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Tests of the efficiency of an augmented distorted planewave basis in electronic structure calculations

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Abstract

An augmented distorted planewave plus local orbital basis set has been developed and implemented in a simple fashion in order to test its efficiency for electronic structure calculations. It is based on the idea of using distorted planewaves (Gygi 1993 *Phys. Rev. B* **48** 11692) as basis functions in the interstitial region instead of ordinary planewaves, as in the usual linearized augmented planewave and augmented planewave plus local orbitals methods. This is shown to lead to a significantly more rapid convergence for open structures as well as a modestly improved convergence for close packed structures.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Planewaves are a common and in a sense a natural choice of basis set in electronic structure calculations for crystals. This stems from the fact that planewaves are a complete and orthonormal set, and that each basis function fulfills the crystal symmetry and has a trivial Fourier transform. The disadvantage is that a large number of planewaves are often needed to converge the wavefunction, charge density and potential, which vary rapidly near the atomic centers even with the softest state-of-the-art pseudopotentials. It is well known that the number of necessary basis functions can be drastically reduced by introducing muffin tin (MT) spheres centered at each atom, on which the planewaves are matched onto a set of local functions, which are solutions to the local spherically averaged potential. This is the commonly used augmented planewave (APW) method, proposed by Slater in 1937 [1], which has meanwhile evolved into the accurate and popular linear augmented planewave (LAPW) method [2] and the related augmented planewave plus local orbital (APW + lo) method [3].

Another way of reducing the number of planewaves required was proposed by Gygi in 1993 [4]. By using planewaves on adaptive curved space coordinates, Gygi showed that it is possible to substantially reduce the number of basis functions needed to describe the electronic structure

of solids, molecules and atoms. In this original approach the arbitrary coordinate transformation was used as an additional variational freedom. An alternative formulation was later proposed by Gygi, in which the coordinate transformations were explicit and linked to the atomic positions [5, 6].

In this paper we suggest a combination of APW-like methods and the distorted space method and present tests of this basis set. We keep the basis functions unchanged in the atomic vicinity where we already have powerful methods for finding good basis functions [2, 7, 3], but use planewaves on a distorted space mesh in the interstitial region in order to improve convergence, especially for open systems. After a short introduction to the APW-like methods, we review the concept of distorted planewaves and describe how they can be utilized in the augmentation technique. In this paper we then study the efficiency of this basis using a simplified implementation of the resulting augmented distorted planewave (ADPW) method. We finish with a conclusion and the outlook for future implementations.

1.1. APW + lo basis set

In the APW + lo method, the APW part of the basis set consists of planewaves in the interstitial region, augmented in the MT_α sphere of atom α to radial functions times spherical

harmonics:

$$\phi_{\mathbf{G}}(\mathbf{k}; \mathbf{r}) = \begin{cases} \frac{1}{\sqrt{\Omega}} e^{i(\mathbf{G}+\mathbf{k})\cdot\mathbf{r}}, & \mathbf{r} \in \text{I} \\ \sum_{\ell, m\alpha} a_{\ell m\mathbf{G}}^{\alpha} f_{\ell m}^{\alpha}(r) Y_{\ell m}(\hat{\mathbf{r}}), & \mathbf{r} \in \text{MT}_{\alpha}. \end{cases} \quad (1)$$

The radial functions $f_{\ell m}^{\alpha}(r)$ are solutions to the radial Schrödinger equation (in Hartree atomic units)

$$\left[-\frac{1}{2} \frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} + V(r) - \epsilon_{\ell m}^{\alpha} \right] r f_{\ell m}^{\alpha}(r) = 0, \quad (2)$$

$$f_{\ell m}^{\alpha}(R_{\text{MT}}^{\alpha}) \neq 0,$$

where R_{MT}^{α} is the MT radius of atom α and $\epsilon_{\ell m}^{\alpha}$ is the so-called linearization energy. The matching between the planewaves and the augmentation wavefunctions of an atom at \mathbf{r}_{α} with a MT-sphere radius R_{MT}^{α} is made by the analytical expansion of the planewaves in spherical harmonics, which gives matching coefficients

$$a_{\ell m}^{\alpha} = \frac{4\pi}{f_{\ell m}^{\alpha}(R_{\text{MT}}^{\alpha})\sqrt{\Omega}} e^{i\mathbf{G}\cdot\mathbf{r}_{\alpha}} i^l j_l(|\mathbf{G}|R_{\text{MT}}^{\alpha}) Y_{\ell m}^*(\hat{\mathbf{G}}). \quad (3)$$

