Comment on "Quantum Mechanics in Metric Space: Wave Functions and their Densities"

In a recent Letter, D'Amico *et al.* [1] report a positive correlation between two distances defined for quantum-mechanical N-particle systems, one among wave functions, the other among their particle densities, thereby offering a very interesting new perspective on density functional theory. Given states $|1\rangle$ and $|2\rangle$ and their corresponding real and positive-defined particle densities $\rho_1(\mathbf{x})$ and $\rho_2(\mathbf{x})$ ($\mathbf{x}$ indicates position and spin), the distance between states is defined [2] as

$$D(1|2) = \sqrt{\langle 1|1\rangle + \langle 2|2\rangle - 2|\langle 1|2\rangle|} \tag{1}$$

and the one between their densities they define as

$$D_\rho(1|2) = \int |\rho_1(\mathbf{x}) - \rho_2(\mathbf{x})| d\mathbf{x}. \tag{2}$$

If normalizing densities to N and states to $\sqrt{N}$, the metric spaces arising through these distances are argued to display an onionlike structure, the different onion shells corresponding to the different values of N, growing from $N = 0$ at the center (see Fig. 1 in [1]).

Within a given N shell the mentioned correlation is less general than apparent in Ref. [1]. For $N = 1$ any two plane waves are maximally distant wave-functions and have minimally distant densities. For large N, the dimension of configuration space makes the largest distances exponentially more likely for wave functions than for densities. The D_ρ vs D curves would thus tend to a step function, as indeed observed in Fig. 2(c) of [1] for ground states of model Hamiltonians [3] with up to $N = 8$. If a metric could be defined from $D^{1/N}$ it might recover a significant correlation with D_ρ for larger N. As it stands it should be useful for few-particle systems.

For different values of N the case rests on two points: (i) If defining vacuum at the onion center as $\Psi = 0$ and $\rho(\mathbf{x}) = 0$ in each metric space, the distance from any N state to the center is $\sqrt{N}$, and N for its density. (ii) The "minimum distance" between states with different N values is *defined* as $|\sqrt{N} - \sqrt{N'}|$, and as $|N - N'|$ for the densities. We show here that the intershell aspect of the onion paradigm is valid for the density (actually a stronger case than originally stated), while it is not so for Fock space. Starting with the density, the fact that $\rho(\mathbf{x}) = 0$ for $N = 0$ is easy to validate, since $\rho(\mathbf{x})$ is a function defined on the same $\mathbf{x}$ space for any N, trivially extending to $\rho(\mathbf{x}) = 0$ (e.g. $\rho(\mathbf{x}) = \langle \Psi|\psi^\dagger(\mathbf{x})\psi(\mathbf{x})|\Psi\rangle$, with the ψ's as the relevant field operators, and $|\Psi\rangle$ any N-particle state, including the vacuum state).

The second supporting argument as stated in Ref. [1] is weak, since the minimal distance for densities in different N shells is defined irrespective of Eq. (2). It is easy to see, however, that the minimal distance for densities for N and M particles is $|N - M|$ as a direct consequence of the original definition in Eq. (2) extended to variable N. Taking $N > M$, the minimal distance between a N density and a M density, $D_\rho(1^N|2^M)$, happens when $\rho_1^N(\mathbf{x}) \geq \rho_2^M(\mathbf{x})$ everywhere, in which case $D_\rho(1^N|2^M) = N - M$ exactly (the argument also holds for $N = M$, for which the condition $\rho_1^N(\mathbf{x}) \geq \rho_2^M(\mathbf{x})$, $\forall\, \mathbf{x}$ is only fulfilled if both densities are equal everywhere). The density onion case is further supported by the authors' argument that maximum distance occurs for locally nonoverlapping densities ($\rho_1(\mathbf{x})\rho_2(\mathbf{x}) = 0$, $\forall\, \mathbf{x}$). It generalizes trivially to $N \neq M$, giving $D_\rho(1^N|2^M) = N + M$, consistent with the onion. D_ρ varies smoothly from $|N - M|$ to $N + M$.

Now for interstate distances [Eq. (1)] among different shells. If considering states with well defined particle number, Eq. (1) yields $D(1^N|2^M) = \sqrt{N + M}$. This is actually consistent with the onion picture as the maximum distance between states with N and M particles: In the hemispheric picture of Fig. 1(b) of Ref. [1] the maximum distance is that between a state in the pole and a state in the equator, which, for spheres of radii $\sqrt{N}$ and $\sqrt{M}$, gives precisely $\sqrt{N + M}$. It furthermore confirms the radius of the sphere to $\sqrt{N}$, by taking $M = 0$. The problem is that $\sqrt{N + M}$ is the distance for *any* two states of N and M particles, very much against the onion-shell paradigm, and in contradiction with their definition of a minimal distance of $|\sqrt{N} - \sqrt{M}|$. Alternative definitions to Eq. (1) could be built by substituting $|\langle 1|2\rangle|$ by a (suitably normalized) expression like (for $N_1 = N_2 + 1$):

$$\min_\phi |\langle 1|c_\phi^\dagger|2\rangle|, \quad \text{with} \quad c_\phi^\dagger = \int d\mathbf{x}\, \phi(\mathbf{x})\psi^\dagger, \tag{3}$$

for any 1-particle wave function $\phi(\mathbf{x})$. D then takes values between $\sqrt{|N_1 - N_2|}$ and $\sqrt{N_1 + N_2}$. As it stands, however, the wave-function metric based on Eq. (1) is inconsistent with the onion geometry.

Emilio Artacho
Department of Earth Sciences
University of Cambridge
Downing Street, Cambridge CB2 3EQ, United Kingdom

Received 25 February 2011; published 27 October 2011
DOI: 10.1103/PhysRevLett.107.188901
PACS numbers: 03.65.−w, 03.67.−a, 31.15.ec, 71.15.Mb

[1] I. D'Amico, J. P. Coe, V. V. França, and K. Capelle, Phys. Rev. Lett. **106**, 050401 (2011).
[2] L. Longpré and V. Kreinovich, Int. J. Theor. Phys. **47**, 814 (2007).
[3] The set of ground states is incorrectly said not to be a Hilbert space: any $|\Psi\rangle$ in a Hilbert space is the ground state of some operator (take $\hat{H} = -|\Psi\rangle\langle\Psi|$). The set of ground states of an arbitrary set of Hamiltonians conforms to the arguments of the authors.

