8 HIGHLIGHT OF THE MONTH

Electronic Structure using Wavelets

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8.1 Introduction

In July of this year J. Bernholc and I organised a workshop at CECAM with the theme of "Grid, Multigrid and Wavelet Methods in Electronic Structure Computation." About 25 researchers from Europe, USA and Japan came to discuss new approaches to electronic structure calculations based upon these ideas. The goal was to develop a next generation of DFT codes for total energy and molecular dynamics calculations which would work entirely in real-space. Rather than traditional real-space quantum chemistry basis sets, such as Gaussians, the workshop focussed entirely on grid based methods. The motivation being that such methods retain complete flexibility in the form of the wave functions. Many of the methods discussed are well known in other numerically intensive computing fields, such as finite elements, multigrids and wavelets, but so far have not been widely used in electronic structure. From the progress reported at the workshop it seems clear that some of these methods will indeed play an important role in the future.

In this article I intend to give a brief overview of the motivation behind this work. Then I shall describe in more detail one particular approach, based on the elegant mathematics of wavelet theory. Hopefully this article will highlight some of the advances which have been made, as well as the difficulties which have yet to be overcome.

8.2 Motivation

The readers of this newsletter will, of course, be well aware of the capabilities of modern electronic structure algorithms. Using the Car Parinello algorithm together with a plane wave basis set and separable norm-conserving pseudoptentials accurate ab initio calculations are now possible for very complex systems with several hundred inequivalent atoms. The impressive examples shown by Parinello and others at the Ψ_k network conference included direct simulation of liquids, reaction dynamics of large molecules, and determining the structure of biological molecules.

The plane wave basis sets used in these calculations have many advantages, in particular:

1. The speed of the Fast Fourier Transform (FFT).
2. The ability to compute the Hellman Feynman forces on the ions.
3. The plane wave cut-off can be easily adjusted to ensure convergence.

These have made plane wave pseudopotential methods very popular because they are fairly simple to implement, fast, and relatively straightforward to run.

However, despite these advantages the plane wave basis set also has several disadvantages or factors which limit potential applications. These problems include (in no particular order):

1. Each basis state extends throughout the whole unit cell.
2. The FFT requires a uniform spacing of grid points everywhere in the unit cell.
3. The boundary conditions must be periodic and hence the unit cell must be charge neutral.
4. The FFT is not convenient for massively parallel computation.
5. 'Hard pseudopotential' atoms, such as transition metals, are expensive to include.

Problems 1-3 are specifically due to the nature of plane waves and of the FFT. In particular, problem 1 means that plane wave basis sets are not useful for O(N) algorithms, for which the computational time is proportioal to system size. Standard plane wave algorithms, such as Car Parinello, scale with N^3 for large systems because of the time to keep the occupied wave functions orthogonal to each other. The various O(N) algorithms build in the 'near-sightedness' of the total energy by working with real-space representations of the density-matrix. Real space bases are thus essential.

Problem 4, the difficulty of parallelization, is a consequence of 1, the global nature of the plane wave basis. Of course parallel FFTs do exist, however, unless each computer node has enough memory to store the whole FFT grid for all the occupied states for a given k point, significant data communication between nodes is inevitable. In contrast the O(N) algorithms are naturally parallel since the near-sightedness implies that distant regions of space are quite independent, and so can be handled in parallel. In fact any real-space basis set makes parallelization relatively simple by domain decomposition, reducing communication to only the data associated with the boundaries between domains.

Problem 5, the hard pseudopotential problem, is difficult to surmount with any completely general basis set. Of course LMTO and LAPW methods are very successful for transition metals. However, forces are difficult for molecular dynamics applications. Soft pseudopotential methods are now making some transition metal systems quite feasible with Car Parinello type methods. To some extent the real problem with these systems is the requirement of a uniform grid spacing (problem 2 above). The higher cut off involved in adding even one transition metal atom to a system requires a denser grid everywhere throughout the cell. On the other hand, this problem would be overcome by using finite elements, adaptive grids or wavelets. These methods allow the program to (automatically) allocate more grid points where needed so reducing to a minimum the computationl cost ascociated with hard pseudopotential atoms.