In order to incorporate the energy dependence of the local functions $f_{\ell m}^{\alpha}$ some local orbitals are added to the basis set

$$\phi_{\ell m\alpha}^{\text{lo}}(\mathbf{r}) = \begin{cases} 0, & \mathbf{r} \in \text{I} \\ \left(a_{\ell m}^{\text{lo},\alpha} f_{\ell m}^{\text{lo},\alpha}(r) + b_{\ell m}^{\text{lo},\alpha} f_{\ell m}^{\alpha}(r) \right) Y_{\ell m}(\hat{\mathbf{r}}), & \mathbf{r} \in \text{MT}_{\alpha}, \end{cases} \quad (4)$$

where $f_{\ell m}^{\text{lo},\alpha}(r)$ are solutions to the same scalar relativistic version of equation (2) as $f_{\ell m}^{\alpha}(r)$, but with different energy parameters $\epsilon_{\ell m}^{\text{lo},\alpha}$. The matching condition gives $a_{\ell m}^{\text{lo},\alpha} f_{\ell m}^{\text{lo},\alpha}(R_{\text{MT}}^{\alpha}) + b_{\ell m}^{\text{lo},\alpha} f_{\ell m}^{\alpha}(R_{\text{MT}}^{\alpha}) = 0$.

While the necessary local orbitals are in practice fixed and determined by the number of atoms in the unit cell, the number of APWs scales with the unit cell volume. However, the convergence of the APW is determined by the matching at the MT boundary and an empirical rule of thumb is that a sufficiently large basis set is obtained with a planewave cut-off of $G_{\text{max}} = \max_{\alpha} \{2(\ell^{\alpha} + 2)/R_{\text{MT}}^{\alpha}\}$, where ℓ^{α} is the largest open shell azimuthal quantum number for atom α .

We emphasize that in this method, radial functions, generated by numerical solution of the wave equation are used inside atom centered spheres, and that planewaves, while present throughout space, are only used in the interstitial region outside the spheres. Thus in the APW method there are two regions where planewaves provide more variational freedom than needed: (1) far from the atomic centers, as in conventional planewave calculations, and (2) within the MT spheres. On the other hand a very accurate solution is needed at the sphere boundaries in order to obtain proper matching for the augmentation.

2. New basis for the interstitial region

In 1993 Gygi [4] realized that by using planewaves on a distorted space mesh $\mathbf{r}'(\mathbf{r})$, the planewaves could be made to look more like atomic centered basis functions close to the atomic sites:

$$\eta_{\mathbf{G}}(\mathbf{k}; \mathbf{r}) = \eta_{\mathbf{G}}(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} = \frac{1}{\sqrt{\Omega}} e^{i\mathbf{k}\cdot\mathbf{r}} \left| \frac{\partial \mathbf{r}'}{\partial \mathbf{r}} \right|^{1/2} e^{i\mathbf{G}\cdot\mathbf{r}'}, \quad (5)$$

where Ω is the unit cell volume and $|\partial \mathbf{r}'/\partial \mathbf{r}|$ is the determinant of the Jacobian matrix of the coordinate transform. These distorted planewaves (DPW) form a complete and orthonormal basis set [4]. In contrast to earlier studies, we have chosen to break out the Bloch phase factor for reasons which will become clear later on.

As suggested by Gygi in 1995 [5, 6], we will let each atom distort space around it through a distorting function F and element specific parameters, i.e. the strength, A , and the range, R_0 of the distortion:

$$\mathbf{r}' = \mathbf{r} + \sum_{\alpha} A^{\alpha} \frac{(\mathbf{r} - \mathbf{r}^{\alpha})}{R_0^{\alpha}} F \left(\left| \frac{\mathbf{r} - \mathbf{r}^{\alpha}}{R_0^{\alpha}} \right| \right). \quad (6)$$

The distorting function F should be chosen in a way that enhances the number of nodes of the basis functions in the vicinity of a nucleus and reduce the number of nodes in the interstitial. The function F should then have a maximum either at the nuclear position or, in our case, at least inside the MT spheres. The distorting function should be smooth and not too rapidly varying to avoid numerical instabilities. Gygi suggests several nuclear centered distorting functions in his papers [4–6]. One of them is

$$F(x) = \text{sech}(x), \quad (7)$$

which is the one we have focused upon in this study. However, a related distorting function with maximum distortion close to the MT-sphere boundary,

$$F(x) = \text{sech}(x) \tanh(x), \quad (8)$$

is suggested too. The choice of distorting function might significantly alter the efficiency of the method and further studies to find the most suitable distorting function may be useful.

