Quantum Mechanics in Metric Space: Wave Functions and Their Densities

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Hilbert space combines the properties of two different types of mathematical spaces: vector space and metric space. While the vector-space aspects are widely used, the metric-space aspects are much less exploited. Here we show that a suitable metric stratifies Fock space into concentric spheres on which maximum and minimum distances between states can be defined and geometrically interpreted. Unlike the usual Hilbert-space analysis, our results apply also to the reduced space of only ground states and to that of particle densities, which are metric, but not Hilbert, spaces. The Hohenberg-Kohn mapping between densities and ground states, which is highly complex and nonlocal in coordinate description, is found, for three different model systems, to be simple in metric space, where it becomes a monotonic and nearly linear mapping of vicinities onto vicinities.

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It is a fundamental tenet of quantum mechanics that the space of the proper wave functions of an N-particle quantum system is a Hilbert space: a complete vector space of (complex) functions among which a scalar product is defined [1]. Mathematically, a Hilbert space combines the properties of two fundamentally different types of spaces: a vector space and a metric space. In short, a vector space is one in which linear combinations of its elements can be formed, while a metric space is one in which to each two elements one can assign a distance.

The vector-space aspects of Hilbert space are widely known, and routinely exploited in quantum mechanics. Wave functions are added, and multiplied by real or complex numbers, to form new wave functions, and the degree of similarity of two wave functions is measured by their overlap, which in turn is obtained from their scalar product. Much less exploited in quantum mechanics are the metric-space aspects of Hilbert space. In the present Letter we explore the space of quantum-mechanical wave functions from the point of view of metric spaces, in which the similarity of two wave functions is characterized by a suitable metric (a measure of distance [2]).

Our analysis reveals several deep and useful properties of wave functions that are obfuscated by the more common analysis in terms of vector spaces and scalar products. Notably, ground-state (GS) wave functions on their own do not form a Hilbert space, while they still *do* form a metric space. Similarly, particle densities do not form a Hilbert space but another metric space. (These affirmations are explained and proven below.) The characterization of the set of GS wave functions and densities as metric spaces also provides a new perspective on the Hohenberg-Kohn one-to-one mapping between GS wave functions and their densities.

This Letter has three parts. In the first part we describe the geometry of the space of wave functions and their densities from the viewpoint of metric space. In the second part we focus on the special case of GS wave functions. In the last part we present results from numerical investigations of three model systems, illustrating and corroborating our analytical considerations.

1. Geometry of the space of wave functions and their densities.—We adopt the convention that the N-particle wave function is normalized to the total particle number [3] and define the distance between any two N-particle wave functions as

$$D_\psi(\psi_1, \psi_2) = \min_\phi \tilde{D}_\psi(\psi_1, \psi_2) \tag{1}$$

$$= \min_\phi \sqrt{\int |\psi_1(\boldsymbol{x}) - \psi_2(\boldsymbol{x})|^2 d\boldsymbol{x}} \tag{2}$$

$$\sqrt{\int (|\psi_1|^2 + |\psi_2|^2) d\boldsymbol{x} - 2\left|\int \psi_1^* \psi_2 d\boldsymbol{x}\right|}. \tag{3}$$

where $\boldsymbol{x} = (x_1, \ldots, x_N)$ represents spatial and spin coordinates, in any dimensionality, and the phase ϕ is defined through $\int \psi_1^* \psi_2 d\boldsymbol{x} = e^{i\phi} |\int \psi_1^* \psi_2 d\boldsymbol{x}|$ [4].

Such a distance has been used for wave functions previously [5] and can be identified as a special case of the Bures distance [6] applied to pure states [7]. In particular, the triangular inequality

$$D_\psi(\psi_1, \psi_2) \leq D_\psi(\psi_1, \psi_3) + D_\psi(\psi_3, \psi_2) \tag{4}$$

is satisfied, and the space of all wave functions, with this measure of distance, becomes a metric space [2].

