have employed that ψ and ψ' lead to the same $\rho(\mathbf{r})$. Since ψ and ψ' also lead to the same $\mathbf{j}(\mathbf{r})$, we have on equating (6) and (10) that

$$\mathbf{A}'(\mathbf{r}) = \mathbf{A}(\mathbf{r}). \tag{11}$$

From the variational principle for the energy for a nondegenerate ground state,

$$E \;=\; <\psi|\hat{H}|\psi> \;\;<\;\; <\psi'|\hat{H}|\psi'>. \tag{12}$$

Now, in general

$$\begin{aligned} <\psi'|\hat{H}|\psi'> \;=\; & <\psi'|\hat{T}+\hat{U}+\hat{V}'+\int \hat{\mathbf{j}}'(\mathbf{r})\cdot\mathbf{A}'(\mathbf{r})d\mathbf{r} - \frac{1}{2}\int \hat{\rho}(\mathbf{r})A'^2(\mathbf{r})d\mathbf{r}|\psi'> \\ & + <\psi'|\hat{V}-\hat{V}'|\psi'> \\ & + <\psi'|\int[\hat{\mathbf{j}}(\mathbf{r})\cdot\mathbf{A}(\mathbf{r}) - \hat{\mathbf{j}}'(\mathbf{r})\cdot\mathbf{A}'(\mathbf{r})]d\mathbf{r}|\psi'> \\ & - \frac{1}{2}<\psi'|\int \hat{\rho}(\mathbf{r})[A^2(\mathbf{r}) - A'^2(\mathbf{r})]d\mathbf{r}|\psi'>. \end{aligned} \tag{13}$$

(This equation should replace Eq. (36) of [1]).

For ψ' real, employing Eq. (11) we see that the last term of Eq. (13) vanishes. Next

$$\begin{aligned} <\psi'|\hat{\mathbf{j}}(\mathbf{r})|\psi'> \;&=\; \mathbf{j}'_p(\mathbf{r}) + \rho'(\mathbf{r})\mathbf{A}(\mathbf{r}) \qquad (14)\\ &=\; \rho(\mathbf{r})\mathbf{A}(\mathbf{r}), \qquad (15) \end{aligned}$$

where we have employed Eq. (9) and that $\rho'(\mathbf{r}) = \rho(\mathbf{r})$. Thus,

$$<\psi'|\int \hat{\mathbf{j}}(\mathbf{r})\cdot\mathbf{A}(\mathbf{r})d\mathbf{r}|\psi'> = \int \rho(\mathbf{r})A^2(\mathbf{r})d\mathbf{r}. \tag{16}$$

Similarly,

$$\begin{aligned} <\psi'|\hat{\mathbf{j}}'(\mathbf{r})|\psi'> \;&=\; \mathbf{j}'_p(\mathbf{r}) + \rho'(\mathbf{r})A'(\mathbf{r}) \qquad (17)\\ &=\; \rho(\mathbf{r})A(\mathbf{r}), \qquad (18) \end{aligned}$$

where we have employed Eq. (9) and Eq. (11) and $\rho'(\mathbf{r}) = \rho(\mathbf{r})$. Consequently,

$$<\psi'|\int \hat{\mathbf{j}}'(\mathbf{r})\cdot\mathbf{A}'(\mathbf{r})d\mathbf{r}|\psi'> = \int \rho(\mathbf{r})A^2(\mathbf{r})d\mathbf{r}. \tag{19}$$

Thus, employing Eqs. (16) and (19), the term of Eq. (13)

$$< \psi'| \int [\hat{\mathbf{j}}(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r}) - \hat{\mathbf{j}}'(\mathbf{r}) \cdot \mathbf{A}'(\mathbf{r})] d\mathbf{r} |\psi' >= 0. \tag{20}$$

Therefore,

$$\begin{aligned} < \psi'|\hat{H}|\psi' > &= E' + \int \rho'(\mathbf{r})[v(\mathbf{r}) - v'(\mathbf{r})] d\mathbf{r} && (21) \\ &= E' + \int \rho(\mathbf{r})[v(\mathbf{r}) - v'(\mathbf{r})] d\mathbf{r}, && (22) \end{aligned}$$

since $\rho'(\mathbf{r}) = \rho(\mathbf{r})$. Thus, Eq. (12) is

$$E \ < \ E' + \int \rho(\mathbf{r})[v(\mathbf{r}) - v'(\mathbf{r})] d\mathbf{r}. \tag{23}$$

