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Contract/Grant Number N00014-92-J-1752

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MATRIX/SECOND-PHASE-PARTICLE INTERFACES

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K. Cho, T. Arias, J. Joannopoulos and P. Lam, "Wavelets in Electronic Structure Calculations", submitted to Phys. Rev. Letters 1993.

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6 May 1993

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Dear George:

This letter is meant to be a progress report for the period March 1, 1992 to February 28, 1993 of our grant with ONR #N00014-92-J-1752. I am also enclosing a PPPH report for your records.

Although this is the first year of this proposal, we have already made significant progress towards our goal to be able to accurately theoretically model and understand the strengths of Matrix/Second-phase-particle Interfaces. Our accomplishments have been along two directions. The first involves using our state-of-the-art ab-initio dynamics approach to calculate the properties of the bare Cu(100) surface. This is needed as a test before we may begin to study the interfaces with the second-phase-particles. The results of our calculations of some structural properties are summarized in Table I.

Table I

Comparison between theory and experiment of various ground state properties of bulk Cu and its (100) surface

Properties of Cu	Theory	Experiment
Lattice constant in bulk (Å)	3.63	3.60
Bulk modulus (M Bu)	1.56	1.42
Bulk cohesive energy (eV/atom)	3.91	3.50
Surface layer relaxation	-4%	-3%
Surface energy (eV/atom)	0.84	0.74 ± .2

As you can see the agreement between theory and experiment is excellent. This is particularly true when you consider that no experimental input enters the theory except for the atomic number of Cu. The electronic charge density of the (100) surface is shown at the top panel of Fig. 1. In order to get a better understanding of the effects of the s-electron and d-electron contributions to this density we show at the bottom of Fig.1 the density obtained by subtracting off the atomic d-electrons. The s-electrons are seen to be very nearly uniformly spread out, almost as if they were free-electron like. This feature could be used in modeling the region away from the Cu interface as a jellium system.

As far as the details of the interface are concerned, we have discovered that we can theoretically design a Cu(100) - TiO₂ interface that is lattice-matched to less than 0.5%! The interface supercell is $\sqrt{13} \times \sqrt{13}$ for Cu and 2×2 for TiO₂. This system will than provide a tractable and interesting interface to study using our ab-initio techniques, and is also possibly an interface that could be made experimentally. We are consistently in contact with Professor Warren Garrison and his group at Carnegie-Mellon and have suggested this new interface as an interesting system to study. Professor Garrison has recently finished some interesting studies of secondary crystallization and most recently has gone on to prepare materials that are internally oxidized. It appears that both theory and experiment are now at the point to begin studies of the interphase interfaces.

The second accomplishment this past year involves the introduction of a new theoretical method that appears to be extremely promising for performing ab-initio calculations of complex material systems. Although the technique is still in a very preliminary form, and not yet capable of studies of the types of material systems of interest for this proposal, it has great potential. The technique involves the introduction of Wavelet Theory and Multi-resolution Analysis to the electronic structure arena. Test calculations on reproducing the 1s states of all the atoms in the periodic table, as well as the ground state of the hydrogen molecule ion, successfully demonstrate the potential power of this new technique. The results for the hydrogen molecule ion are show in Fig. 2. Here the open circles represent the *exact* solution. We have already written a

paper on this subject and sent it out for publication, a copy of which is enclosed with this letter.
We are very excited about the prospects of this new approach, and plan to pursue it vehemently.

I hope this is sufficient. If you need any additional information please let me know.