Wave functions differing only by a constant phase are assigned distance zero by the metric (2). Without the minimization over ϕ, the distance between two wave functions differing only by a constant phase, ψ_1 and $\psi_2 = \psi_1 e^{i\phi}$, would be $\tilde{D}_\psi(\psi_1, \psi_2) = 2\sqrt{N}|\sin(\phi/2)|$, which also satisfies the mathematical requirements for a metric, but as a function of ϕ takes on any value from 0 to $2\sqrt{N}$. The alternative measure of distance $\tilde{D}_\psi$ thus discriminates between different gauge copies of the same wave function, which is unphysical.

The density of an N-particle wave function is

$$\rho(x) = \int |\psi(x, x_2, \ldots, x_N)|^2 dx_2 \cdots dx_N, \tag{5}$$

where $\int \rho(x)dx = N$. We define the distance between any two densities as

$$D_\rho(\rho_1, \rho_2) = \int \sqrt{|\rho_1(x)|^2 + |\rho_2(x)|^2 - 2\rho_1(x)\rho_2(x)}dx, \tag{6}$$

which satisfies the triangular inequality

$$D_\rho(\rho_1, \rho_2) \leq D_\rho(\rho_1, \rho_3) + D_\rho(\rho_3, \rho_2). \tag{7}$$

With this definition, the space of all densities forms a metric space [2], although densities do not form a vector space, and much less a Hilbert space.

Definitions (2) and (6) are derived in the standard way from the characteristic norm of the quantities of interest and determine the geometry of wave function and density spaces, without making use of Hilbert-space concepts such as scalar products or linear combinations. From Eq. (6) it follows that all densities integrating to the same fixed number N of particles lie in density space on a sphere of radius N, centered at the zero-density function $\rho^{(0)}(x) \equiv 0$, because $D_\rho(\rho, \rho^{(0)}) = N$. Similarly, from Eq. (2) it follows that all N-particle wave functions lie in wave function space on spheres of radius $\sqrt{N}$ centered at the zero-wave-function $\psi^{(0)} \equiv 0$. Both the space of all densities and the space of all wave functions can thus be visualized as concentric spheres, i.e., an onion-shell-like geometry, illustrated in Fig. 1. The direct sum of all N-particle Hilbert spaces is frequently denoted Fock space. From the metric point of view, Fock space is thus stratified into an infinite number of concentric spheres, each of which represents an N-particle metric space.

An upper bound to the maximum distance between two N-particle densities can be deduced from the normalization together with the triangular inequality (7), by taking $\rho_3 = \rho^{(0)}$:

$$D_\rho(\rho_1, \rho_2) \leq D_\rho(\rho_1, \rho^{(0)}) + D_\rho(\rho^{(0)}, \rho_2) = 2N, \tag{8}$$

which is in agreement with the radius of the sphere being N. This upper bound is attained in the limiting case of nonoverlapping densities. This can be seen from Eq. (6) by noting that $\rho_1(x)\rho_2(x) \geq 0$, and that the maximum of the right-hand side is obtained when $\rho_1(x)\rho_2(x) \equiv 0$, so that $D_\rho^{\max} = \int \rho_1(x)dx + \int \rho_2(x)dx = 2N$. Maximally distant densities are thus found to be nonoverlapping densities.

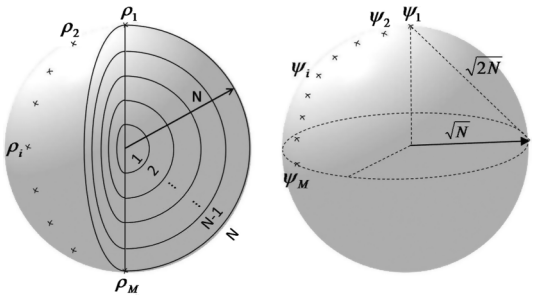

FIG. 1. Sketch of the metric spaces for particle densities (left) and wave functions (right). The onion-shell-like geometry is explicitly displayed for the particle densities. One set of particle densities and one of wave functions are presented: their distance from the reference state—at the north pole—increases with their labeling index, up to maximum distance.

