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REGULAR ARTICLE

Toward a fuzzy atom view within the context of the quantum theory of atoms in molecules: quasi-atoms

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Abstract The notion of quasi-atoms is introduced within the context of the quantum theory of atoms in molecules. Being a subset of the quantum divided basins that were introduced previously, quasi-atoms are the quantum subsystems that are practically indistinguishable from the topological atoms; thus, revealing the continuous evolution of quantum divided basins into topological atoms. This indistinguishability is rooted in the limited accuracy of chemical observations; they are not sensitive to discriminate a topological atom from its associated quasi-atoms. In this regard, it is disclosed that the set of quantum atoms is in a wide-range including members other than topological atoms; the quasi-atoms are concrete examples. Finally, the idea of the fuzzy set of atoms that is foreign to the disjoint partitioning schemes for which the orthodox QTAIM is a classic example is extended employing the set of quasi-atoms.

Keywords Real space quantum subsystems · Quantum theory of atoms in molecules · Quantum divided basins · Fuzzy atoms · Topological atoms

1 Introduction

In a recent study, a new set of real space quantum subsystems termed the quantum divided basins (QDB) was scrutinized [1]. They emerged as a result of our ongoing investigations [2–6] on the foundations of the quantum theory of atoms in molecules (QTAIM) [7, 8]. This set of subsystems includes all 3D regions satisfying the net zero-flux equation, $\int_{\Omega}\nabla^2\rho(r)\mathrm{d}\tau = 0$, except from those of the topological atoms that are the orthodox objects within the context of the QTAIM. In this regard, a general framework namely the quantum theory of proper open subsystems (QTPOS) was devised to study these novel objects [1]. Whereas a subset of the QDB, namely the bundles, was considered previously by different authors [9–12], the set of QDB generally contains diverse and sometimes bizarre objects [1], Fig. 1. The morphology of these objects is completely different from that of the set of the topological atoms; thus, based on the reported computational results, it seems that there is a clear distinction between the members of these two sets. However, in contrast to all previous reports, this letter presents a subset of QDB that is practically indistinguishable from the topological atoms. This subset is termed quasi-atoms (QA); the 3D regions derived from the net zero-flux equation that does not satisfy the local zero-flux equation, $\vec{\nabla}\rho(r)\cdot\vec{n}(r) = 0$, but are quite similar to the topological atoms. The existence of these subsystems set the stage for the introduction of a novel version of fuzzy atom methodology within the context of the QTAIM. This fuzzy set conclusively confirms the non-equivalence of the set of quantum and topological atoms as conjectured previously [2]; that is, the topological atoms are only a subset of the general set of quantum atoms.

2 The quasi-atoms

It was recently demonstrated that apart from the topological atoms other "consistent" real space quantum subsystems, which were collectively called QDB, also emerge "naturally" from the general framework of the quantum

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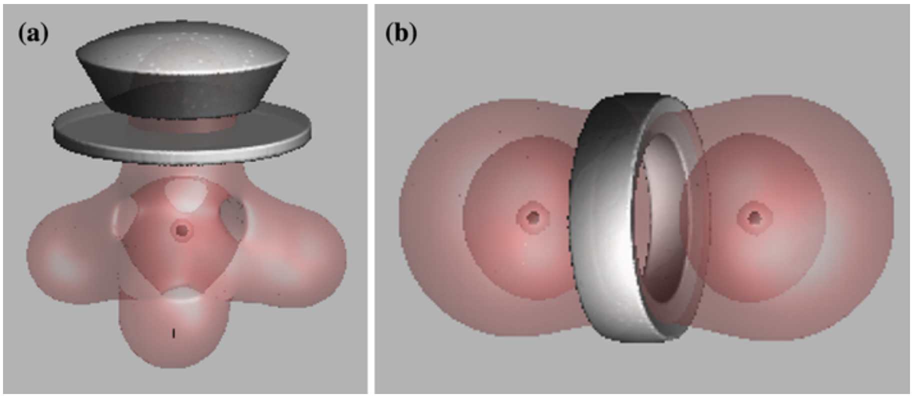