Sincerely,

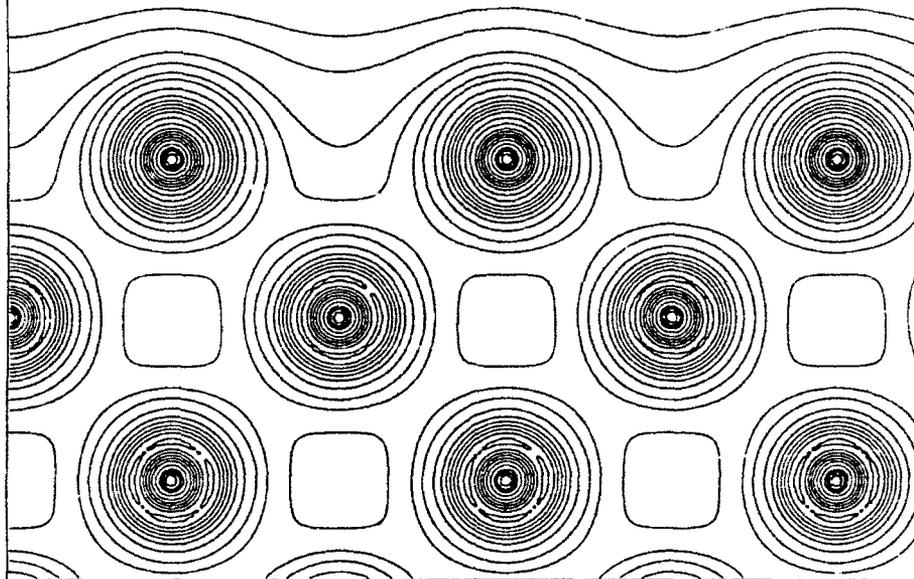


John D. Joannopoulos
Professor of Physics

JDJ:ia

Cu (100) : Total Valence Electron Density

Vacuum



Cu (100) : Total Valence Electron Density minus
Atomic d-Electron Density

Vacuum

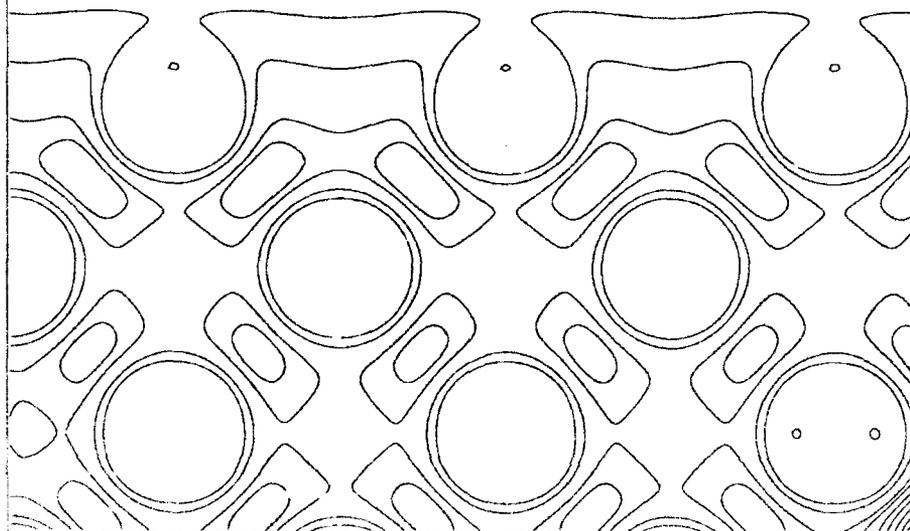


Fig. 1.

Hydrogen Molecule ion

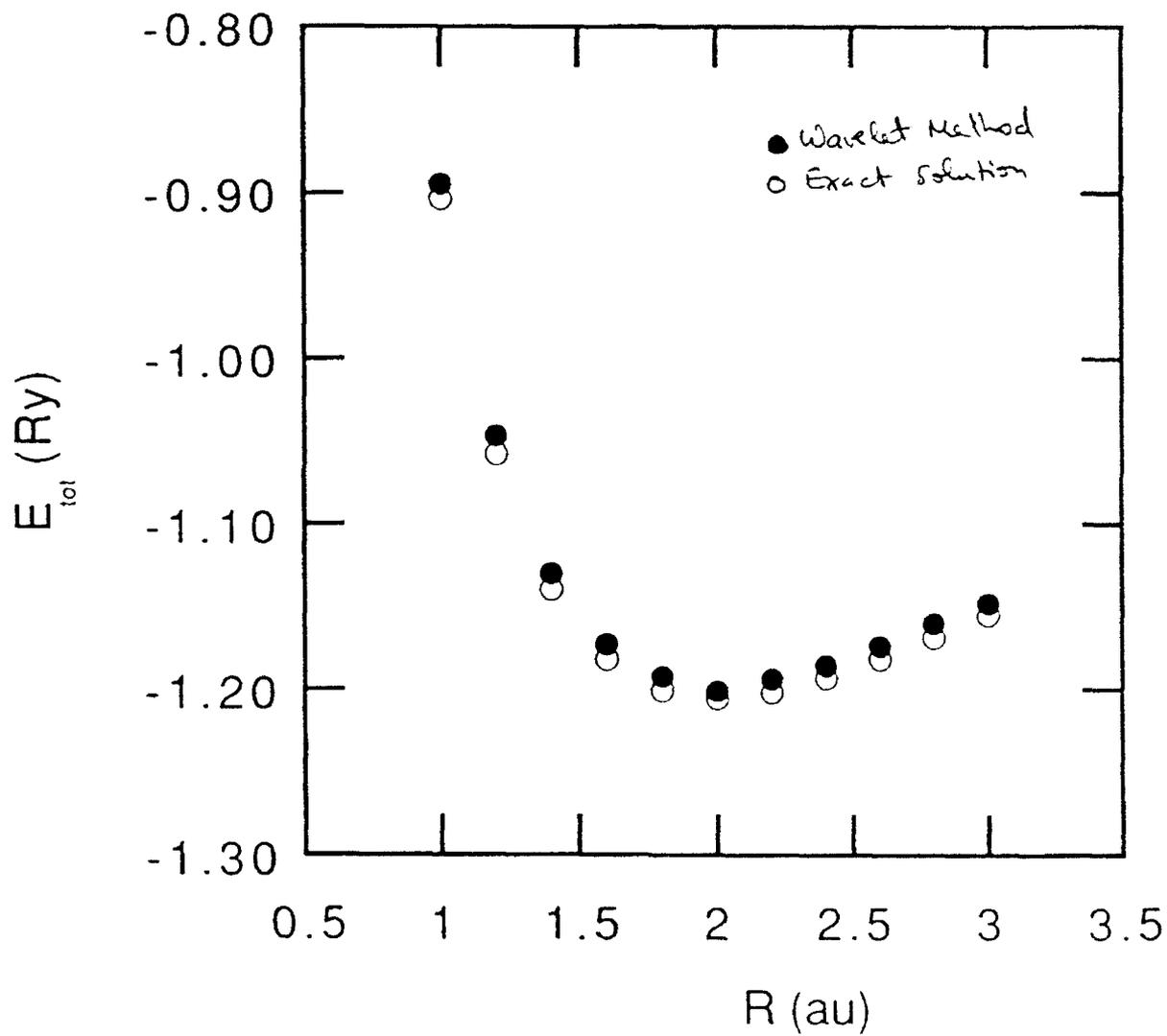


Fig. 2.