2.1. Augmented distorted planewaves

In the same way as the PW before, the DPW may be augmented in the MT spheres, giving rise to *augmented distorted planewaves* (ADPW)

$$\psi_{\mathbf{G}}(\mathbf{k}; \mathbf{r}) = \begin{cases} \eta_{\mathbf{G}}(\mathbf{k}; \mathbf{r}), & \mathbf{r} \in \text{I} \\ \sum_{\ell m\alpha} \tilde{a}_{\ell m\mathbf{G}}^{\alpha} f_{\ell m}^{\alpha}(r) Y_{\ell m}(\hat{\mathbf{r}}), & \mathbf{r} \in \text{MT}_{\alpha}. \end{cases} \quad (9)$$

Difficulties arise from the fact that we no longer have planewaves in the interstitial region. For instance, the matching must be done by numerical expansion of the DPWs in spherical harmonics, solving Poisson's equation for the interstitial region

is no longer trivial and the surface contribution to the kinetic energy has to be calculated in a different way. Although difficult, these are all problems that can be solved. However, prior to a full implementation, it is desirable to determine if the basis set is sufficiently efficient to justify it. This is the purpose of the present study. Here, since we are mainly interested in investigating the potential gain with this new basis, we use another simpler approach, which circumvents these problems. The DPWs can be expressed as an expansion of ordinary plane waves

$$\eta_{\mathbf{G}'}(\mathbf{k}; \mathbf{r}) = \exp(i\mathbf{k} \cdot \mathbf{r}) \sum_{\mathbf{G}} \exp(i\mathbf{G} \cdot \mathbf{r}) U_{\mathbf{G}\mathbf{G}'}, \quad (10)$$

where $U_{\mathbf{G}\mathbf{G}'}$ are the inverse Fourier transform coefficients of $\eta_{\mathbf{G}'}(\mathbf{r})$. It is in order to facilitate this transform that we redefined the DPW with an explicit Bloch wave factor. Now, by using the known matching coefficients for the PW, we get a transformation between APW and ADPW

$$\psi_{\mathbf{G}'}(\mathbf{k}; \mathbf{r}) = \sum_{\mathbf{G}} \phi_{\mathbf{G}}(\mathbf{k}; \mathbf{r}) U_{\mathbf{G}\mathbf{G}'}. \quad (11)$$

Furthermore, the ADPW Hamiltonian (or overlap) matrix can be directly described in terms of the APW Hamiltonian (or overlap) matrix

$$\tilde{H}_{pq} = \langle \psi_{\mathbf{G}'_p} | H | \psi_{\mathbf{G}'_q} \rangle = \sum_{ij} U_{\mathbf{G}'_i \mathbf{G}'_p}^* \langle \phi_{\mathbf{G}_i} | H | \phi_{\mathbf{G}_j} \rangle U_{\mathbf{G}_j \mathbf{G}'_q} \quad (12)$$

or in short

$$\tilde{H} = U^\dagger H U. \quad (13)$$

Notice, that since the local orbital part of the APW + lo basis set is unchanged, the transformation matrix is a unit matrix in terms of this part of the basis. Hence, we can set up the Hamiltonian and overlap matrices in undistorted space in terms of APW and then transform it into an ADPW basis. This give us a secular problem:

$$\{\tilde{H} - \varepsilon_{\mathbf{k}} \tilde{O}\} \tilde{\mathbf{c}} = \{U^\dagger (H - \varepsilon_{\mathbf{k}} O) U\} U^\dagger \mathbf{c} = 0. \quad (14)$$

The transformation matrices U are \mathbf{k} independent and only have to be calculated once. The distorted space, implicitly incorporated in the ADPW, can lead to a faster convergence in terms of the number of basis functions. That is, in practice we can use a rectangular $N \times M$ transformation matrix U , in order to reduce the secular matrix from N to M dimensions. After the diagonalization we back transform the eigenvector

$$\mathbf{c}_{\mathbf{G}} = \sum_{\mathbf{G}'} U_{\mathbf{G}\mathbf{G}'} \tilde{\mathbf{c}}_{\mathbf{G}'}, \quad (15)$$

and can construct the charge density etc in ordinary space. As already mentioned, this implementation does not provide the full gain in computational effort of the ADPW method, since the set-up time is longer not shorter than for the APW method, but it gives us the opportunity to carefully investigate the efficiency of this new basis set.