Fig. 1 Several representative QDB: **a** of CH_4 molecule (a shared and an exclusive QDB) **b** of N_2 molecule (only a shared QDB). The *pink* contours encompassing the nuclei (*black dots*) are the zero value Laplacian surfaces of the one-electron density

theory of proper open subsystems (QTPOS) [1]. These subsystems persist against external perturbations, i.e. external fields and nuclear excursions, so, in addition to preserving their identity, they are also observable (at least in principle) employing diffraction data [1]. They originate from the layered structure of the Laplacian of the one-electron density, $\nabla^2\rho(r)$; this scalar field is generally composed of alternative positive and negative regions [7], allowing to "design" various 3D objects for which the net Laplacian content is null. Figure 2a pictorially presents the general strategy for designing the QDB. It is evident from this figure that it is possible to have arbitrarily small QDB and this fact is employed in designing the QA.

At first the qualitative construction of a QA is described by a hypothetical example. Figure 2b presents a simplified zero Laplacian surface of a typical covalently bonded homo-nuclear diatomic species as well as the inter-atomic surface (IAS), which is the zero-flux surface dividing the molecule into two equal topological atoms. Attached to the IAS, within the basin of the topological atom (TA) that is placed in the right-hand side of this figure, an exclusive cylindrical QDB is constructed. By assuming the cylindrical QDB as part of the left hand side atomic basin, the combined region is also a QDB satisfying the net zero-flux equation ($TA_{LHS} + QDB_{cylindrical} = QDB_{LHS}$). On the other hand, the remaining part of space is also a QDB since it satisfies the net zero-flux equation ($TA_{RHS} - QDB_{cylindrical} = QDB_{RHS}$). Because of the fact that the cylindrical QDB can be made arbitrarily small, the resulting QDB_{RHS} as well as QDB_{LHS} and their properties can be also arbitrarily similar to the original topological atoms. The two regions thus obtained with properties similar to the corresponding topological atoms are examples of the QA. The partitioning of a diatomic into a pair of QA is "exhaustive"; thus, the sum of their properties is equal to the corresponding molecule's properties. The utility of this procedure and its generality are explicitly demonstrated for the nitrogen molecule as a typical example.

In order to confirm this qualitative reasoning in practice, various cylindrical as well as Gaussian shaped exclusive QDB are considered in the nitrogen molecule as two distinct sets of the QDB. Figure 3 depicts their morphologies and geometrical parameters schematically, whereas Tables 1 and 2 present their detailed geometrical

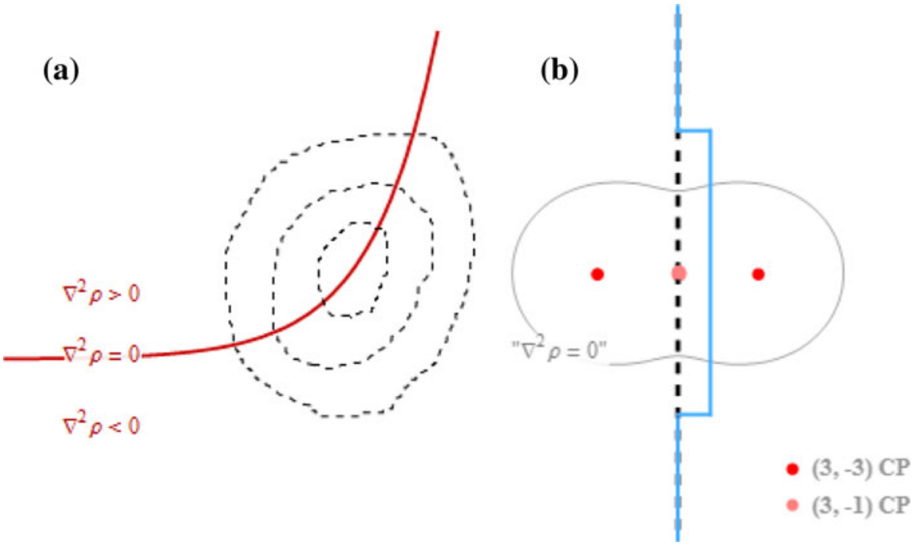

Fig. 2 **a** A schematic representation of QDB; regions containing equal portions of positive and negative Laplacian of the one-electron density. **b** A schematic 2D representation of two typical quasi-atoms (for a diatomic homo-nuclear molecule in a plain containing both nuclei) the boundary of which is delineated by the *blue line*; the *dashed line* represents the orthodox zero-flux surface delineating the boundary of two identical topological atoms for the same molecule