Apr 20, 1993

Wavelets in Electronic Structure Calculations

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A three dimensional (3D) wavelet analysis is employed to develop a new formalism for electronic structure calculations. The wavelet formalism provides a systematically improvable and tractable description of electronic wavefunctions and overcomes limitations of conventional basis expansions. The potential power of the wavelet formalism for *ab initio* electronic structure calculations is demonstrated by a calculation of 1s states for all the naturally occurring nuclei on the periodic table and the interaction energies of the hydrogen molecule ion.

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Spectral analysis using the Fourier transform (FT) is a powerful method for solving many problems in science and engineering. This method, however, is not appropriate for problems that require a localized description in real space *and* in Fourier space. Although several techniques, such as the windowed Fourier transform, have been invented to attempt to overcome this limitation, by far the most promising new technique is the wavelet transform (WT) [1]. Unlike the plane wave (PW) basis functions of the FT, the wavelet basis functions are localized both in real space *and* in Fourier space [1-4]. Furthermore, multiresolution analysis (MRA) of the WT provides a systematic successive approximation scheme for practical applications [1,2]. Applications of the WT have focussed primarily on digital signal processing (1D), compact image coding (2D), and related fast mathematical algorithms [3]. Most recently the WT has been applied to the analysis of chaotic behavior and turbulence in 2D, the coherent states of quantum optics and quantum field theory, and to real space renormalization group theory [4].

In this letter, we introduce a new method for the application of WT, in 3D, to electronic structure investigations of material properties. The traditional *ab initio* total energy density functional pseudopotential methods for electronic structure calculations use either LCAO-type (*e.g.* atomic, Gaussian, or Slater) basis sets or PW basis sets [5]. LCAO-type basis sets typically are capable of describing the electronic structure with a small number of basis functions, but lack an explicit and well-defined procedure for systematic improvement [6], and generally complicate the calculation of forces because of the presence of Pulay terms [7]. On the other hand, PW basis sets provide a systematic expansion of electronic wavefunctions, and simple algorithms for calculating forces, but suffer from the same limitations as the FT method. Specifically, the description of the rapid variations of the electronic wavefunction close to the atomic nuclei (atomic core) requires a large number of PW functions even though

the volume of the atomic core is only a small part of the total volume of the system. In addition PW basis sets are, in principle, not well suited for the description of isolated molecules and surfaces. This is because the periodic nature of the basis introduces unnecessary periodic images and a redundant high resolution description of the vacuum regions.

The "best of all worlds" then would be to have a basis set that, unlike a PW basis, can zoom into the atomic core regions and does not introduce unnecessary periodic images, *and*, unlike an LCAO-type basis, does not have Pulay terms and provides an explicit prescription for complete expansion of the electronic wavefunctions. The wavelet basis has all these desired properties: multiscale decomposition of the wavefunction, the localized description of the rapid variations, and systematically complete expansion similar to the PW expansion. Therefore, as we demonstrate in this letter, the wavelet basis overcomes the limitations of both conventional basis sets and retains only their advantages.

We begin our discussion with a brief review of the basic concepts underlying wavelets. We then extend the wavelet formalism to the solution of the Schrödinger equation with the introduction of spherically symmetric basis functions. As a simple example we apply our technique to the study of a hydrogen atom. We then demonstrate that a *single* small basis set is capable of calculating accurately the 1s states of all the nuclei from Hydrogen through Uranium! Finally we demonstrate that a wavelet basis can easily describe covalent bonding and illustrate its use with the hydrogen molecule ion (H_2^+). We conclude with a discussion of the straightforward extension of the current analysis to periodic systems and all electron calculations.

The wavelet transform and multiresolution analysis. - Given a square integrable function space $L^2(R^3)$, wavelets impose a hierarchical structure of subspaces with different resolutions which forms a multiresolution analysis. The space of functions at

resolution 2^{-j} (or more simply at resolution j) is represented by $V_j(R^3)$, and spanned by the basis set of *scaling functions* at resolution j , $\{\phi_{j,n}(\mathbf{r})\}$, where n specifies the center of the basis function. The hierarchical structure is then

$$\cdots V_{-2} \subset V_{-1} \subset V_0 \subset V_1 \subset V_2 \cdots \quad (1)$$

The *approximation* space V_j is decomposed into a sum of the coarser approximation space V_{j-1} and the *wavelet* space W_{j-1} which describes the detail at resolution j ($V_j = V_{j-1} \oplus W_{j-1}$) and is spanned by the basis set of the *wavelet functions* at resolution j , $\{\psi_{j,n}(\mathbf{r})\}$. With a repetition of this decomposition, the $L^2(R^3)$ space can be expressed as either the sum of the wavelet spaces of all resolutions or the sum of one approximation space and the wavelet spaces of higher resolutions:

$$\bigoplus_j W_j = V_{j_0} \oplus \bigoplus_{j=j_0} W_j = L^2(R^3). \quad (2)$$

Therefore, any square integrable function $f(\mathbf{r})$ can be expanded either as a sum of the wavelet functions of all resolutions or as a sum of the scaling functions at resolution $j = j_0$ and the wavelet functions of all finer resolutions $j \geq j_0$. In this work, we will use the latter expansion because it introduces approximations only at the high resolution cutoff in practical applications.