The above simplified scheme has been implemented in the open source APW + lo code EXCITING [8].

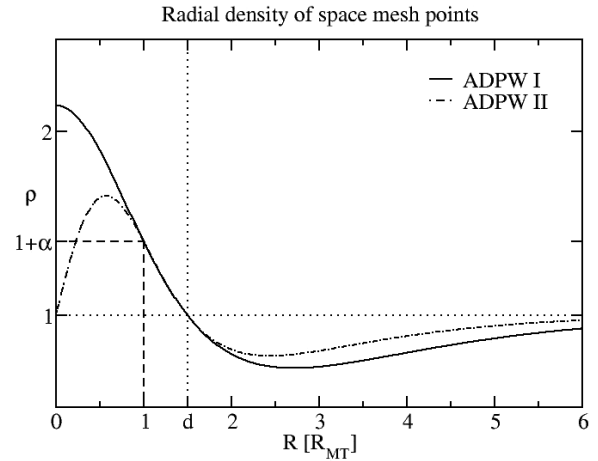


Figure 1. Radial density of space points ρ due to distortion from a single nucleus, given by equation (6), using the atom centered distortion function (ADPW I) and the MT optimized distortion function (ADPW II). The dimensionless parameters α and d could be interpreted as the strength and range of the distortion.

3. Results and discussion

As mentioned earlier, the efficiency of the basis set will depend on the distorting function used and the choice of parameters A and R_0 . To find the best choice of parameters and distorting function we compare calculations of single atoms of different species using a range of parameters and the atom centered distorting function from equation (7), and a modified version, with maximum distortion around the muffin tin sphere from equation (8). To facilitate the comparison between the two distorting functions we use the dimensionless parameters α and d defined by the relations

$$\left. \frac{dr'}{dr} \right|_{r=dR_{MT}} = 1, \quad (16)$$

$$\alpha = \left. \frac{dr'}{dr} \right|_{R_{MT}}. \quad (17)$$

For any distorting function the parameter d is the number of MT-sphere radii from the nucleus where the radial density of space points due to the distortion from the nucleus is equal to the density of space points in undistorted space. The parameter α is the relative radial density of space points at the MT-sphere boundary.

An interpretation of the two parameters and the radial density of space points for the two distorting functions investigated in this paper (ADPW I given by equation (7) and ADPW II given by equation (8)) is illustrated in figure 1. Using the same d and α for the two different distorting functions gives a similar distortion around the MT spheres. To find the best choice of parameters we have investigated a range of parameters α and d for two extreme systems, free atoms of some chosen atomic species and the close packed structure for the same species. In figure 2 the results of ADPW calculations for single atoms (treated as a simple cubic lattice with large lattice parameter) of copper and potassium using a range of parameters α and d are shown. Here we start from a converged