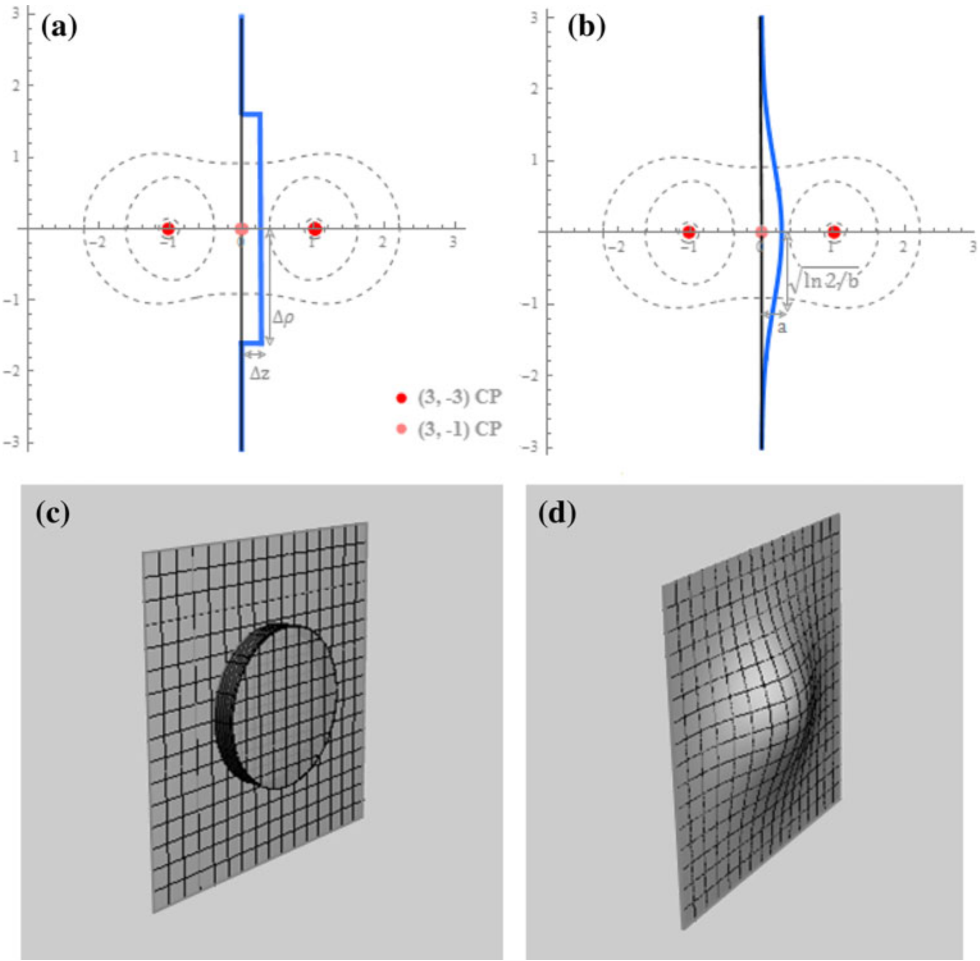

Fig. 3 **a, b** A schematic 2D representation of two quasi-atoms (delineated by the *blue line*) for the N_2 molecule in the plane containing the two nuclei. The parameters *a* and *b* are parameters of the $a\,\mathrm{Exp}(-br^2)$ function representing the Gaussian bulge where $\Delta\rho$ and Δz are the radius and height of the cylindrical bulge, respectively. The *black line* is the intra-atomic surface (IAS) dividing the molecule into two identical topological atoms; also, the critical points (CP) of the one-electron density as well as the zero value Laplacian surfaces (the *dashed* contours) are depicted for clarity. **c, d** A schematic 3D representation of the surfaces delineating the boundary of the quasi-atoms for the N_2 molecule