Why are grid methods to be preferred over other real space basis sets such as Gaussian orbitals? Gaussian basis sets are ubiquitous in quantum chemistry, and are also well known in solid state calculations. Tight binding LMTO and screened KKR methods also provide ab initio real-space basis sets. The main motivation for the grid based methods is their complete flexibility. The calculation will be gauranteed to converge to the exact answer for all atomic geometries without user input based on 'physical intuition'. Physical intuition may help in choosing 'good' basis sets, but can also be misleading if the intuition is wrong! For those of us who have difficulty in visualizing wave functions in 100 atom non-periodic systems it is very helpful to have a single parameter, say a grid spacing h, and know that $h \to 0$ is always the exact answer. Standardized Gaussian basis sets are certainly useful to obtain 'chemical accuracy' $\sim 0.01 - 0.1$eV/atom, but for problems requiring higher precision (e.g. energy differences between polytypes, magnetic coupling, testing DFT functionals) it can be important to ensure that basis set error is negligible. To some extent grids methods and Gaussians can be useful as complimentary methods, for example using accurate grid calculations to benchmark Gaussian basis sets, or using novel grid methods to improve the speed of Gaussian based calculations.

At the CECAM workshop several different grid based methods were discussed. These included real-space finite difference methods [1, 2], adaptive curvilinear coordinate methods [3, 4], finite element methods [5], multigrid methods, [6] interpolets [7], and wavelets [8, 9, 10, 11]. The limited space here does not allow me to describe them all. Below I shall focus entirely on the wavelet approach. Wavelets are a simple and elegant mathematical concept, as I shall try to show below. Applying wavelet ideas to electronic structure calculations is far from complete at the present time (although several groups are working on development), however I shall try to give some general ideas about how wavelet ideas can be applied in practical electornic structure calculations.

8.3 The Wavelet Concept

'Wavelet theory' became a substantial field of mathematics following some key developments in the early 1980's. The original ideas built on physics concepts, such as scaling transfomations and localized wave packets, developing a powerful mathematical formalism from these concepts [12, 13]. Very quickly the wavelet ideas were applied in signal analysis and image compression problems. Work on a variety of ordinary and partial differential equations also developed. The first application of wavelet concepts to electronic structure calculation was by Cho et al. [8]

.and more recently by Wei and Chou [9].

The central idea is the concept of a multi-resolution analysis. Normally in signal analysis one samples a signal $f(x)$ at a constant rate, corresponding to a uniform set of points, $f(x_n)$, $x_n = nh$. Obviously h defines a fixed resolution and Fourier components of $f(x)$ can be found up to $\pm\pi/h$. The similarity with plane wave pseudopotential calculations is clear. To do better than this one would like to adjust the resolution h depending on whether $f(x)$ is slowly or quickly varying in a given place. In a **multiresolution analysis** one divides $f(x)$ into component parts, where each component contains the data expressed as well as possible at a given resolution length scale.

The multiresolution analysis process is remarkably similar to the Kadanoff block spin transformation in phase transition theory. The idea is to develop a nested sequence of Hilbert spaces corresponding to coarser and coarser length scales. Suppose there are N function values $f_0(x_n)$, $x_n = nh = nL/N$. The set of all possible function values is an N dimensional vector space, V_0. Using a block-spin idea we can easily imagine transfomations where we eliminate 'fast modes' and define $N/2$ new function values $f_1(x_n)$, $x_n = nh$ for even values of n. The space of such functions f_1 obeys

$$V_0 > V_1 \tag{1}$$

Repeating the process to decimate again and again we can generate a sequence of spaces on coarser and coarser scales

$$V_0 > V_1 > V_2 > V_3 > \ldots. \tag{2}$$

Space V_p has dimension $N/2^p$. The sequence obvously ends when there is only a single data point left. A specific example of such scaling transfomation might be an average or sum of adjacent points

$$f_{p+1}(x_n) = f_p(x_n) + f_p(x_{n+d}) \tag{3}$$

where $d = 2^p$ the spacing of points in function f_p is $2^p h$. For simplicity I assume periodic boundary conditions, $n + N \equiv n$. The coarse grained functions f_p contain all of the information present in the function at the given scale of resolution.