Interestingly, for wave functions the situation is not that simple. We can deduce a similar upper bound to the distance between two N-particle wave functions from the triangular inequality (4), taking $\psi_3 = \psi^{(0)}$:

$$D_\psi(\psi_1, \psi_2) \leq D_\psi(\psi_1, \psi^{(0)}) + D_\psi(\psi^{(0)}, \psi_2) = 2\sqrt{N}, \tag{9}$$

which is in agreement with the radius of the sphere being $\sqrt{N}$. However from Eq. (3) it is clear that the maximum distance between two N-particle wave functions is reached for nonoverlapping functions, and is $\sqrt{2N}$. The upper bound coming from the triangular inequality is thus not attained if distances between wave functions are measured by D_ψ. By contrast, if measured by the alternative metric $\tilde{D}_\psi$ (which assigns nonzero distance to wave functions differing by a constant phase), the maximum distance of $2\sqrt{N}$ is reached for $\phi = \pi$, i.e., for ψ and $-\psi$.

This situation has a simple geometric interpretation, illustrated in Fig. 1. Start with some arbitrary wave function ψ on the N-particle sphere and call it the north pole. The distance D_ψ from the north pole to any wave function that does not overlap with it is the locus of points on the sphere at linear distance $\sqrt{2N}$. Since the diameter of the sphere is $2\sqrt{N}$ and $\cos\alpha = \sqrt{2N}/(2\sqrt{N})$ implies $\alpha = \pi/4$, this locus is the equator. According to $\tilde{D}_\psi$, on the other hand, the wave function that is maximally distant from the north pole is just $-\psi$, i.e., the south pole [8]. The geometrically intuitive interpretation of maximum distance from the north pole is thus only recovered if gauge copies of the initial wave function are considered to be distinct wave functions, which is unphysical. The same characterization of maximally distant wave functions according to D_ψ (at the equator) and maximally distant wave functions according to $\tilde{D}_\psi$ (at the south pole) holds for any arbitrary wave function taken to be the north pole, and repeats itself on any of the infinite number of concentric spheres in wave function metric space [9].

The minimal distance among wave functions (or densities) with same N is obviously zero. According to Eqs. (2) and (6) distances between wave functions or densities with different numbers of particles are not defined in general. We can, however, define a ''minimal'' distance as the difference between the radii of the corresponding spheres, i.e. $D_\rho^{\min}(\rho^N, \rho^{N'}) := |N - N'|$ and $D_\psi^{\min}(\psi^N, \psi^{N'}) := |\sqrt{N} - \sqrt{N'}|$. In particular, the ''minimal'' distance between an N and an $N + 1$ particle density is 1 for all N, while that between the corresponding wave functions is $\sqrt{N+1} - \sqrt{N}$, which goes to zero for large N. In this sense, densities provide a better resolution for quantifying distances between large systems than wave functions, which is a very interesting property in view of the other advantages densities have over wave functions for large systems [10].

2. Geometry of the space of ground-state wave functions.—All of the above applies to any proper wave function of a nonrelativistic N-body quantum system. In the remainder of this Letter we take a closer look at what may be the most important subset of wave functions, namely, those describing ground states.

One key property of a vector space is that it is closed with respect to any possible linear combination, i.e., its elements can be summed, and multiplied by scalars, and the result of these operations is still an element of the same space. This property is fundamental for quantum mechanics, where linear combinations of wave functions abound. We note, however, that *ground-state* wave functions on their own do not satisfy this requirement: the sum of two GS wave functions is guaranteed to be another wave function, but not necessarily another GS wave function. Hence, the set of all GS wave functions *is not a vector space*, much less a Hilbert space. Nevertheless, it is still a metric space, and all of our above considerations apply just as well when restricted to ground states even if degenerate.