description and properties. It is evident from these tables that arbitrarily small bulges and dips are conceivable on the orthodox IAS. Also, Fig. 4 offers the inter-dependence of the geometrical parameters of each set of QDB demonstrating their "continuous" geometrical evolution. The five smaller QDB of each set are used to construct the "probable QA". Table 3 offers their properties as well as those of the corresponding topological atoms. Indeed, the QA constructed from the smallest QDB in each set are quite similar to the topological atoms. Literally speaking, one may imagine that the boundary surface of the two subsystems continuously deforms like a membrane during a hypothetical vibration in a way that all the resulting deformed objects satisfy the net zero-flux equation; so, the QA are the result of low amplitude vibration. In the case that this boundary surface becomes a zero-flux surface, it is equivalent to the IAS yielding two identical topological atoms; however, in other cases, it delineates the boundary of two QDB which by having similar properties to the topological atoms are called QA. This procedure also illustrates the continuous evolution of the QDB into the topological atoms unveiling the relationship of these two sets of real space quantum subsystems. Considering the fact that the strategy used for constructing the QA of the nitrogen molecule is quite general and taking the common patterns of the Laplacian maps into account [13], it appears that the notion of QA is easily extendable to other species. This provides an opportunity for introducing the set of fuzzy atoms within the context of the QTAIM. However, before considering this issue in detail, a rigorous definition of the QA is offered.

The QA were recognized as a subset of QDB that are sufficiently similar to the reference topological atom. In order to quantify this similarity for deriving the QA, one needs to first enumerate the probable QA and then define index(es) to explicitly measure the resemblance of these QDB to the reference topological atom. Based on the considered example and remembering the fact that there is unlimited number of QDB, it is assumed that the probable QA are discernable by a continuous index (real number), *p*, which is assumed to be zero for the reference topological atom (this index could be a single or a combined geometrical parameter). Also, taking into account that the experimental measurement of all regional properties has a limited accuracy [14], it is possible to devise a set of precision parameters, $\{\alpha\}$, for the measurement of a finite

Table 1 The properties (volume $V(\omega)$, population $N(\omega)$ and the Hamiltonian and Lagrangian kinetic energies, $K(\omega)$ and $G(\omega)$, in atomic units) as well as geometrical description of several QDB of the N_2 molecule at its equilibrium geometry (computed at HF/6-31*g*(*d*) computational [1])