With the introduction of two projection operators, \hat{A}_j (approximation operator) and \hat{D}_j (detail operator), which project a function into V_j and W_j , respectively, one may express $f(\mathbf{r})$ as

$$f(\mathbf{r}) = \hat{A}_{j_0} f(\mathbf{r}) + \sum_{j=j_0} \hat{D}_j f(\mathbf{r}). \quad (3)$$

The approximation and the detail of a function $f(\mathbf{r})$ at resolution j are expanded in terms of the basis functions,

$$\hat{A}_j f(\mathbf{r}) = \sum_{\mathbf{n}} a_{j,\mathbf{n}} \phi_{j,\mathbf{n}}(\mathbf{r}), \quad (4)$$

$$\hat{D}_j f(\mathbf{r}) = \sum_{\mathbf{n}} d_{j,\mathbf{n}} \psi_{j,\mathbf{n}}(\mathbf{r}). \quad (5)$$

Combination of Eqns. (3)-(5) and truncation at the finest resolution j_{max} leads to the wavelet expansion of $f(\mathbf{r})$ as

$$f(\mathbf{r}) = \sum_{\mathbf{n}} a_{j_0, \mathbf{n}} \phi_{j_0, \mathbf{n}}(\mathbf{r}) + \sum_{j=j_0}^{j_{max}} \sum_{\mathbf{n}} d_{j, \mathbf{n}} \psi_{j, \mathbf{n}}(\mathbf{r}). \quad (6)$$

This expansion still contains an infinite number of basis functions associated with the lattice $\{\mathbf{n}\}$. Since the scaling functions and the wavelet functions are spatially localized, one may retain only the basis functions that have significantly large coefficients in Eqn (6) for the problem at hand. This leads to an expansion with a finite number of basis functions and allows one to use different resolutions for different spatially localized regions. In particular, for the description of the rapid oscillations of the electronic wavefunction in an atomic core region, one need add higher resolution scales *only* to the core region and thereby systematically improve the calculation.

Construction of a wavelet basis set. - Although the wavelet and scaling functions are far from unique, we found that the following forms are particularly convenient in practical applications. The wavelet functions $\psi_{j, \mathbf{n}}(\mathbf{r})$ are chosen to be the Mexican-hat functions (the Laplacians of Gaussians) which form a fairly tight frame [1]. The scaling function $\phi_{0, \mathbf{n}}(\mathbf{r})$ corresponding to the Mexican-hat function is chosen to be a Gaussian function. Both the Mexican-hat functions and the Gaussian functions are spherically symmetric. The relationship between the Gaussian scaling function and the Mexican-hat wavelet function is not exact, but is quite a good approximation as discussed in Ref. 1. These localized basis functions are spatially arranged so that their centers form a simple cubic lattice [8]. This is shown schematically in the top panel of Fig. 1. The lattice spacing d_0 at resolution $j = 0$ is chosen small enough to give a fairly tight frame [1,9]. The basis functions with resolution j are arranged correspondingly on the lattice sites with lattice spacing $d_0/2^j$. The centers of basis functions for different resolutions are selected so as not to overlap, and the

centers of *all* the basis functions form a simple cubic lattice with spacing $d_0/2^{j_{max}}$. In order to construct a *finite* basis set we collect the most important basis functions by introducing spheres of finite support radii at each nuclear center. This is illustrated schematically at the bottom panel of Fig. 1. Correspondingly smaller support radii are chosen for correspondingly higher resolutions so that deep core regions have more resolution scales. We designate this finite basis set as $\{\phi_{0,n}(\mathbf{r}), \psi_{j,n}(\mathbf{r}); j_{max} \geq j \geq 0\}$ or more compactly as $\{b_i(\mathbf{r})\}$ where i is a simplified notation for $\{j, n\}$.

Solution of Schrödinger equation. - The Schrödinger equation, $\hat{H}|\Psi\rangle = \epsilon|\Psi\rangle$, for electronic structure calculations becomes a generalized eigenvalue problem in a general nonorthogonal wavelet basis. Expansion of the wavefunction in terms of the basis function ($|\Psi\rangle = \sum_i c_i |b_i\rangle$) leads to the secular equation,

$$\sum_i \langle b_j | \hat{H} | b_i \rangle c_i = \epsilon \sum_i \langle b_j | b_i \rangle c_i. \quad (7)$$

With our choice of wavelet and scaling functions, all the matrix elements in Eq. (7) can be calculated analytically. Solution of Eq. (7) may then proceed by a number techniques including square root matrix diagonalization [10], Cholesky decomposition [11], molecular dynamics [5], and conjugate gradients [5] approaches. In this work we have used both square root matrix diagonalization and conjugate gradients approaches.