The above scaling transformation 'coarse grains' the function onto longer and longer length scales. However it is not invertible, since we have not yet defined a way to go back form the coarse grained data to a finer scale. The wavelet transformation does that, making an invertible (and in some cases unitary) transform. What is needed is to retain information about the high frequency components. For example to invert Eq. 3 we obviously need to retain information about the differences:

$$h_{p+1}(x_{n+d}) = f_p(x_n) - f_p(x_{n+d}), \tag{4}$$

with $d = 2^p$. This defines a new sequence of functions h_p $p = 1, 2, ...$ containing only the high frequency data. In terms of the Hilbert spaces, the $N/2^p$ dimensional space V_p has been divided into two spaces of half the size:

$$V_p = V_{p+1} \oplus W_{p+1} \tag{5}$$

where W_p is the space of possible functions h_p. Scaling several times, the original function N dimensional space V_0 has been divided into spaces of dimension $N/2$, $N/4$, ...

$$V_0 = W_1 \oplus W_2 \oplus \ldots \oplus W_P \oplus V_P. \tag{6}$$

The final space V_P can contain as little as one point.

The 'fast wavelet transform' (FWT) of a function $f_p(x_n)$ in this example is a band matrix multiplication:

$$\begin{pmatrix} f_{p+1}(x_0) \\ h_{p+1}(x_d) \\ f_{p+1}(x_{2d}) \\ h_{p+1}(x_{3d}) \\ \cdots \\ \cdots \end{pmatrix} = \begin{pmatrix} 1 & 1 & 0 & 0 & \cdots\cdots \\ 1 & -1 & 0 & 0 & \cdots\cdots \\ 0 & 0 & 1 & 1 & \cdots\cdots \\ 0 & 0 & 1 & -1 & \cdots\cdots \\ \cdots & \cdots & & & \\ \cdots & \cdots & & & \end{pmatrix} \begin{pmatrix} f_p(x_0) \\ f_p(x_d) \\ f_p(x_{2d}) \\ f_p(x_{3d}) \\ \cdots \\ \cdots \end{pmatrix}. \tag{7}$$

This is obviously unitary, apart from an overall factor of $1/\sqrt{(}2)$. The inverse transform is thus also simply a matrix multiply, using the transpose of the above matrix. To scale from the original function from f_0 to f_P requires repeating the above matrix multiplication to $p = 0$, $p = 1$, $p = 2, \ldots p = P - 1$. If the original data has N points, the CPU time to do this is of order $N + N/2 + N/4 + \ldots \approx 2N$. The FWT is thus an $O(N)$ algorithm, rather than the $O(N \log N)$ FFT. The particular form for the matrix in Eq. 7 is called the Haar wavelet transform. The Daubechies wavelet transforms are also unitary band matrix multiplications, only with a longer bandwidth of 4, 6 or higher. Coding subroutines to do these transforms is simple. Examples are given in Numerical Recipes (2nd Edition only!) [13] or are available form the author. [11]

What is the physical meaning of the coefficients $h_p(x_n)$? They are the coefficients of the function expanded in a new basis, the wavelet basis. This is just like Fourier coefficients which are expansion coefficients of a function in a basis of plane waves. Hence there exist functions $\psi_1(x_n)$, $\psi_2(x_n)$ etc. such that

$$\begin{aligned} f(x_n) = \quad & \textstyle\sum_m h_1(x_m)\psi_{1m}(x_n) + & (8) \\ & \textstyle\sum_m h_2(x_m)\psi_{2m}(x_n) + & (9) \\ & \ldots + & (10) \\ & \textstyle\sum_m h_P(x_m)\psi_{Pm}(x_n) + & (11) \\ & \textstyle\sum_m \phi_{Pm}(x_n) f_P(x_m). & (12) \end{aligned}$$

