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ND-Wavelets Derived from Anti-symmetric Systems of Isolated Particles using the Determinant of Slater

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Abstract—Wavelets are known to be closely related to atomic orbital. A new approach of 2D, 3D and multidimensional wavelet system is proposed from a parallel with anti-symmetric systems of isolated particles. The theory of fermionic states is used to generate new n-dimensions wavelets, $n \geq 2$, by the determinant of Slater. As pioneering paper in exchanging formalism between particle wave-functions and wavelets, it opens some perspectives for further adaptations derived from the physics of particles in the wavelet analysis scope.

Keywords—3D wavelets, anti-symmetric wavelets, orbital wavelets, image analysis.

I. Introduction

Wavelet transforms methods are now standard tools in image processing due to their capabilities of multiresolution analysis and image decomposition [6], [18]. Wavelet-based image processing is a routinely and largely adopted approach in texture image decomposition, subband coding, fast image segmentation [1], [3], [13], [16], [31], even for 3D [30]. There are also plenty of applications of wavelet in computer graphics [20], [23], [25], [27].

There is a rooted [2], but not fully explored link between quantum mechanics and wavelets. The wave nature of light can be deduced from the phenomenon of interference, the photoelectric effect, however, seems to suggest a corpuscular nature of light. Theoretical physicists struggled to include observations like the photoelectric effect and the wave-particle duality into their formulations [29]. Erwin Schrödinger, an Austrian physicist, was using advanced mechanics to deal with these phenomena and developed a equation that relates the space-time in quantum mechanics, in an attempt to get the analog of the classical mechanics. Because wavelets are localized in both time and frequency they offer significant advantages for the analysis of problems in quantum mechanics. In this paper, we shed some light on some of these relations. Rather than seeking at wavelet features on particles or waves, we adapted some concepts of quantum mechanics to a novel wavelet decomposition for still images.

Initially, we introduce in Section II the motivation to build these wavelets, with inspiration in "Particle Physics" [4], [11]. In Section III, we introduce the construction of orbital wavelets for the image decomposition, starting from a single mother wavelet. It is shown this construction actually generates two-dimensional wavelets. Section IV includes the main lines for an extension to the 3D-case and to higher dimensions. Finally, the concluding remarks are presented in Section VI.

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II. MOTIVATION ARISING FROM PARTICLE PHYSICS

Usual wavelet image analysis combines one-dimensional (1D) wavelets to generate a two-dimensional (2D) wavelet [1], [31]. This is equivalent to the analysis by the matrix:

$$\begin{bmatrix} LL & HL \\ LH & HH \end{bmatrix}, \tag{1}$$

where L and H denote {low- and high}-pass bands, respectively [28].

The combinations LL and HH naturally exhibit a symmetry (even): $\varphi(x)\cdot\varphi(y)=\varphi(y)\cdot\varphi(x)$, ditto for $\psi(x)\cdot\psi(y)=\psi(y)\cdot\psi(x)$. Now, the combination of $\varphi(\cdot)$ and $\psi(\cdot)$ resulting in two different analyzes and non-commutative, namely, $\varphi(x)\cdot\psi(y)$ and $\psi(x)\cdot\varphi(y)$. The combination of $\varphi(\cdot)$ and $\psi(\cdot)$ should result in asymmetry (odd symmetry), and the exchange of the coordinates $x\leftrightarrow y$ just swap the direction of observation. The combined $\varphi_-\psi$ wave should be such that:

$$\varphi_{-}\psi(x,y) = -\varphi_{-}\psi(y,x). \tag{2}$$

The proposal then is to define the orbital combination between φ and ψ by the following wave function:

$$\varphi_{-}\psi(x,y) := \frac{1}{\sqrt{2}} [\varphi(x)\psi(y) - \psi(x)\varphi(y)], \tag{3}$$

instead of merely $\varphi(x) \cdot \psi(y)$ (*LH*) or $\psi(x) \cdot \varphi(y)$ (*HL*). It should be noted that it now hold Equation (2).

Worth nothing that the subtraction of the standard images *LH - HL* results in exactly the picture of the orbital decomposing, as well as its negative, on the secondary diagonal of the decomposition matrix of Equation (1).

III. ORBITAL WAVELET FOR THE 2D CASE

The wave functions describing electronic orbital can be combined generating "atomic orbitals." The "equivalent" in the scope of wavelets, also characterized by wave functions, would be combination of different spatial wavelets [7]. In the case of particles is typically assumed the combination of antisymmetric particles without interaction [11]. The combination of α and β states should not depend on which of the particles (1 or 2) is in one of the particular states. This is called "exchange degeneracy." It corresponds to a probability density of two particles, being one in the alpha state and another in the beta state not knowing where a particular state. There are two ways to achieve this [10]:

$$\psi_S(r_1, r_2) := \frac{1}{\sqrt{2}} [\psi_{\alpha\beta}(r_1) + \psi_{\beta\alpha}(r_2)],$$
 (4)

and

$$\psi_A(r_1, r_2) := \frac{1}{\sqrt{2}} [\psi_{\alpha\beta}(r_1) - \psi_{\beta\alpha}(r_2)].$$
 (5)

where r_1 and r_2 are the positions of particle 1 and 2, and α and β are particular states, respectively.