The hydrogen atom. - In order to gain a sense of the optimal values of the various parameters of the formalism, we chose to study the hydrogen atom as a simple test case. After performing calculations using many different resolution scales and different support radii, we find that a satisfactory minimal basis set for the Hydrogen atom contains 25 basis functions with four resolution scales: (7 scaling functions for $j = 0$, plus 6 wavelets for $j = 0$, plus 6 wavelets for $j = 1$, plus 6 wavelets for $j = 2$) which we designate simply as (7 + three 6's). These correspond respectively to support

radii of $1au$, $0.5au$, $0.25au$, and $0.125au$. The calculated $1s$ eigenenergy is within 2% of the exact value, and the calculated $1s$ radial wavefunction is shown in Fig. 2 (top panel). The calculated wavefunction differs from the exact one primarily near the origin (within the resolution limit j_{max}). The small difference at $r = 2au$ is due to the finite support radii used for the basis set. By increasing the support radii, the difference at $r = 2au$ disappears as shown in the bottom panel of Fig. 2. The result in the bottom panel of Fig. 2 corresponds to a basis set of 85 basis functions with three resolution scales (33 + two 26's) with support radii ($2au$, $1au$, and $0.5au$), and gives the $1s$ eigenenergy to within 0.5% of the exact value.

Hydrogen to Uranium. - By adding more resolution scales, one can calculate the wavefunctions of heavier nuclei *within the same accuracy* as follows. As the atomic number increases, the Coulomb potential becomes stronger, and consequently higher resolution scales are needed in the core region. However, only *one* additional resolution scale needs to be added each time the atomic number doubles. Therefore, for the description of $1s$ wavefunctions from Hydrogen to Uranium, one needs to use a basis set with eleven resolution scales (7 + ten 6's). Using this fixed basis set consisting of *only* 67 basis functions, one can calculate (to within 3%) the $1s$ eigenvalues of all the naturally occurring nuclei on the periodic table! The results are shown in Fig. 3 and include, for simplicity, only the even nuclei. Note that the eigenvalue for each nucleus is larger than the exact value by very nearly a constant percentage so that the results appear to lie on a straight line as expected.

The hydrogen molecule ion. - We now investigate the efficiency of the wavelet basis for the description of chemical bonds. As a simple example, we consider the energy of an H_2^+ molecule as a function of the separation R between the two protons. The total energy (electronic eigenenergy plus the Coulomb potential energy) is plotted as a function of R in Fig. 4. The basis set for the calculation is selected using the same

support radii as for the hydrogen atom calculation with the larger basis set (Fig. 2 bottom panel), and the total number of basis functions varies between 141 and 167 [12] depending on R . It is important to note that the centers of the basis functions are *not* following the nuclei as the separation R changes; *i.e.*, the underlying infinite basis set is not correlated to the ionic positions. Rather, it is the support spheres, which are attached to each nucleus, that designate and determine the finite basis set as illustrated in the bottom panel of Fig. 1. This property of the basis set does not lead to Pulay forces, and allows the wavelet functions to overcome the limitations of LCAO-type basis functions [7]. Finally we note that the calculated values in Fig. 4 are larger than the exact values [13] by a nearly constant amount of 1%. This implies that the wavelet basis also gives an excellent representation of ionic forces.

Conclusions. - We have developed a 3D wavelet formalism that is applicable in general to electronic structure investigations of materials, and have demonstrated its potential power by performing calculations of the deepest core states of all the nuclei on the periodic table and the interaction energy of an H_2^+ molecule. The wavelet expansion with a small number of basis functions gives an accurate description of the wavefunction both in an atomic core region and in a chemical bond. To extend this approach to many-electron systems within LDA, one can simply use traditional techniques for inclusion of Hartree and exchange-correlation interactions. In particular, schemes developed for localized basis sets [14] provide one natural framework for this extension. Finally, the extension of the current analysis to periodic systems is straightforwardly achieved by introducing a Bloch transformation of the wavelet functions [15]. With the extensions to many-electron systems and periodic systems, the wavelet formalism can open a completely new direction of the development for *ab initio* total energy calculations.

Acknowledgment. - This work was supported in part by ONR Grant No. N00014-

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- ² Charles K. Chui, *An Introduction to Wavelets* (Academic Press, Boston, 1992).
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- ⁴ M. B. Ruskai *et al* (Eds.), *Wavelets and their Applications* (Jones and Bartlett, Boston, 1992).
- ⁵ M. C. Payne, M. P. Teter, D. C. Allan, T. A. Arias, and J. D. Joannopoulos, *Rev. Mod. Phys.* **64**, 1045 (1992).
- ⁶ Improvement of LCAO-type basis sets is an art requiring experience and knowledge of the system under study. In contrast PW basis sets offer guaranteed systematic convergence merely by increasing the kinetic energy of the basis set.
- ⁷ P. Pulay, *Mol. Phys.* **17**, 197 (1969).
- ⁸ We have also tested fcc and bcc lattices and obtain similar results to the sc lattice.
- ⁹ For the examples treated in this work d_0 is chosen to be $1au$, and the Gaussian width is $1.35au$.
- ¹⁰ This technique reduces a generalized eigenvalue problem to a standard eigenvalue problem by use of the square root of the diagonalized overlap matrix.
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¹² Note that this procedure leads naturally to a linear scaling of the basis set size with the number of atoms in the calculations.

¹³ D. R. Bates, K. Ledsham, and A. L. Stewart, *Phil. Trans. Roy. Soc. London* **246**, 215 (1953).

¹⁴ W. J. Hehre, L. Radom, P. v.R. Schleyer, and J. A. Pople, *Ab initio Molecular Orbital Theory* (John Wiley and Sons, New York, 1986).

¹⁵ The theory of *periodized* wavelets is discussed in Ref. 3.