The function has thus been decomposed by the FWT into its components on the different basis functions ψ_{1m}, ψ_{2m} .... At the longest lengthscale there is a wavelet ψ_{Pm}, and also a second function, ϕ_{Pm}, usually called the scaling function. (Another more picturesque name is the 'mother wavelet' ψ_{Pm} and the father wavelet ϕ_{Pm}. The smaller scale wavelets ψ_{pm} are then 'daughter' wavelets. There are no sons!) Figure 1 shows the father wavelet, mother wavelet and some daughters for the Daubechies D-4 wavelet transform.

For the Haar and Daubechies wavelet transforms these basis functions are orthonormal. This follows simply because the wavelet transform is unitary. (Recall that unitary transformations, such as Hermitian matrix diagonalization, always preserve the orthonormality of basis vectors). Thus the vectors $\psi_{pm}(x_n)$ and $\psi_{p'm'}(x_n)$ are orthogonal to each other under translation, $m \neq m'$, and under changes of scale, $p \neq p'$. The wavelets, $\psi_{pm}(x_n)$, are also orthogonal to the scaling function ϕ_{Pm} on the longest scale.

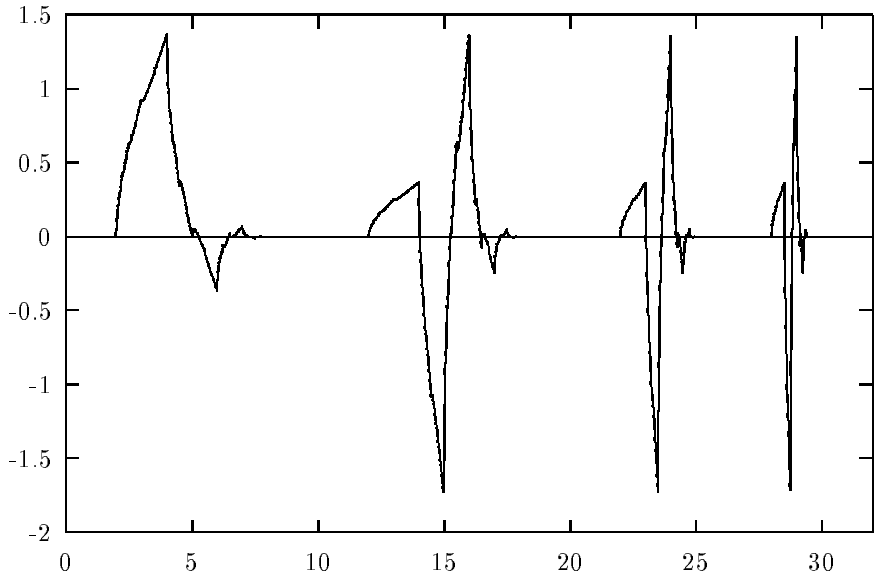

Figure 1: Daubechies D-4 wavelets and scaling function. From left to right: the scaling function (or father wavelet), $\phi_{Pm}(x)$, the longest scale wavelet (or mother wavelet), $\psi_{Pm}(x)$, and two smaller scale (daughter) wavelets, $\psi_{pm}(x)$. The heights have been rescaled for clarity in the plot.