The metric-space viewpoint also sheds new light on the famous mapping between GS wave functions and their densities, whose existence is the content of the Hohenberg-Kohn (HK) theorem [11]. Since GS wave functions by themselves do not form a Hilbert space, this mapping can be considered as one between mere sets, i.e., structureless collections of objects. We have just seen, however, that both GS wave functions and densities form spaces with a metric structure. This metric structure can be used to further analyze the density-wave function mapping.

By Eq. (5), a wave function uniquely determines its density. The inverse is much less trivial, and actually is the content of the HK theorem: to each GS density corresponds a unique GS wave function in Eq. (5). Since any metric $D(x, y)$ satisfies $D(x, y) = 0 \Leftrightarrow x = y$, the HK theorem implies that GS wave functions with nonzero distance are mapped onto densities with nonzero distance.

Because of the enormous complexity of the HK $\psi - \rho$ mapping (which is highly nonlinear and nonlocal in coordinate description) and the endless variety of possible functions it connects, analytical results on the geometry and topology of the mapping are very hard to obtain. However, further progress can be made by numerical calculations for model systems.

3. Numerical calculations—In this last part of the Letter we consider three different nontrivial model systems, taken from different realms of quantum mechanics: the one-dimensional Hubbard model, the Helium isoelectronic series, and a parabolically confined two-electron system (sometimes known as Hooke's atom). For each of these we calculate numerically highly precise or analytical GS wave functions and densities, and investigate how a change from one wave function to another affects the corresponding densities. To this end we adopt one or few states of each system as a reference state and then vary some system parameters (atomic number Z for the He atom, the frequency ω of the confining potential for parabolic confinement, and the frequency ω of the confining potential for different particle numbers N and interactions U for the Hubbard model). This variation produces paths on the respective metric spheres, i.e., families of GS wave functions and densities, the distance of which from the reference states we quantify by the respective metrics. We then calculate D_ρ as a function of D_ψ, as the system parameters are varied (see Fig. 2).

The HK theorem guarantees that the graph of D_ρ as a function of D_ψ starts with positive slope at the origin (where $D_\psi = D_\rho = 0$) and then never reaches the horizontal (D_ψ) axis again. For nonzero D_ψ, the curves display various additional remarkable features that are not automatic consequences of the HK theorem.

First, in all investigated systems the initial slope is ≤ 45 degrees, because the density is an integrated functional of the wave function, and as such D_ρ should be affected at most as much as D_ψ by a small change in the wave function. Also, the slope remains positive for the entire range of D_ψ, i.e., all curves increase monotonically. At least for these three systems, the HK mapping thus consistently maps nearby densities onto nearby wave functions, and distant densities onto distant wave functions.

Second, after starting at the origin, the density distance does not only increase monotonically as a function of the wave function distance, but even almost linearly. In this sense, the HK mapping is as simple as it could be: an increase in the distance between two densities is followed by a proportional increase in the distance between the two wave functions associated with the densities via the HK theorem. This near linearity has apparently not been noted, and much less exploited, in the literature on density-functional theory or on quantum mechanics.

Third, this linearity persists up to values of D_ψ that are close to the maximum possible distance of $\sqrt{2N}$, derived above. Only for wave functions that are close to maximally distant (i.e., nearly nonoverlapping, according to our above analysis) do the corresponding density distances depart from linearity and grow rapidly towards their own