This idea can be used in the decomposition of Equation (1). ψ_S is employed in the main diagonal and ψ_A in the secondary diagonal. Interestingly, employing the combination symmetric diagonally main results in

$$LL(x,y) := \frac{1}{\sqrt{2}} [\varphi^*(x)\varphi(y) + \varphi^*(y)\varphi(x)], \tag{6}$$

and

$$HH(x,y) := \frac{1}{\sqrt{2}} [\psi^*(x)\psi(y) + \psi^*(y)\psi(x)]. \tag{7}$$

This definition allows, in particular, analyzing images using continuous complex wavelets (see also [14]). In the case of real wavelets, simplification collapses to the usual $\varphi(x) \cdot \varphi(y)$ or $\psi(x) \cdot \psi(y)$. For the sake of simplicity, we often drop the variables x and y and denote by (LL) and (HH) as introduced in Equation (1). The orbital-based 2D analysis is shown in Appendix.

The initial proposal for "combination" of two wavelets was adopted for image analysis (2D) considering the same orthogonal mother wavelet, but at different scales of multiresolution. The two wavelets are $\psi_{a_1,b}(.)$ and $\psi_{a_2,b}(.)$ and the approach for simultaneous analysis in two different scales corresponds to the following set-up: Consider a 1D orthogonal [7], [15], [17] wavelet mother $\psi(x)$ equipped with her daughters $\{\psi_{a,b}(x)\}_{a\neq 0,b\in R}$.

Definition 1: The function 2D-orbital at the scales $\{a_1, a_2\}$ is defined by:

$$\psi_A(x,y) := \frac{1}{\sqrt{2}} \det \begin{bmatrix} \psi_{a_1,b}^*(x) & \psi_{a_1,b}^*(y) \\ \psi_{a_2,b}(x) & \psi_{a_2,b}(y) \end{bmatrix}, \tag{8}$$

which can be rewritten

$$\psi_{A}(x,y) = \frac{1}{\sqrt{2|a_{1}||a_{2}|}} \psi^{*} \left(\frac{x-b}{a_{1}}\right) \psi \left(\frac{y-b}{a_{2}}\right) - \frac{1}{\sqrt{2|a_{1}||a_{2}|}} \psi \left(\frac{x-b}{a_{2}}\right) \psi^{*} \left(\frac{y-b}{a_{1}}\right).$$
(9)

The condition $a_1 \neq a_2$ eliminates the degeneration into $\psi_A(x,y) = 0$. This is to some extent in connection to the Pauli Exclusion Principle [10]. It state that with a singlevalued many-particle wavefunction is equivalent to requiring the wavefunction to be antisymmetric. An antisymmetric twoparticle state is represented as a sum of states in which one particle is in state α and the other in state β . Besides, the relationship $\psi_A(y,x) = -\psi_A(x,y)$ ensures the desired asymmetry. Here, we use the same wavelet-mother, but on different scales. It will be seen that the orthogonality requirements correspond to the "dual" of particles without interaction. If the wavelets are orthogonal on any two scales, one can perform

a decomposition of an image "simultaneously" in both scales. The decomposition 2D sated in Definition 1 results in a strict 2D-wavelet.

Hypothesis 1: If the wavelets $\{\psi_{a,b}(t)\}$ are orthogonal, then the inner product $\langle \psi_{a_1,b}, \psi_{a_2,b} \rangle = 0$ and the following integrals cancel out $\forall a_1 \neq a_2$:

$$\int_{-\infty}^{\infty} \psi_{a_{1},b}(x) \cdot \psi_{a_{2},b}^{*}(x) dx = \int_{-\infty}^{\infty} \psi_{a_{1},b}^{*}(x) \cdot \psi_{a_{2},b}(x) dx = 0.$$
(10)

It is also noteworthy that

$$\langle \psi_{a_1,b}, \psi_{a_2,b} \rangle^* = \langle \psi_{a_2,b}, \psi_{a_1,b} \rangle. \tag{11}$$

Proposition 1: The previously defined 2D-orbital function has oscillatory behavior satisfying the following properties:

- 1) $\int_{-\infty}^{\infty} \psi_A(x, y) dx = 0,$ 2) $\int_{-\infty}^{\infty} \psi_A(x, y) dy = 0,$ 3) $\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \psi_A(x, y) dx dy = 0.$