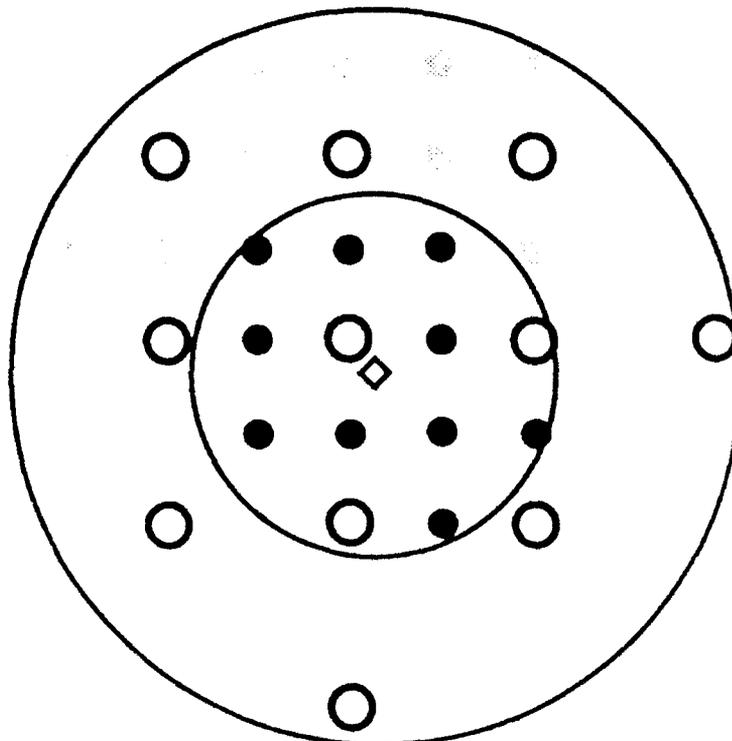
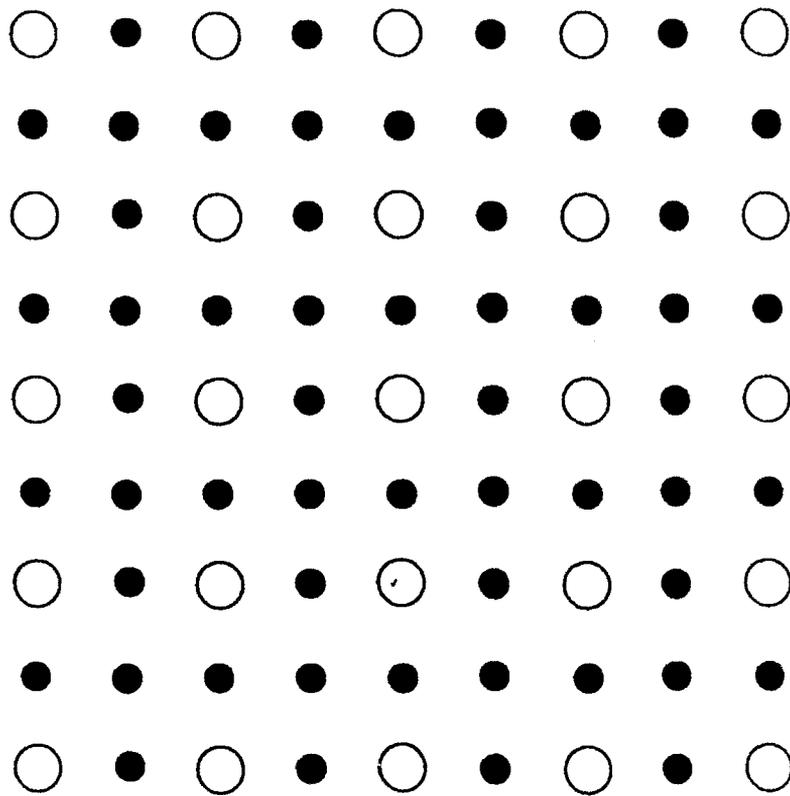
FIGURES