QDB[a]	Geometrical description[b]			$V(\omega)$	$N(\omega)$	Kinetic energy		$L(\omega)$[c]	α[d]
	$\Delta\rho$	$\Delta\varphi$	Δz			$K(\omega)$	$G(\omega)$		
1	0–2.0934	0–2π	0–0.2	2.75	0.45	0.4361	0.4361	9.6×10^{-10}	$\sim 10^8$
2	0–2.0792	0–2π	0–0.19	2.58	0.43	0.4127	0.4127	-1.7×10^{-9}	$\sim 10^8$
3	0–2.0658	0–2π	0–0.18	2.41	0.40	0.3895	0.3895	1.4×10^{-9}	$\sim 10^8$
4	0–2.0532	0–2π	0–0.17	2.25	0.38	0.3665	0.3665	3.9×10^{-10}	$\sim 10^8$
5	0–2.0414	0–2π	0–0.16	2.09	0.36	0.3438	0.3438	2.2×10^{-9}	$\sim 10^7$
6	0–2.0304	0–2π	0–0.15	1.94	0.34	0.3212	0.3212	4.5×10^{-10}	$\sim 10^8$
7	0–2.0201	0–2π	0–0.14	1.79	0.31	0.2989	0.2989	-9.7×10^{-10}	$\sim 10^8$
8	0–2.0106	0–2π	0–0.13	1.65	0.29	0.2768	0.2768	1.1×10^{-9}	$\sim 10^8$
9	0–2.0019	0–2π	0–0.12	1.51	0.27	0.2548	0.2548	-1.6×10^{-9}	$\sim 10^7$
10	0–1.9939	0–2π	0–0.11	1.37	0.24	0.2330	0.2330	9.4×10^{-10}	$\sim 10^8$
11	0–1.9867	0–2π	0–0.1	1.24	0.22	0.2113	0.2113	-3.6×10^{-10}	$\sim 10^8$
12	0–1.9802	0–2π	0–0.09	1.11	0.20	0.1898	0.1898	-2.1×10^{-9}	$\sim 10^7$
13	0–1.9743	0–2π	0–0.08	0.98	0.18	0.1684	0.1684	4.7×10^{-10}	$\sim 10^8$
14	0–1.9692	0–2π	0–0.07	0.85	0.16	0.1471	0.1471	-9.0×10^{-10}	$\sim 10^7$
15	0–1.9648	0–2π	0–0.06	0.73	0.13	0.1259	0.1259	-4.0×10^{-10}	$\sim 10^8$
16	0–1.9611	0–2π	0–0.05	0.60	0.11	0.1048	0.1048	-9.0×10^{-10}	$\sim 10^7$
17	0–1.9580	0–2π	0–0.04	0.48	0.09	0.0838	0.0838	9.8×10^{-10}	$\sim 10^7$
18	0–1.9557	0–2π	0–0.03	0.36	0.07	0.0628	0.0628	8.7×10^{-11}	$\sim 10^8$
19	0–1.9540	0–2π	0–0.02	0.24	0.04	0.0418	0.0418	3.0×10^{-10}	$\sim 10^7$
20	0–1.9530	0–2π	0–0.01	0.12	0.02	0.0209	0.0209	-1.6×10^{-9}	$\sim 10^6$
21	0–1.9527	0–2π	0–0.001	0.01	2.2×10^{-3}	0.0021	0.0021	-5.8×10^{-10}	$\sim 10^6$
22	0–1.9526	0–2π	0–0.0001	1.2×10^{-3}	2.2×10^{-4}	0.0002	0.0002	6.9×10^{-10}	$\sim 10^5$

[a] A schematic representation of these cylindrical-shaped QDB is conceivable in Fig. 3a. It is the region bounded between the intra-atomic surface (black line) and the other boundary (blue line)

[b] The geometrical description is based on the cylindrical coordinate system, (ρ, φ, z), where its z-axis goes through the two nuclei and its origin is fixed on the midpoint between them. The z-coordinate of the two nitrogen nuclei are 1.0189 and −1.0189, respectively

[c] $L(\omega) = -(1/4)\int_\omega \nabla^2\rho(r)$ is the net flux integral (see [1] for details)

[d] Considering the fact that for each QDB $L(\omega)$ contains equal amounts of the net positive and negative fluxes (see [1] for details) $L(\omega) = L^+(\omega) + L^-(\omega) = 0$, this column represents the approximate value of the $\alpha = |L^+(\omega)/L(\omega)| = |L^-(\omega)/L(\omega)|$

number, say N, of regional properties, $\{M(\Omega)\}$. All QDB having properties within the acceptable bounds (the probable QA), $M^K(\Omega) \pm \alpha^K$, are identified as the QA associated to the reference topological atom. These may also be compressed in a formal language.

Let $\{\alpha\}$ be the set of precision parameters for the set of regional properties $\{M(\Omega)\}$, and Π be the set of all probable QA, $\Pi = \{p \in R | p_{\min} \leq p \leq p_{\max}, p \neq 0\}$, such that for each regional property, i.e. each $K(1 \leq K \leq N)$,

$$\left| M_p^K(\Omega) - M_0^K(\Omega) \right| \leq \alpha^K \qquad (1)$$

In this way, one may introduce the set of QA associated to a reference topological atom as follows:

$$\sum_{\{\alpha\}}^{p=0} = \{p | p \in \Pi \wedge \text{Inequality (1) is satisfied}\} \qquad (2)$$

The inequality (1) states that the regional properties of a QA and the reference topological atom, $M_P^K(\Omega)$ and $M_0^K(\Omega)$, are experimentally indistinguishable, so $\sum_{\{\alpha\}}^{p=0}$ must be regarded as a mathematical neighborhood with the center at the reference topological atom and the radius $\{\alpha\}$ such that all of its members are practically equivalent: the set of QA.