On interchanging the unprimed and primed quantities, we have

$$E' \ < \ E + \int \rho(\mathbf{r})[v'(\mathbf{r}) - v(\mathbf{r})] d\mathbf{r}, \tag{24}$$

so that on addition of Eqs. (22) and (23) we obtain the contradiction

$$E + E' < E + E'. \tag{25}$$

The original assumption that $\psi \neq \psi'$ is thus erroneous, and therefore $\psi = \psi'$. This means that

$$\rho(\mathbf{r})\Big|_{\psi} = \rho'(\mathbf{r})\Big|_{\psi'}. \tag{26}$$

However, the corresponding physical current densities are *not* the same:

$$\mathbf{j}(\mathbf{r})\Big|_{\psi} \neq \mathbf{j}'(\mathbf{r})\Big|_{\psi'}, \tag{27}$$

because $\mathbf{A}(\mathbf{r}) \neq \mathbf{A}'(\mathbf{r})$. This proves that the original assumption that there exists a $\{v', \mathbf{A}'\}$ that leads to the same $\{\rho, \mathbf{j}\}$ as that due to $\{v, \mathbf{A}\}$ is incorrect. *This is the step which takes into account that there could exist many $\{v, \mathbf{A}\}$ that lead to the same nondegenerate ground state ψ.* Hence, there exists only one $\{v, \mathbf{A}\}$ that leads to a $\{\rho, \mathbf{j}\}$. The bijectivity of Eq. (1) is therefore proved. We conclude by reiterating that in the presence of a magnetostatic field $\mathbf{B}(\mathbf{r})$, the relationship between $\{v, \mathbf{A}\}$ and ψ can be many-to-one. Our proof of bijectivity explicitly takes into consideration this possibility.

For the case when ψ is complex, with the same original assumptions that ψ and ψ' lead to the same $\rho(\mathbf{r})$ we have

$$< \psi'|\hat{\mathbf{j}}(\mathbf{r})|\psi' > \; = \; \mathbf{j}'_p(\mathbf{r}) + \rho(\mathbf{r})\mathbf{A}(\mathbf{r}). \tag{28}$$

and

$$< \psi'|\hat{\mathbf{j}}'(\mathbf{r})|\psi' > \; = \; \mathbf{j}'_p(\mathbf{r}) + \rho(\mathbf{r})\mathbf{A}'(\mathbf{r}). \tag{29}$$

Therefore

$$< \psi'|\int \hat{\mathbf{j}}(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r})d\mathbf{r}|\psi' > \; = \; \int \mathbf{j}'_p(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r})d\mathbf{r} + \int \rho(\mathbf{r})A^2(\mathbf{r})d\mathbf{r}, \tag{30}$$

and

$$< \psi'|\int \hat{\mathbf{j}}'(\mathbf{r}) \cdot \mathbf{A}'(\mathbf{r})d\mathbf{r}|\psi' > \; = \; \int \mathbf{j}'_p(\mathbf{r}) \cdot \mathbf{A}'(\mathbf{r})d\mathbf{r} + \int \rho(\mathbf{r})A'^2(\mathbf{r})d\mathbf{r}, \tag{31}$$

so that in Eq. (13) the term

$$\begin{aligned} &< \psi'|\int [\hat{\mathbf{j}}(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r}) - \hat{\mathbf{j}}'(\mathbf{r}) \cdot \mathbf{A}'(\mathbf{r})]d\mathbf{r}|\psi' > \\ &= \int \mathbf{j}'_p(\mathbf{r}) \cdot [\mathbf{A}(\mathbf{r}) - \mathbf{A}'(\mathbf{r})]d\mathbf{r} + \int \rho(\mathbf{r})[A^2(\mathbf{r}) - A'^2(\mathbf{r})]d\mathbf{r}. \end{aligned} \tag{32}$$

Finally, employing again that $\rho'(\mathbf{r}) = \rho(\mathbf{r})$,

$$\begin{aligned} &\frac{1}{2} < \psi'|\int \hat{\rho}(\mathbf{r})[A^2(\mathbf{r}) - A'^2(\mathbf{r})]d\mathbf{r}|\psi' > \\ &\qquad = \frac{1}{2}\int \rho(\mathbf{r})[A^2(\mathbf{r}) - A'^2(\mathbf{r})]d\mathbf{r}. \end{aligned} \tag{33}$$