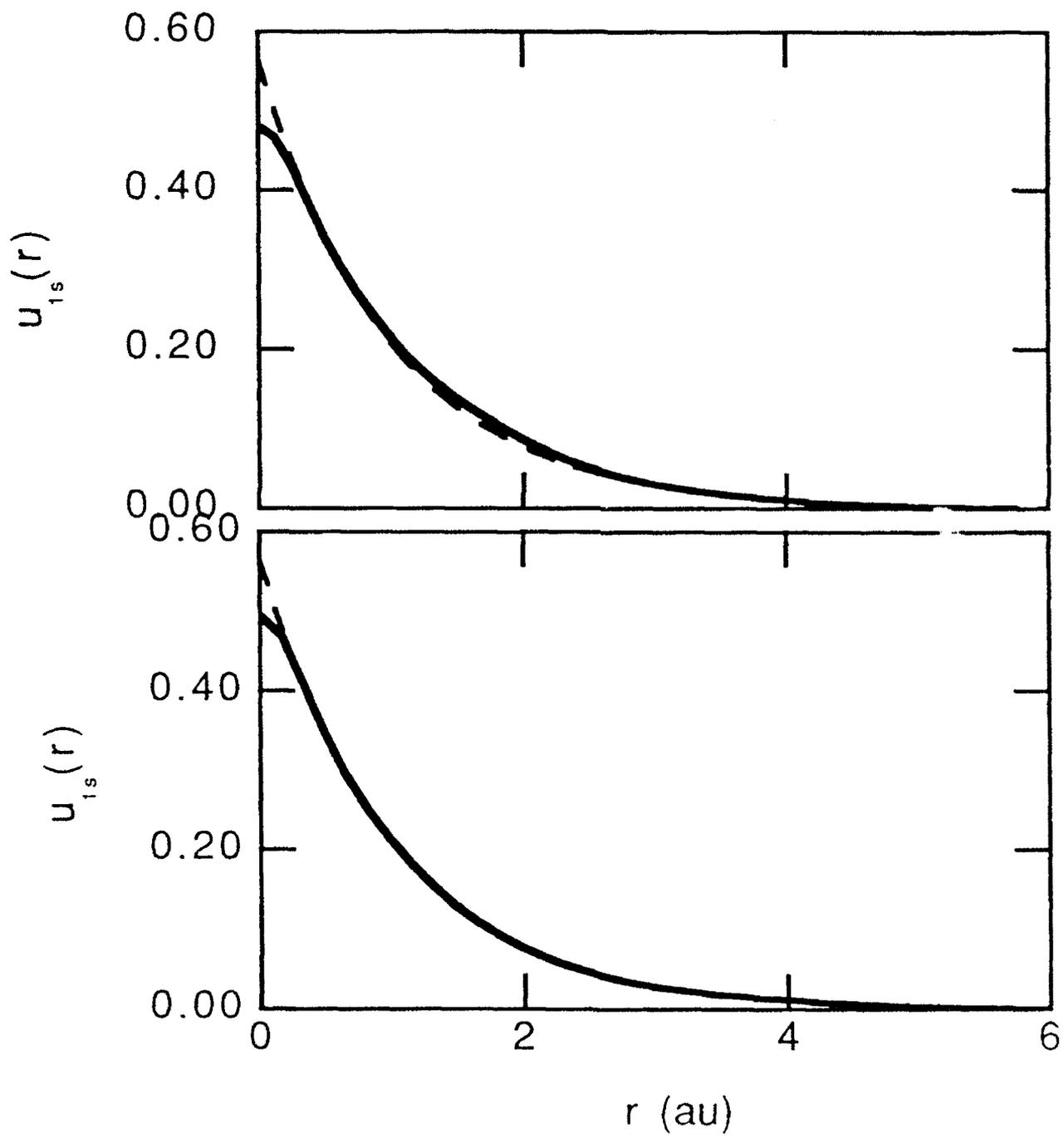
FIG. 1. Top panel shows a two dimensional arrangement of the centers of basis functions on a simple square lattice. Open circles are the centers of the basis functions at resolution $j = 0$, and filled circles are the centers of the basis functions at resolution $j = 1$. Bottom panel shows the basis functions that lie within each support radius that is centered on an atomic position (diamond-symbol). The larger (smaller) radius corresponds to $j = 0$ ($j = 1$) resolution.

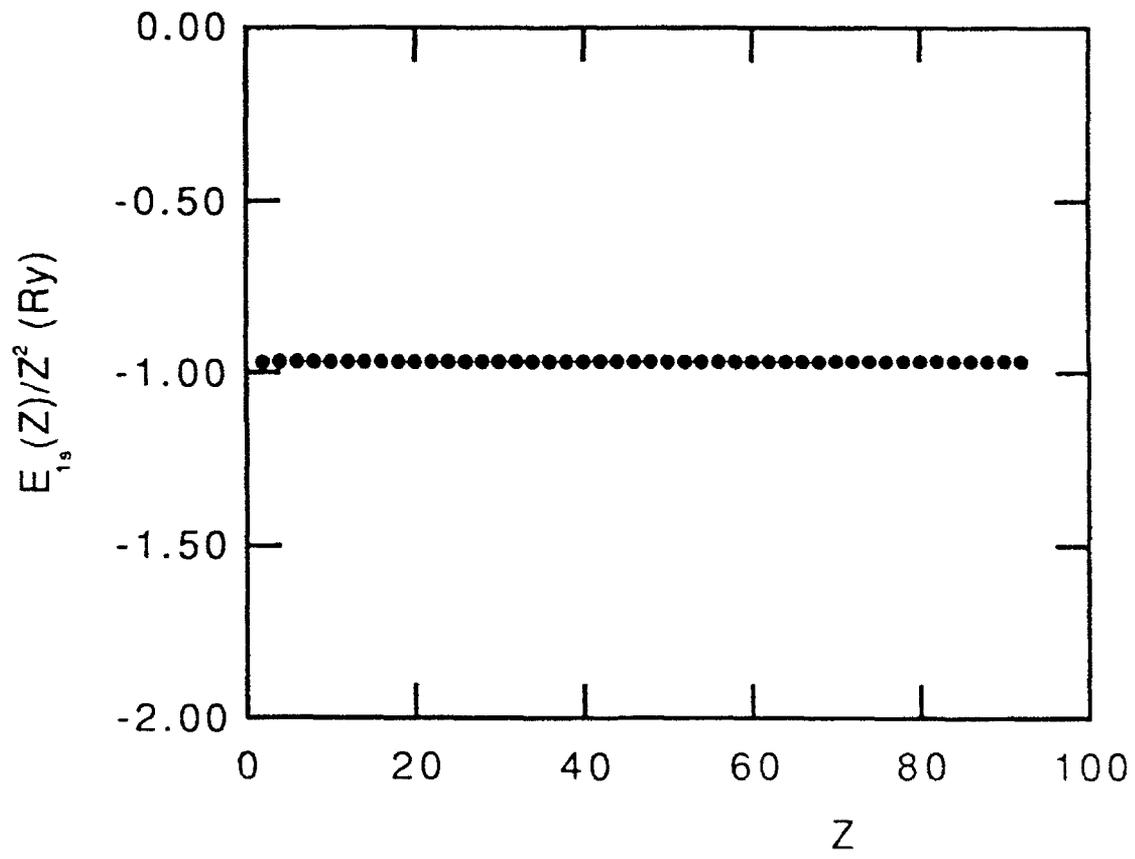
FIG. 2. Top panel shows the 1s radial wavefunction of a hydrogen atom calculated with 25 basis functions (7 + three 6's). Bottom panel shows the 1s radial wavefunction of a hydrogen atom calculated with 85 basis functions (33 + two 26's). The continuous lines are from the wavelet calculations, and the broken lines are the exact wavefunctions.