This orthogonality persists after **any** number of scaling transforms. An amazing consequence of this is that there is a continuum limit $N \to \infty$ in which the Daubechies wavelet is defined for all x, $\psi_{pm}(x)$, not just on a set of discrete points. These continuum functions are compact (vanish exactly outside a finite interval), and are again orthonormal under all integer translations and scaling by powers of 2:

$$\int \psi_{pm}(x)\psi_{p'm'}(x) = \delta_{mm'}\delta_{pp'} \tag{13}$$

with

$$\psi_{pm}(x) = 2^{-p/2}\psi(2^{-p}x - m). \tag{14}$$

The Daubechies wavelets (plus the scaling functions) defined in this way form a complete orthonormal set of functions. Using the Haar wavelet transform of Eq. 7 the base wavelet turns out to be just:

$$\psi(x) = \begin{cases} +1 & 0 < x < 1/2 \\ -1 & 1/2 < x < 1 \\ 0 & otherwise \end{cases} . \tag{15}$$

It is easy to see that this function obeys the orthogonality relations 13 under scaling by any power of two, or under translation by any integer. The Daubechies D-4 wavelets in Fig. 1 do not have a simple analytic formula, but can also be proved to be orthonormal under scaling and translation. Unlike the Haar wavelet they are also continuous functions, but unfortunately are not differentiable. Higher order Daubechies wavelets (D-6, D-8 , ...) exist and are smoother, at the expense of being wider in their range of support.

These wavelet bases are useful because of the way they separate contributions from different length scales. If a function is smooth then the high frequency components ($h_p(x_m)$ for small p) will be negligible. However, unlike simple Fourier filtering of the high frequencies the wavelets also retain spatial information. If $f(x)$ has rapid variation in some region, say near x_0, and is

smooth elsewhere then the wavelet coefficients $h_p(x)$ will be negligible except near x_0. Retaining the big coefficients near x_0 and dropping the others one can represtent $f(x)$ very compactly. Because high frequencies are retained where needed the function retains its sharp fetures, while saving storage by eliminating high frequenciy components where the function is smooth. It is for this reason that wavelets have found important applications in image compresson algorithms. One minimizes storage by efficiently representing the regions where the image varies slowly, while still retaining sharp edges where the function varies rapidly. Typically wavelet methods can effectively reduce image data set sizes to of order 1%. In the electonic structure context the analog is clear. One wants to represent the regions where the wave function is smooth using relatively few coefficients, while retaining high frequency components where the wave function has rapid variation, e.g. near the atomic cores.

8.4 Cubic B-spline Wavelets

There are many different types of wavelet optimized for various properties. The Daubechies wavelets have the advantage of compactness (vanishing exactly outside some interval) and orthonormality. However the Daubechies wavelets are not very smooth, as Fig. 1 shows for the D-4 wavelets. The higher order Daubechies wavelets are smoother, but at the expense of extending over a longer range. Wei and Chou recently applied D-6 wavelets to electronic structure calcualtions.

I have chosen to work with wavelets derived from cubic B-splines [14]. These are a good compromise between smoothness and compactness. They are not orthogonal, but this is not necessarily a problem in quantum mechanics applications. A B-spline (basis-spline) is a localized function made out of smoothly joined polynomials [15]. For evenly spaced points (called spline knots), spacing h, and using cubic polynomials the basic B-spline is simply

$$b_0(x) = \begin{cases} (2 + x/h)^3/6 & -2h < x \leq -h \\ (4 - 6(x/h)^2 - 3(x/h)^3)/6 & -h < x \leq 0 \\ (4 - 6(x/h)^2 + 3(x/h)^3)/6 & 0 < x \leq h \\ (2 - (x/h))^3/6 & h < x \leq 2h. \end{cases} \tag{16}$$

By construction $b_0(x)$ is compact and twice differentiable. Making a set of N functions by translation (again with periodic b.c.),

$$b_{0m}(x) \equiv b_0(x - x_m)) \tag{17}$$

for $x_m = mh$, yields an N dimensional Hilbert space. A function in this space is of the form

$$f(x) = \sum_m f_m b_{0m}(x). \tag{18}$$

Any such function is obviously a cubic polynomial between the knots, x_m, and is continuous and smooth at the knots. I.e the function is a spline function, such as those found by spline fits interpolation of N evenly spaced data points, $f(x_m)$). The Hilbert space spanned by the B-splines is the space of all such spine functions.