As mentioned previously, by employing the set of QA, it is feasible to introduce the notion of the “fuzzy set of atoms” within the context of the QTAIM. The original idea of a fuzzy atom was first introduced by Hirshfeld [15] and has elaborated considerably by others since then [16–24] (see [25] for an up-to-date review). Its core idea lies in assuming that atoms in a molecule do not have sharp boundaries and each point in the molecular space is part of all atoms in the molecule with different “weights” or “sharing percentages” (best described as “stockholder

Table 2 The properties (volume $V(\omega)$, population $N(\omega)$ and the Hamiltonian and Lagrangian kinetic energies, $K(\omega)$ and $G(\omega)$, in atomic units) as well as geometrical description of several QDB of the N_2 molecule at its equilibrium geometry (computed at HF/6-31*g*(*d*) computational level [1])

QDB[a]	Geometrical description[b]		$V(\omega)$	$N(\omega)$	Kinetic energy		$L(\omega)$[c]	α[d]
	a	*b*			$K(\omega)$	$G(\omega)$		
1	0.2	0.0772	8.14	0.44	0.4150	0.4150	5.8×10^{-10}	$\sim 10^{9}$
2	0.19	0.0799	7.47	0.41	0.3921	0.3921	3.9×10^{-11}	$\sim 10^{10}$
3	0.18	0.0826	6.84	0.39	0.3694	0.3694	-8.6×10^{-10}	$\sim 10^{8}$
4	0.17	0.0853	6.26	0.37	0.3471	0.3471	2.6×10^{-10}	$\sim 10^{9}$
5	0.16	0.0878	5.72	0.34	0.3250	0.3250	-1.2×10^{-10}	$\sim 10^{9}$
6	0.15	0.0903	5.22	0.32	0.3033	0.3033	8.9×10^{-10}	$\sim 10^{8}$
7	0.14	0.0927	4.75	0.30	0.2818	0.2818	1.0×10^{-10}	$\sim 10^{9}$
8	0.13	0.0949	4.30	0.28	0.2606	0.2606	-1.7×10^{-9}	$\sim 10^{8}$
9	0.12	0.0970	3.88	0.25	0.2396	0.2396	1.8×10^{-9}	$\sim 10^{8}$
10	0.11	0.0990	3.49	0.23	0.2188	0.2188	-1.2×10^{-9}	$\sim 10^{8}$
11	0.1	0.1009	3.11	0.21	0.1983	0.1983	8.7×10^{-10}	$\sim 10^{8}$
12	0.09	0.1026	2.76	0.19	0.1779	0.1779	-1.3×10^{-9}	$\sim 10^{8}$
13	0.08	0.1042	2.41	0.17	0.1577	0.1577	1.1×10^{-9}	$\sim 10^{8}$
14	0.07	0.1055	2.08	0.15	0.1376	0.1376	1.9×10^{-9}	$\sim 10^{8}$
15	0.06	0.1068	1.77	0.13	0.1177	0.1177	-4.2×10^{-9}	$\sim 10^{7}$
16	0.05	0.1078	1.46	0.10	0.0979	0.0979	2.1×10^{-9}	$\sim 10^{7}$
17	0.04	0.1086	1.16	0.08	0.0782	0.0782	7.4×10^{-10}	$\sim 10^{8}$
18	0.03	0.1093	0.86	0.06	0.0586	0.0586	1.6×10^{-9}	$\sim 10^{7}$
19	0.02	0.1098	0.57	0.04	0.0390	0.0390	-1.4×10^{-9}	$\sim 10^{7}$
20	0.01	0.1101	0.29	0.02	0.0195	0.0195	2.4×10^{-10}	$\sim 10^{8}$
21	0.001	0.1102	0.03	2.1×10^{-3}	0.0020	0.0020	-4.2×10^{-10}	$\sim 10^{6}$
22	0.0001	0.1102	2.8×10^{-3}	2.1×10^{-4}	0.0002	0.0002	-3.3×10^{-10}	$\sim 10^{6}$