Hence, in the general case of ψ complex,

$$\begin{aligned} E < E' + \int \rho(\mathbf{r})[v(\mathbf{r}) - v'(\mathbf{r})]d\mathbf{r} \; &+ \; \int \mathbf{j}'_p(\mathbf{r}) \cdot [\mathbf{A}(\mathbf{r}) - \mathbf{A}'(\mathbf{r})]d\mathbf{r} \\ &+ \; \frac{1}{2}\int \rho(\mathbf{r})[A^2(\mathbf{r}) - A'^2(\mathbf{r})]d\mathbf{r}. \end{aligned} \tag{34}$$

On interchanging the primed and unprimed quantities,

$$\begin{aligned} E' < E + \int \rho(\mathbf{r})[v'(\mathbf{r}) - v(\mathbf{r})]d\mathbf{r} \; &+ \; \int \mathbf{j}_p(\mathbf{r}) \cdot [\mathbf{A}'(\mathbf{r}) - \mathbf{A}(\mathbf{r})]d\mathbf{r} \\ &+ \; \frac{1}{2}\int \rho(\mathbf{r})[A'^2(\mathbf{r}) - A^2(\mathbf{r})]d\mathbf{r}. \end{aligned} \tag{35}$$

On adding Eq. (34) and Eq. (35) one obtains

$$E + E' < E + E' + \int [\mathbf{j}'_p(\mathbf{r}) - \mathbf{j}_p(\mathbf{r})] \cdot [\mathbf{A}(\mathbf{r}) - \mathbf{A}'(\mathbf{r})]d\mathbf{r}. \tag{36}$$

It is evident from Eq. (36) that since by assumption $\psi \neq \psi', \mathbf{j}'_p(\mathbf{r}) \neq \mathbf{j}_p(\mathbf{r})$, that $\mathbf{j}'_p(\mathbf{r}) - \mathbf{j}_p(\mathbf{r}) \neq 0$. Further, by assumption $\mathbf{A}(\mathbf{r}) \neq \mathbf{A}'(\mathbf{r})$. Thus, the term of Eq. (36)

$$\int [\mathbf{j}'_p(\mathbf{r}) - \mathbf{j}_p(\mathbf{r})] \cdot [\mathbf{A}(\mathbf{r}) - \mathbf{A}'(\mathbf{r})] d\mathbf{r} \neq 0. \tag{37}$$

It is evident that the *reductio ad absurdum* argument is not applicable. Eq. (36) may be rewritten as follows. From Eqs. (4) and Eq. (8) (with $\rho'(\mathbf{r}) = \rho(\mathbf{r})$, and $\mathbf{j}'(\mathbf{r}) = \mathbf{j}(\mathbf{r})$) we have

$$\mathbf{j}_p(\mathbf{r}) = \mathbf{j}(\mathbf{r}) - \rho(\mathbf{r})\mathbf{A}(\mathbf{r}) \tag{38}$$

and

$$\mathbf{j}'_p(\mathbf{r}) = \mathbf{j}(\mathbf{r}) - \rho(\mathbf{r})\mathbf{A}'(\mathbf{r}), \tag{39}$$

so that

$$\mathbf{j}'_p(\mathbf{r}) - \mathbf{j}_p(\mathbf{r}) = \rho(\mathbf{r})[\mathbf{A}(\mathbf{r}) - \mathbf{A}'(\mathbf{r})]. \tag{40}$$

Substituting Eq. (40) into Eq. (36) leads to the alternate expression

$$E + E' < E + E' + \int \rho(\mathbf{r})[\mathbf{A}(\mathbf{r}) - \mathbf{A}'(\mathbf{r})]^2 d\mathbf{r}. \tag{41}$$

Again, since by assumption $\mathbf{A}(\mathbf{r}) \neq \mathbf{A}'(\mathbf{r})$, the last term of Eq. (40) does not vanish. Eq. (41) is equivalent to Eq. (72) of Tellgren et al [3]. (Our error in [1] was that in the present Eq. (13) we assumed the equivalence of $< \psi'|\hat{\mathbf{j}}(\mathbf{r})|\psi' >$ and $< \psi'|\hat{\mathbf{j}}'(\mathbf{r})|\psi' >$, or equivalently that the physical current density operator was unique, *i.e.* $\hat{\mathbf{j}}(\mathbf{r}) = \hat{\mathbf{j}}'(\mathbf{r})$. This then led to the erroneous Eq. (38) of [1].)