Proof. It follows that

$$\int_{-\infty}^{\infty} \psi_{A}(x,y) dx = \frac{1}{\sqrt{2}} \psi_{a_{2},b}(y) \cdot \overline{\psi_{a_{1},b}^{*}(x)} - \frac{1}{\sqrt{2}} \overline{\psi_{a_{2},b}(x)} \cdot \psi_{a_{1},b}^{*}(y),$$
(12)

where

$$\overline{\psi_{a,b}(x)} := \int_{-\infty}^{\infty} \psi_{a,b}(x) dx.$$
 (13)

Therefore, item 1 derives from the fact that $\psi_{a,b}(x)$, (where $a = \{a_1, a_2\}$) are individual wavelets. Proof of item 2 is similar, by considering that

$$\int_{-\infty}^{\infty} \psi_{A}(x,y) dy = \frac{1}{\sqrt{2}} \overline{\psi_{a_{2},b}(y)} \cdot \psi_{a_{1},b}^{*}(x) - \frac{1}{\sqrt{2}} \psi_{a_{2},b}(x) \cdot \overline{\psi_{a_{1},b}^{*}(y)}.$$
(14)

Now the condition $\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \psi_A(x,y) \mathrm{d}x \mathrm{d}y = 0$ follows from Fubini's theorem [24], regardless of the order of integration.

Proposition 2: The 2D-orbital functions have normalized

Proof. Computing $|\psi_A(x,y)|^2 = \psi_A(x,y) \cdot \psi_A^*(x,y)$, we find

$$|\psi_{A}(x,y)|^{2} = \frac{1}{2} |\psi_{a_{1},b}(x)|^{2} \cdot |\psi_{a_{2},b}(y)|^{2} \times |\psi_{a_{1},b}(y)|^{2} \cdot |\psi_{a_{2},b}(x)|^{2}$$
(15)

and therefore

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} |\psi_A(x,y)|^2 dx dy = 1.$$
 (16)

If, by hypothesis, $\psi_{a_1,b}(t) \perp \psi_{a_2,b}(t)$ holds, then all cross terms are void, concluding the proof. It is possible (more easily) to combine orthogonal 1D-wavelets and use them to build a new 2D-wavelet.

Proposition 3: The 2D-orbital function is a 2D wavelet.

Proof. Starting from $\psi(t) \leftrightarrow \Psi(w)$ and the fact that the

admissibility condition holds [5], [6], $C_{\psi} := \int_{-\infty}^{\infty} \frac{\left|\Psi(w)\right|^2}{|w|} dw < +\infty, \text{ and similarly for their daughter wavelets } \psi_{a,b}(t) \leftrightarrow \Psi_{a,b}(w) \text{ results in }$ $\int_{-\infty}^{\infty} \frac{|\Psi_{a,b}(w)|^2}{|w|} dw < \infty, \text{ since } \Psi_{a,b}(w) = \sqrt{|a|} \Psi(aw) e^{-jwb}$ [8]. Let us now evaluate the condition for the 2D case. If the Fourier transform pair $\psi_A(x,y) \leftrightarrow \Psi_A(u,v)$ do exist, the 2Dspectrum of ψ_A can be computed in terms of the 1D-spectrum of ψ :

$$\Psi_A(u,v) = \frac{\sqrt{|a_1 a_2|}}{\sqrt{2}} \left[\Psi(a_1 u) \Psi^*(a_2 v) - \Psi(a_2 u) \Psi^*(a_1 v) \right]. \tag{17}$$

From the generalized Parseval-Plancherel energy theorem [6], [24], the cross-terms vanish due to the orthogonality,

$$\begin{split} \left|\Psi_{A}(u,v)\right|^{2} &= \\ \frac{\left|a_{1}a_{2}\right|}{2}\left|\Psi(a_{1}u)\right|^{2}\left|\Psi(a_{2}v)\right|^{2} + \frac{\left|a_{1}a_{2}\right|}{2}\left|\Psi(a_{2}u)\right|^{2}\left|\Psi(a_{1}v)\right|^{2}. \end{split} \tag{18}$$

Letting

$$C_{\psi_A} := \int \int_{-\infty}^{\infty} \frac{\left|\Psi_A(u,v)\right|^2}{\left|u\right| \cdot \left|v\right|} du \ dv, \tag{19}$$

the proof that $C_{\psi_A} < +\infty$ follows directly from the marginal admission conditions of the 1D daughter-wavelets.

IV. THE 3D-ORBITAL WAVELETS

For extension of the results in the 3D case (or even higher dimensions), one might consider the following definition inspired by the "Slater determinant" [26], which is used for antisymmetric systems of several isolated particles (fermionic state).