[a] A schematic representation of the Gaussian shaped QDB is conceivable in Fig. 3b. It is the region bounded between the intra-atomic surface (black line) and the Gaussian curve (blue line)

[b] The parameters *a* and *b* describe the height and width of the Gaussian surface (see Fig. 3b) which is one of the boundary surfaces of the QDB. The other boundary surface is the $z = 0$ surface, inter-atomic surface. In addition, the z-coordinate of the two nitrogen nuclei are 1.0189 and –1.0189, respectively

[c] $L(\omega) = -(1/4)\int_{\omega} \nabla^2 \rho(r)$ is the net flux integral (See [1] for details)

[d] Considering the fact that for each QDB $L(\omega)$ contains equal amounts of the net positive and negative fluxes (see [1] for details) $L(\omega) = L^{+}(\omega) + L^{-}(\omega) = 0$, this column represents the approximate value of the $\alpha = |L^{+}(\omega)/L(\omega)| = |L^{-}(\omega)/L(\omega)|$

partitioning" [15]). Consequently, this idea is not generally applicable, at least not in its original form, to the disjoint partitioning schemes that the set of topological atoms is an example of. However, by viewing the QA plus the reference topological atom, $\sum_{\{\alpha\}}^{p=0} \cup TA$, as the set of acceptable "quantum atoms", the set of fuzzy atom is definable within the context of the QTAIM. In line with the orthodox paradigm of fuzzy atoms, a weight function, *f*(*p*), is introduced that determines the relative importance of each member of the fuzzy set.

$$\int f(p)\mathrm{d}p = 1 \quad 0 \leq f(p) \leq 1 \tag{3}$$

For each regional property, this weight function is used to compute the corresponding property of the fuzzy set:

$$\bar{M}^{K}(\Omega) = \int_{p_{\min}}^{p_{\max}} f(p) M_{p}^{K}(\Omega)\mathrm{d}p \tag{4}$$

Since the weight function is not derivable from the very formalism of the QTAIM, it must be determined "externally". As an illustration, the orthodox regional properties of the topological atoms are retrievable, employing the following step-function as the weight function:

$$f(p) = \begin{cases} 1 & p = 0 \\ 0 & p \neq 0 \end{cases} \tag{5}$$

Thus, upon selecting a proper weight function, all required ingredients of the fuzzy atom paradigm are gathered and practical computations may be done easily.

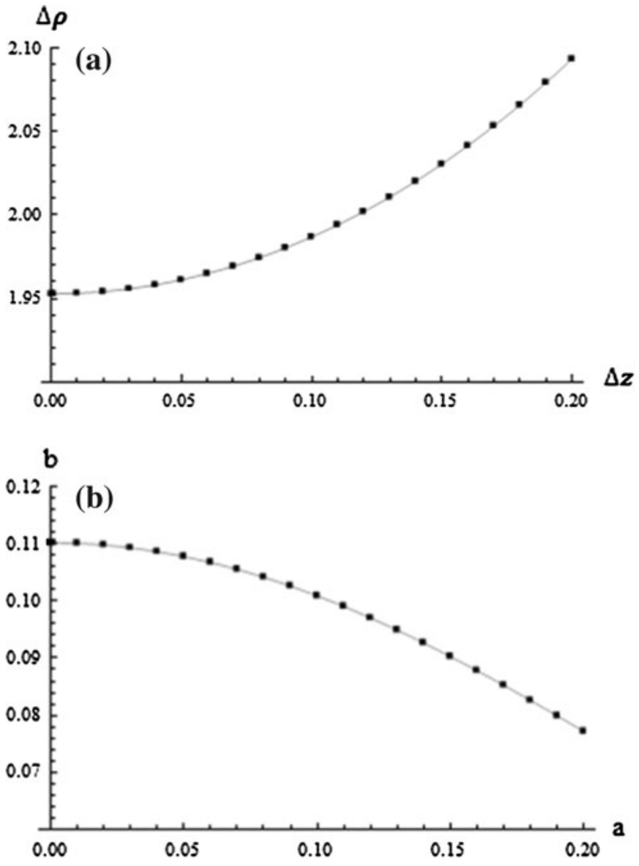

Fig. 4 The continuous evolution of the quasi-atoms constructed employing the QDB gathered in **a** Table 1 and **b** Table 2 by plotting the two geometrical coordinates of each set ($\Delta\rho$ and Δz for cylindrical case and a and b for Gaussian case) versus each other