This Hilbert space is convenient for doing quantum mechanics since all functions in the space are necessarily twice differentiable. Furthermore smooth wave functions are well represented in

this basis set because they are locally close to polynomial. A simple estimate of the error in such a basis comes from calculating the kinetic energy of a plane wave $\psi(x) = \exp(ikx)$ represented in the basis. The energy is $\epsilon(k) = k^2/2 + O(k^6h^8)$, showing a very rapid convergene as $h \to 0$, similar to that of a high order finite difference scheme.

The cubic B-splines can be made into a wavelet basis set by considering changes of scale. Defining

$$b_1(x) = b_0(x/2) \tag{19}$$

gives a function exending over range wider by a factor of 2, from -4h to +4h. This function has spline knots at at the even numbered points $x = 2nh$. Translating this function, $b_{1m} = b_1(x - x_m)$ for $n = 0, 2, 4, \ldots$, gives a Hilbert space of dimension $N/2$. This space is exactly contained in the original N dimensional space, since any spline function defined at $N/2$ evenly spaced knots is obviously a special case of splines defined at N knots. We thus have a situation exactly like Eq. 1. In fact one can easily verfy that the B-splines obey the 'scaling equation'

$$b_1(x) = \frac{b_0(x-2h)}{8} + \frac{b_0(x-h)}{2} + \frac{3b_0(x)}{4} + \frac{b_0(x+h)}{2} + \frac{b_0(x+2h)}{8}. \tag{20}$$

Taking a function defined on the original N basis functions b_{0m}, and projecting a function onto the $N/2$ dimensional space defined by the b_{1m} is exactly analogous to the coarse graining in Eq. 3. The corresponding wavelets represent the high frequency information not included in the coarse graining. In this case a suitable compact, smooth and symmetric wavelet is

$$w_1(x) = -\frac{b_0(x-h)}{2} + b_0(x) - \frac{b_0(x+h)}{2}. \tag{21}$$

Repeating the scaling proceeduce produces wavelets on longer and longer length scales w_2, w_3 etc, similar to the Daubechies wavelets. After a B-spline wavelet transform the original function, Eq. 18 is thus expanded in terms of this wavelet basis as follows:

$$\begin{aligned} f(x) = & \sum h_{1m} w_{1m}(x) + \\ & \sum h_{2m} w_{2m}(x) + \ldots \\ & + \sum h_{Pm} w_{Pm}(x) + \sum f_{Pm} b_{Pm}(x) \end{aligned} \tag{22}$$

quite analogously to Eq. 12. The B-spline functions $b_{Pm}(x)$, are $w_{pm}(x)$ are shown in Fig. 2.

One can also scale the other way, to finer and finer scales. This defines wavelelts w_{0m}, w_{-1m}, $w_{-2m}\ldots$. Since w_{pm} corresponds to a spatial resolution $h = 2^p L/N$ this is equivalent to adding points giving higher and higher resolution in the wave function. The basis set is clearly complete in this $h \to 0$ limit.

8.5 Electronic Structure with Wavelets

Applying these wavelet bases to electronic structure problems is simple in principle, but not so easy in practice. The first change from a plane wave pseudopotential method into a wavelet basis is to replace the usual FFT evaluation of the Bloch wave functions

$$\psi_{n\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{\Omega}} \sum_{\mathbf{G}} c_{\mathbf{G}n\mathbf{k}} \exp\left[i(\mathbf{k}+\mathbf{G}).\mathbf{r}\right] \tag{23}$$