Definition 2: The 3D-orbital function at three distinct scales $\{a_1, a_2, a_3\}$ is given by

$$\psi_{A}(x,y,z) = \frac{1}{\sqrt{3!}} \cdot \det \begin{bmatrix} \psi^{*}_{a_{1},b}(x) & \psi^{*}_{a_{1},b}(y) & \psi^{*}_{a_{1},b}(z) \\ \psi_{a_{2},b}(x) & \psi_{a_{2},b}(y) & \psi_{a_{2},b}(z) \\ \psi^{*}_{a_{3},b}(x) & \psi^{*}_{a_{3},b}(y) & \psi^{*}_{a_{3},b}(z). \end{bmatrix}$$
(20)

The general case follows the same lines. Again, ensuring the orthogonality of the 1D wavelet chosen as the starting point is an essential statement. Further generalizations can also be

V. LINEAR COMBINATION OF WAVELETS AS LCAO

This paper presented a way to combine orthogonal wavelets, Equation (4) and (5), using a method similar to the LCAO (Linear Combination of Atomic Orbitals) approach [19]. When there is no orthogonality, one possible solution is to consider the quantity $S \neq 0$, called orbital overlap (or recoating), which defined by:

$$S := \int_{-\infty}^{\infty} \psi_{a_1,b}(x) \cdot \psi_{a_2,b}^*(x) \mathrm{d}x \tag{21}$$

In this cases Equation (4) and Equation (5) are replaced by

$$\widetilde{\psi}_S(r_1, r_2) := \frac{1}{\sqrt{2(1+S)}} [\psi_{\alpha\beta}(r_1) + \psi_{\beta\alpha}(r_2)],$$
 (22)

$$\widetilde{\psi_A}(r_1, r_2) := \frac{1}{\sqrt{2(1-S)}} [\psi_{\alpha\beta}(r_1) - \psi_{\beta\alpha}(r_2)].$$
 (23)

This can clearly be put as a generalization on Definition 1, but now in the wavelet framework. Since LCAO is larged and successful used in molecule studies, this similar wavelet approach can possible be of potential use.

VI. CONCLUDING REMARKS

Even prospective, the main ideas presented here can be explored, taking advantage of the cornucopia of tools available in particle physics and atomic orbitals theory. This paper offers an original and more general approach for image decomposition engendered by asymmetric orthogonal wavelets, which allows much room, somewhat akin to the extension from wavelets to wavelet packets. Despite the focus being essentially on still image, this approach allows a fully scalable multimedia decomposition. It remains to be investigated the potential of this approach in image compressing [9], in 3D processing and scalable coding for multimedia schemes [21]. Applications in other scenarios such as wavelet-based watermarking [12] or steganography [22] also deserve an investigation. As pioneering paper in exchanging formalism between particle wave-functions and wavelets, it opens new perspectives for adaptations derived from the quantum chemistry in the wavelet analysis scope.

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APPENDIX

A general alternative formulation of standard image (2D) wavelet decomposition can be carried out by the following

$$\begin{bmatrix} LL & HL \\ LH & HH \end{bmatrix}$$

where L and H denote low- and high-pass bands, respectively.

$$LL = \varphi \varphi_S(x, y) := \frac{1}{\sqrt{2}} \det \begin{bmatrix} \varphi^*(x) & \varphi^*(y) \\ -\varphi(x) & \varphi(y) \end{bmatrix}.$$

$$HH = \psi_{-}\psi_{S}(x,y) := \frac{1}{\sqrt{2}} \det \begin{bmatrix} \psi^{*}(x) & \psi^{*}(y) \\ -\psi(x) & \psi(y) \end{bmatrix}.$$

$$LH = \varphi_{-}\psi_{A}(x,y) := \frac{1}{\sqrt{2}} \det \begin{bmatrix} \varphi^{*}(x) & \varphi^{*}(y) \\ \psi(x) & \psi(y) \end{bmatrix}.$$

$$HL = \psi \varphi_A(x, y) := \frac{1}{\sqrt{2}} \det \begin{bmatrix} \psi^*(x) & \psi^*(y) \\ \varphi(x) & \varphi(y) \end{bmatrix}.$$

The symmetries involved are:

 $\varphi_{-}\varphi_{S}(x,y)=\varphi_{-}\varphi_{S}(y,x)$ and $\psi_{-}\psi_{S}(x,y)=\psi_{-}\psi_{S}(y,x)$, whereas the antisymmetries are $\varphi_{-}\psi_{A}(x,y)=-\varphi_{-}\psi_{A}(y,x)$ and $\psi_{-}\varphi_{A}(x,y)=-\psi_{-}\varphi_{A}(y,x)$.