3 Summary and conclusion

In the first contribution of this series of papers [2], it was emphasized that there is no a priori reason to believe that the concepts of quantum and topological atoms are equivalent. This study demonstrates that it is possible to conceive QDB arbitrarily similar to the topological atoms; the set of QA. This observation that seems to be quite general destructs the previous sharp distinction between the sets of topological atoms and QDB. On the other hand, the set of QA enlarges the set of known quantum atoms; the set of quantum atoms includes the reference topological atom and associated QA. Accordingly, because of the ubiquitous error bars in experimental measurements [14], one may claim that the chemical observations are compatible with a whole set of conceivable quantum atoms, not just a single member of this set. These quantum atoms are all compatible with both the subsystem variational procedure [1, 2, 4] and the condition of regional kinetic energy uniqueness taking Cohen's kinetic energy set into account [4, 26, 27] (however, see also the recent results of Ayers et al. [28]).

Table 3 The properties (volume $V(\omega)$, population $N(\omega)$ and kinetic energy, $T(\omega)$, in atomic units) of the two topological atoms as well as several quasi-atoms of N_2 molecule at its equilibrium geometry (computed at HF/6-31$g(d)$ computational level [1])

Quantum atoms[a]	$V(\omega)$	$N(\omega)$	$T(\omega)$	$V(\omega)$[b]	$N(\omega)$	$T(\omega)$
Quasi-atoms						
1	121.673	7.066	54.3502	121.948	7.063	54.3460
2	120.952	6.934	54.2246	120.677	6.937	54.2288
Sum	242.625	14.000	108.5748	242.625	14.000	108.5748
1	121.552	7.044	54.3292	121.735	7.042	54.3265
2	121.073	6.956	54.2456	120.890	6.958	54.2484
Sum	242.625	14.000	108.5748	242.625	14.000	108.5748
1	121.432	7.022	54.3083	121.523	7.021	54.3069
2	121.193	6.978	54.2665	121.102	6.979	54.2679
Sum	242.625	14.000	108.5748	242.625	14.000	108.5748
1	121.325	7.002	54.2895	121.334	7.002	54.2894
2	121.301	6.998	54.2853	121.291	6.998	54.2855
Sum	242.625	14.000	108.5748	242.625	14.000	108.5748
1	121.314	7.000	54.2876	121.315	7.000	54.2876
2	121.311	7.000	54.2872	121.310	7.000	54.2872
Sum	242.625	14.000	108.5748	242.625	14.000	108.5748
Topological atoms						
1	121.313	7.000	54.2874	121.313	7.000	54.2874
2	121.313	7.000	54.2874	121.313	7.000	54.2874
Sum	242.625	14.000	108.5748	242.625	14.000	108.5748

[a] The five quasi-atoms on the LHS (RHS) of this table are constructed employing the last five QDB in Table 1 (Table 2). They resemble the one depicted in Fig. 3a (Fig. 3b) having the surface given in Fig. 3c (Fig. 3d) as the boundary surface. In contrast to the topological atoms, the division of system into the quasi-atoms yields two non-equal quantum atoms. In this regard, the first row (indicated by 1) represents the properties of the quasi-atoms having a (cylindrical or Gaussian) bulge, where the other row (indicated by 2) represents the properties of the quasi-atoms with a dip. Similar to the topological atoms, the sum of these two rows reproduces the properties of the total system

[b] Similar to the case of topological atoms, the volume of these quasi-atoms (which has a Gaussian shaped boundary surface) is calculated assuming the 0.001 a.u. iso-surface of the one-electron density as the outer boundary of the molecule

One may compress all these facts and declare that although the topological atoms are usually conceived as the unique partitioning of a molecule into the atoms within the context of the QTAIM [7, 29–35], the set of quasi-atoms undermines this uniqueness.

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