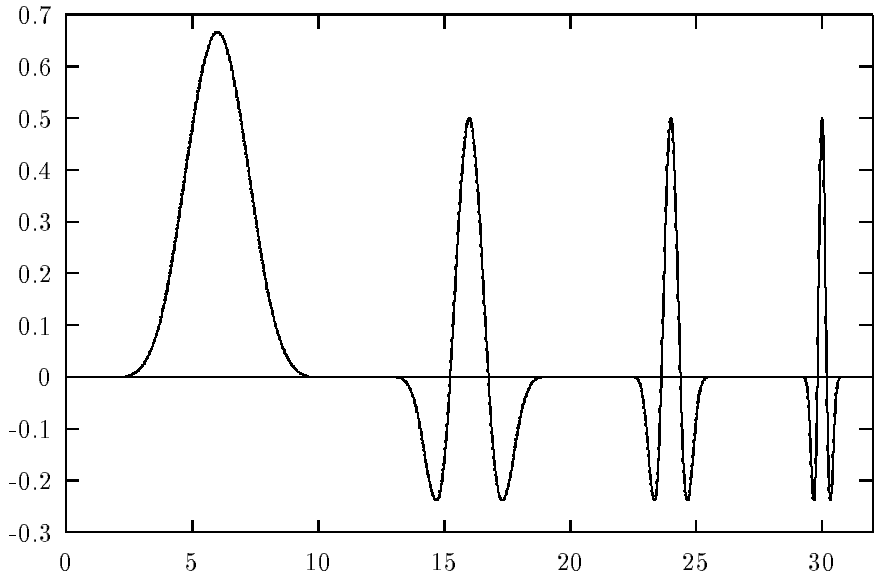

Figure 2: Cubic B-spline scaling function and wavelets of increasing resolution.

with a corresponding fast wavelet transform. In the case of B-spline wavelets this is

$$\psi_{n\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{\Omega}} \left(\sum_{\mathbf{pm}} h_{\mathbf{pm}n\mathbf{k}} w_{\mathbf{pm}}(\mathbf{r}) + \sum_{\mathbf{m}} f_{\mathbf{Pm}n\mathbf{k}} b_{\mathbf{Pm}}(\mathbf{r}) \right). \tag{24}$$

where P is the coarsest scale of wavelets included in the basis set. Here for brevity $\mathbf{p} \equiv (p_1, p_2, p_3)$ and the three dimensional wavelets are just products of 1-d wavelets

$$w_{\mathbf{pm}}(\mathbf{r}) \equiv w_{p_1 m_1}(r_1) w_{p_2 m_2}(r_2) w_{p_3 m_3}(r_3). \tag{25}$$

For general unit cells it is convenient to change variables so that

$$\mathbf{r} = r_1 \mathbf{a}_1 + r_2 \mathbf{a}_2 + r_3 \mathbf{a}_3 \tag{26}$$

where $\mathbf{a}_1$ etc. are the Bravais lattice vectors. In terms of the r_i the unit cell is then just the unit cube $0 \leq r_i < 1$.

Instead of the FFT one uses the wavelet transform Eq. 7 (actually the inverse of Eq. 7) to expand out the long scales and hence evaluate $\psi_{n\mathbf{k}}(\mathbf{r})$ in real space. From $\psi_{n\mathbf{k}}(\mathbf{r})$ one can obtain the charge density $n(\mathbf{r})$, Coulomb potential and so on. Since the wavelet fransform is similar in speed to the the FFT (actually N not $N \log N$)) this is clearly a competitive method. Furthermore the wavelet transform can be made even faster is one can make use of the fact that most of the wavelet expansion coefficients (the h_{pm} in Eq. 12) will be negligible. Thus with a wavelet basis one can hope to save in terms of memory used (only non-zero h_{pm} need be stored) as well as CPU time.

Several groups are now working on wavelet methods in electronic structure [8, 9, 10, 11]. Other closely related approaches, such a multi-grid methods, finite elements and interpolets are also under development. In principle these efficient basis sets can also be combined with the advantages of massively parallel and/or order N algorithms. It will be exciting to see just what sort of physics problems will be solvable in the future with these powerful combinations of techniques!

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