Finally, we note that although our proof that $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$ are the basic variables is restricted to the case of ψ real, our conclusion based on reasons given in [1, 10] that $\{\rho(\mathbf{r}), \mathbf{j}_p(\mathbf{r})\}$ cannot be the basic variables remains unchanged [11, 12]. This conclusion is further buttressed by the fact that for ψ real, $\mathbf{j}_p(\mathbf{r}) = 0$. We reiterate [2] that in any 'density' functional theory, it is imperative to first prove a bijective relationship between the basic variables and the external potentials (for the nondegenerate ground state). Only then can one claim that the wave function is a functional of the basic variables as are the expectation values of all operators. This then also makes possible the mapping to model systems of noninteracting fermions or bosons with the same values of the basic variables as those of the interacting system. As noted earlier, the ground state wave function ψ of the Hooke's atom in a magnetostatic field is real. We have constructed [8] via quantal density functional theory [13] a system of noninteracting fermions that reproduces the $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$ of this atom.

In conclusion, there exists a one-to-one relationship between $\{\rho, \mathbf{j}\}$ and $\{v, \mathbf{A}\}$ for ψ real, and thus within this domain, the basic variables are $\{\rho, \mathbf{j}\}$, and $\psi = \psi[\rho, \mathbf{j}]$. Thus, the expectation of all operators are unique functionals of $\{\rho, \mathbf{j}\}$. As pointed out in [3], $\{\rho, \mathbf{j}\}$ are also the basic variables for one-electron systems.

In their work, employing convex analysis in conjunction with the Lieb [14] constrained-search density matrix functional, Tellgren *et al* [3] conclude, however, that "the most common formulation in terms of $\{\rho, \mathbf{j}_p\}$ is presently the most convenient and viable formulation of CDFT." Although our paper is not a Comment on their work, we make a few brief remarks to put their work in context. The conclusion of Tellgren *et al* is predicated on the following: (a) The assumption that the basic variables in CDFT are $\{\rho, \mathbf{j}_p\}$. Although they state that "In particular, Pan and Sahni have gone far in arguing that the paramagnetic current density, in some sense, cannot correctly be regarded as a basic CDFT variable", they do not address our critique [1, 10] of the Vignale-Rasolt proof [15] that this cannot be the case. (b) Their "basic potentials" in formulating the Lieb functional CDFT are not the external potentials $\{v, \mathbf{A}\}$ but rather $\{u, \mathbf{A}\}$, where $u = v + \frac{1}{2}A^2$. Again, in this new formulation, they *assume* the "basic densities" to be $\{\rho, \mathbf{j}_p\}$. They acknowledge that their "perspective differs from that by Pan and Sahni, who restrict the term *basic variable* to variables that admit an HK (Hohenberg-Kohn [9]) theorem." Our point of view [2] is that it is only after one proves certain gauge invariant properties to be basic variables in the rigorous HK sense that the constrained-search framework is possible. (c) In studying the Lieb functional formulation in terms of the basic densities $\{\rho, \mathbf{j}\}$, they treat the external vector potential $\mathbf{A}(\mathbf{r})$ as a variable. They state that "The constrained-search approach to CDFT with the physical current as the basic variable is substantially complicated by the fact that a wave function does not determine the physical current." In other words, the wave function depends upon the choice of $\mathbf{A}(\mathbf{r})$. We note, however, that in any Rayleigh-Ritz or constrained-search variational calculation, the choice of external potentials $\{v, \mathbf{A}\}$, and thereby the Hamiltonian $\hat{H}$, must remain *fixed* throughout the variational procedure. This is the only way in which a minimum or infimum can be achieved. (Note that the constrained-search procedure is a consequence of application of the Rayleigh-Ritz variational principle. Hence, the constrained-search must be performed with fixed $\{v, \mathbf{A}\}$. Additionally, the constrained-search requires the *a priori* knowledge of the basic variables $\{\rho, \mathbf{j}\}$. As such there is an *implicit* dependence on the external potentials. This follows from the bijective relationship between the external potentials and basic variables. Thus, the constrained-search is intrinsically connected to the specific physical system of interest as defined by the external potentials, in spite of the fact that one is minimizing the expectation value of the operators $\hat{T} + \hat{U}$. (See [2] for further discussion.) Thus, any variational wave function ψ not only determines $\mathbf{j}_p(\mathbf{r})$ but also determines $\mathbf{j}(\mathbf{r})$ since $\mathbf{A}(\mathbf{r})$ is known. For an example of the variational procedure where the external electromagnetic potentials are kept fixed in a Percus-Levy-Lieb functional [14, 16] as taken from time-dependent CDFT in which the basic variables are $\{\rho(\mathbf{r}t), \mathbf{j}(\mathbf{r}t)\}$, see the work of Ghosh-Dhara [17]. The presence of a solely magnetostatic field constitutes a special case.

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