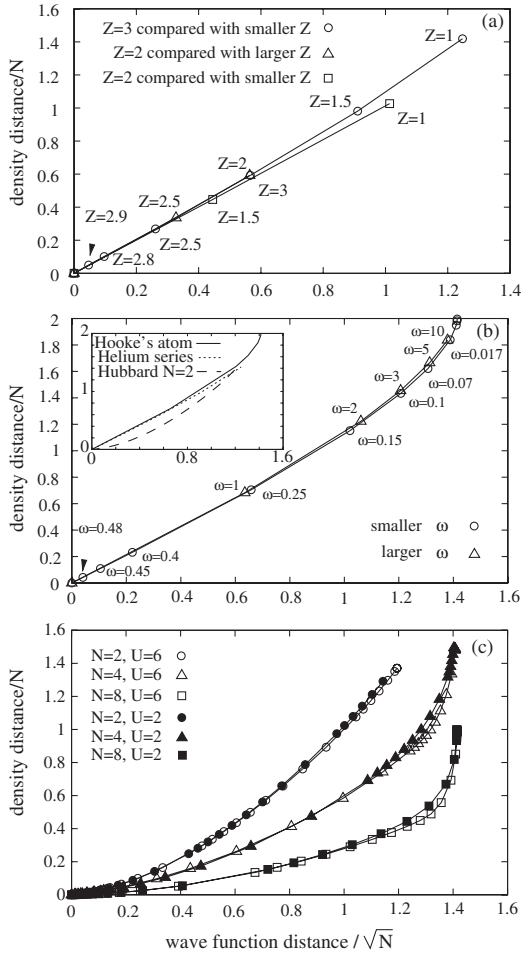

FIG. 2. Density distance vs wave function distance. (a) Helium-like atoms. The reference systems have $Z = 3$ (circles, decreasing Z) and $Z = 2$ (triangles for increasing Z and squares for decreasing Z). (b) Hooke's atom. The reference system has $\omega = 0.5$ (triangles for increasing ω and circles for decreasing ω). (c) Hubbard model. The reference system has $\omega = 4$, and is compared with smaller ω systems with 8 sites and different particle numbers (circles for $N = 2$, triangles for $N = 4$ and squares for $N = 8$) and interactions (filled symbols for $U = 2$ and unfilled for $U = 6$).

maximum value $D_\rho^{\max} = 2N$. In this region a small increase in the distance between two wave functions can produce a large increase in the distance between the two densities. Densities thus appear to be a rather suitable diagnostic tool for distinguishing wave functions, although much explicit information contained in the wave functions is integrated out when calculating the density.

Finally, we note that curves for $N = 2$ in different model systems can be almost superimposed onto each other [see inset of Fig. 2(b)], which hints at universality across different systems in the shape of the mapping. For larger N a similar universality is also suggested by the Hubbard model [Fig. 2(c)], since the mapping is essentially the same for different interactions.

The metric viewpoint can be applied anywhere in quantum mechanics. It could help, e.g., in testing approximate density functionals, which should reproduce the near linearity of the HK mapping. In variational calculations, the existence of a suitable measure of distance between wave functions may complement work such as that of Ref. [12] and help in choosing better trial functions. Another use is in the development of order (N) methods for electronic-structure calculations, as our results show that, for large N, densities provide better resolution for distinguishing physical systems than wave functions. Our findings on the distance between wave functions may complement the use of the fidelity[13] in quantum information theory and in the study of quantum phase transitions. In conclusion, we emphasize that the metric and the vector-space viewpoints are complementary, and that only together do they exhaust the full richness of Hilbert space.

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[8] For $N = 1$ our sphere does not reduce to the Bloch sphere representation of single qubits as defined in quantum information theory, as there orthogonal states reside at the opposite poles of the sphere.
[9] When the N-body wave function is normalized to 1 instead of to N, all these concentric spheres collapse to just one sphere, representing all of Fock space. The maximum distance between any two wave functions becomes 2 (the diameter of that sphere) and that between two nonoverlapping wave functions becomes $\sqrt{2}$. We prefer to normalize to N, because this allows us to split Fock space into subspaces defined by a constant particle number, each subspace being represented by its own sphere, and because in this way the geometry of the metric space of all wave functions is the same as that of the metric space of all densities, i.e., concentric spheres.
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