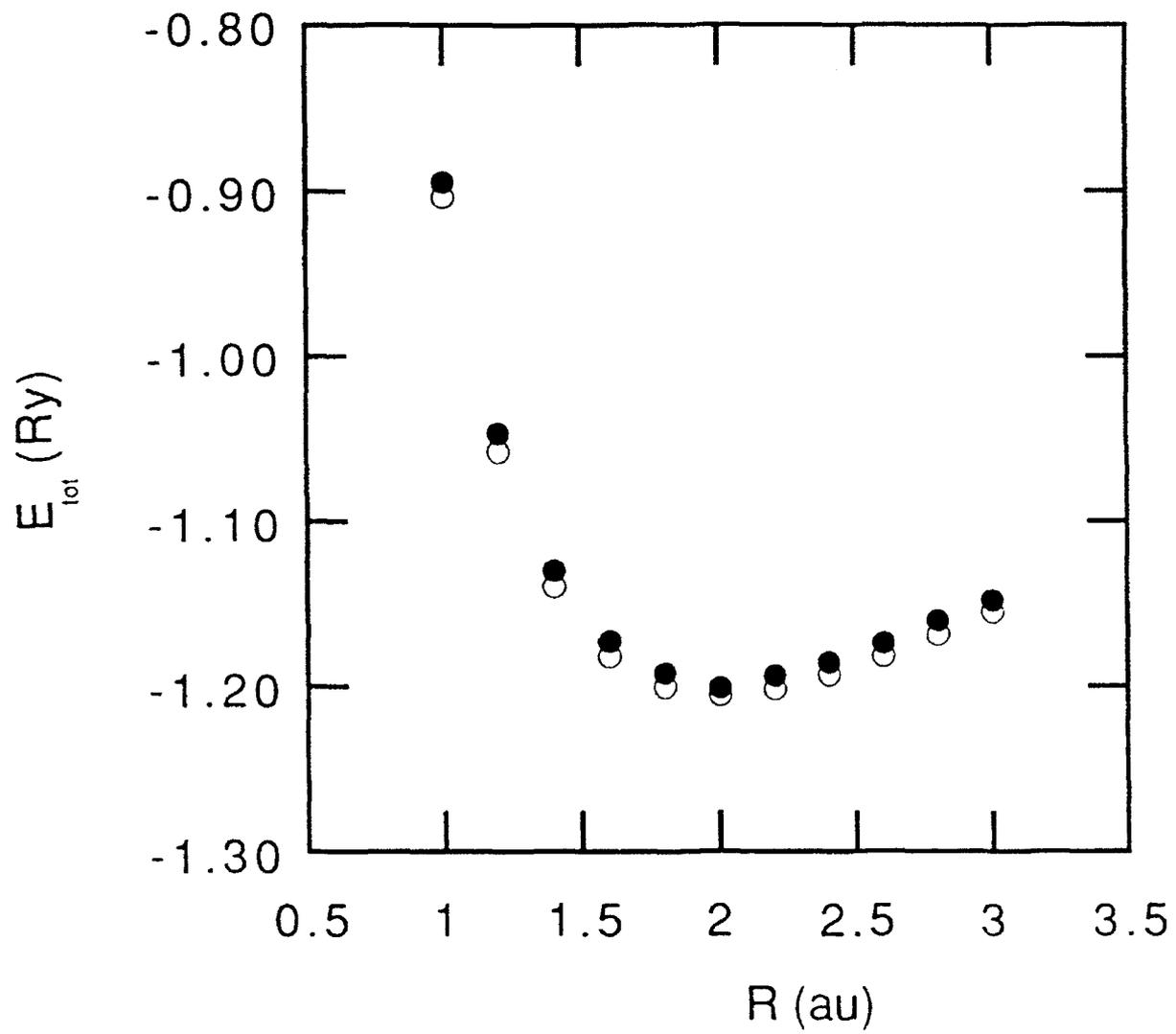
FIG. 3. The filled circles are the 1s eigenenergies of all the nuclei with even atomic numbers on the periodic table ($Z = 2, 4, \dots, 92$) calculated with the fixed 67 basis function set.

FIG. 4. The total energy of a molecular hydrogen ion is shown as a function of the separation between the nuclei. The filled circles are the calculations with 141 to 167 basis functions depending on the separation R . The open circles are the exact values.









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