



A study on quantum similarity in the phase space

J.M. Sellier*, D.Y. Ivanova, I. Dimov

IICT, Bulgarian Academy of Sciences, Acad. G. Bonchev str. 25A, 1113 Sofia, Bulgaria

HIGHLIGHTS

- We discuss a recently proposed definition of quantum similarity in the phase space.
- We investigate the dependence of this quantum similarity on an integer parameter.
- We apply this study to the hydrogen atom in the ground and excited states.

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ABSTRACT

Quantum similarity represents an important concept in the context of many applied disciplines such as physical and quantum chemistry. Nowadays, two definitions exist based, respectively, on the *real* and the *phase* spaces. In this paper, we focus on the second one, which was presented recently, and investigate it. In particular, being its mathematical definition dependent on a given integer s , we study the influence of this parameter on the similarity between two systems. To keep this investigation comprehensible, while still meaningful, we focus on a very simple quantum system represented by a hydrogen atom in the ground and excited states corresponding to the quantum numbers $(n, l, m) = (1, 0, 0)$ and $(n, l, m) = (2, 0, 0)$.

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1. Introduction

Molecular quantum similarity is a mathematical tool which, nowadays, is utilized for practical purposes in many different scientific areas, such as organic, quantum and physical chemistry. A concrete example is provided by research performed in pharmaceutical companies where quantum similarity can provide a systematic way to investigate the relation between the structure of a molecule and its chemical reactivity, thus drastically easing the process of drug design and, at the same time, the reduction of possible side effects. The idea was first proposed in 1980 and has received, since then, a growing interest in the community of Applied Scientists [1]. Different definitions of quantum similarity can be provided depending on many variables, among which the choice of the molecular descriptor, therefore making the problem of providing a universal definition practically impossible. As a matter of fact, recently a new definition has been proposed which exploits the concept of quasi-distribution functions in the phase space [2]. Consequently, it can be applied in the context of phase space formulations of quantum mechanics such as Refs. [3,4].

In this paper, we start from the work recently presented in Ref. [2] and use the definition of quantum similarity based on the quasi-distribution functions of quantum systems. The mathematical expression suggested in the mentioned work depends on an integer which can drastically influence the results. Since no analysis on the impact of such integer has been provided so far, this endeavor tries to fill this “gap”.

* Corresponding author.

E-mail addresses: jeanmichel.sellier@parallel.bas.bg, jeanmichel.sellier@gmail.com (J.M. Sellier).

This paper is structured as follows. We first briefly summarize the analytical results obtained in Ref. [2]. We then proceed with a mathematical investigation of the impact of the integer present in the definition of phase space quantum similarity on the results one might obtain. Finally, we conclude with some comments and a discussion about possible future developments.

2. Molecular descriptor in the phase space formalisms

For the sake of making this paper self-contained, in this section we report the main results previously presented in Ref. [2]. Although we try to be as much detailed as possible, we encourage the interested reader to refer to that previous work for more details.

The concept of molecular quantum similarity can be mathematically defined, given a particular context, by first selecting a *significant* molecular descriptor. In fact, the descriptor could be useful in certain situations but not in others and greatly depends on the specific task one wants to achieve. Therefore, a universal choice good for any situation is, simply said, impossible. Consequently, in practice, one has to choose among many options. To give an idea of the difficulty of this task, a (most likely incomplete) list of possible choices is given below [5]:

- Feature counts. Descriptors consist of a simple counting of some feature, for instance the number of certain atomic species in a molecule.
- Physicochemical parameters. Descriptors are defined in terms of specific physical/chemical features, for instance the partition coefficient.
- Fragment descriptors. Descriptors are based on molecular two-dimensional connection tables and three-dimensional descriptions of the structure for substructure searches.
- Topological indices. Descriptors are atom based and expressed in terms of indices, for example the Wiener index/number.
- Field-based descriptors. Descriptors are based on fields such as the electron density, the electrostatic potential, etc.

Although incomplete, this list already represents a huge set of possible descriptors. The reader should note that none of the concepts presented above involves the use of a quasi-distribution function $f_W = f_W(x; p; t)$, a typical concept of phase space formulations of quantum mechanics suggested by E. Wigner [3] or one of the author of this work [4].

In Ref. [2], we suggested a new mathematical expression of molecular quantum similarity. In particular, given two molecules A and B described, respectively, by the quasi-distribution functions f_W^A and f_W^B , the quantum similarity between these two chemical systems is defined as:

$$d_{AB}(s) = \left(\int d\mathbf{x} \int d\mathbf{p} |f_W^A(\mathbf{x}; \mathbf{p}) - f_W^B(\mathbf{x}; \mathbf{p})|^s \right)^{\frac{1}{s}}, \quad (1)$$

where s is an integer and the integration is performed over the (eventually finite) phase space corresponding to the simulation domain. It is clear from this definition that $d_{AB} \geq 0$, and two molecules are said to be similar only when their distance d_{AB} is close or equal to zero. Conversely, the bigger the number $d_{AB}(t)$ the less similar the molecules are. Finally, it is worth to note that as the integer number s increases, the definition (1) represents a stronger measure. As a matter of fact, when $s \rightarrow +\infty$ one obtains an absolute density descriptor.

Comments. An example underlining the advantages of the definition (1) has been presented for the case $s = 1$ in Ref. [2]. As a matter of fact, it is possible to show that two quantum systems A and B represented by the following quasi-distribution functions (fulfilling the Tatarskii pure state quantum conditions [6])

$$f_W^A(\mathbf{x}; \mathbf{p}) = N_A \rho(\mathbf{x}) e^{-\frac{\left(\frac{p^2}{2m} - E_0^A\right)}{\sigma}},$$

and

$$f_W^B(\mathbf{x}; \mathbf{p}) = N_B \rho(\mathbf{x}) e^{-\frac{\left(\frac{p^2}{2m} - E_0^B\right)}{\sigma}},$$

have a quantum similarity equal to 0 in the real space, but a completely different similarity, i.e. *greater than 0*, in the phase space (where N_A and N_B are two normalization constants, σ is the dispersion in energy of the packet, E_0^A and E_0^B are the peak in energy of the two packets with $E_0^A \neq E_0^B$, and m is the mass of the system). This clearly supports the idea that the phase space similarity represents a richer concept in terms of details if compared to the one based on the real space. This example also shows an interesting fact: two *different* Wigner states corresponding to the same probability density in the real space cannot automatically be considered similar in the phase space.

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