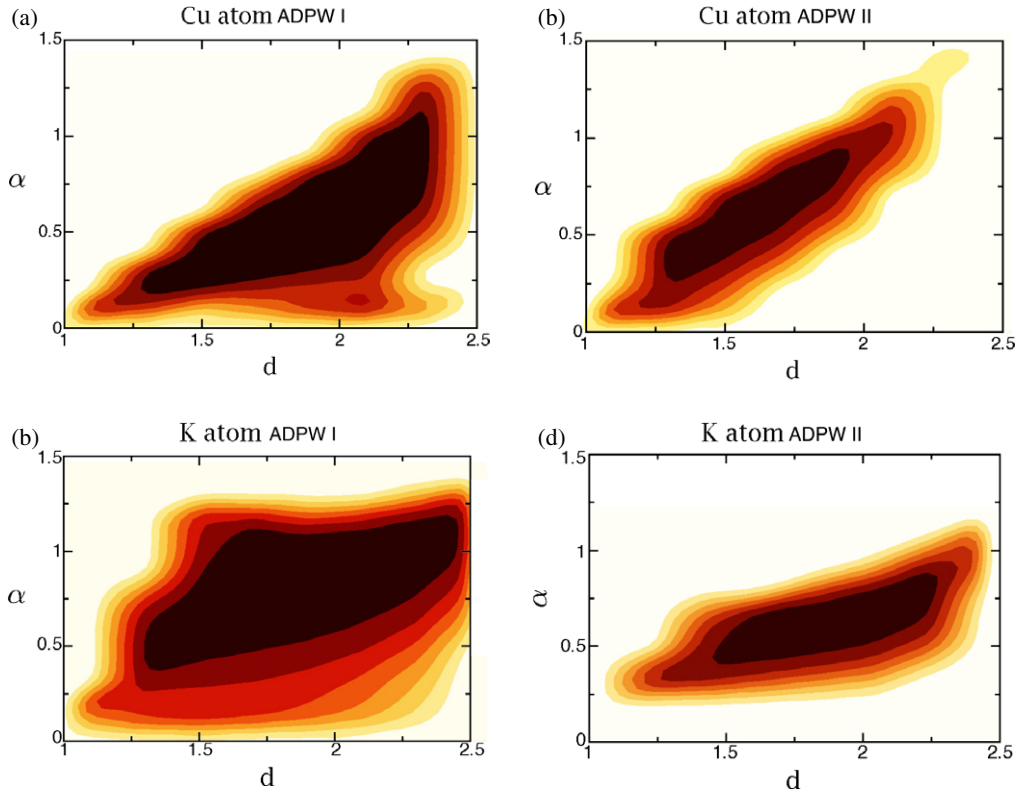


Figure 2. Distortion parameters for single atoms. In the colored region the sum of eigenvalues using M basis functions, expanded in N plane waves is lower than the sum of eigenvalues using M APW basis functions. In the colored region the sum of eigenvalues fulfill $E_{\text{sum}}^{\text{ADPW}}(M) < E_{\text{sum}}^{\text{APW}}(M)$ and in the innermost, darkest region $E_{\text{sum}}^{\text{ADPW}}(M) - E_{\text{sum}}^{\text{APW}}(N) < \frac{E_{\text{sum}}^{\text{APW}}(M) - E_{\text{sum}}^{\text{APW}}(N)}{10}$. Here $\frac{M}{N} \approx 0.9$.

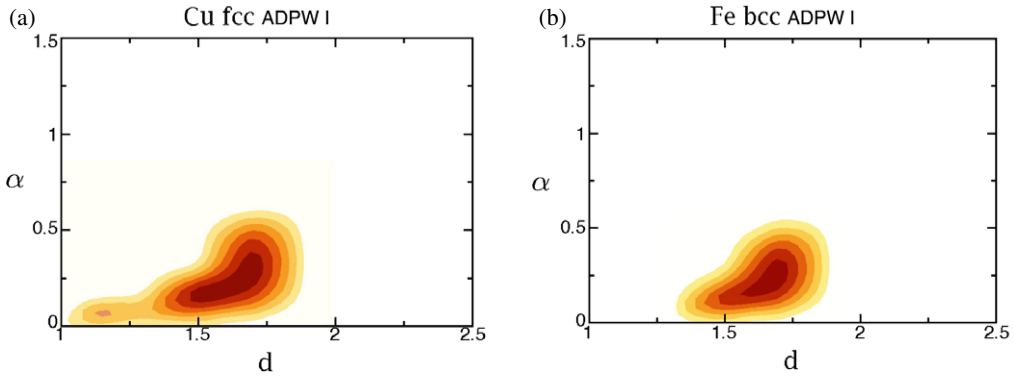


Figure 3. Distortion parameters for close packed structures. The region of acceptable parameters is much smaller due to the influence on the distortion from neighboring atoms.

charge density with N APW plane waves and do one more iteration with M APW plane waves, where $M/N \approx 0.9$ and with M ADPW basis functions and compare the results. The closer the sum of eigenvalues of the smaller ADPW basis calculation is to the sum of eigenvalues of the larger APW basis calculation the better. The parameters in the darkest region in figures 2 and 3 give eigenvalues that fulfill the relation

$$E_{\text{sum}}^{\text{ADPW}}(M) - E_{\text{sum}}^{\text{APW}}(N) < \frac{E_{\text{sum}}^{\text{APW}}(M) - E_{\text{sum}}^{\text{APW}}(N)}{10}. \quad (18)$$

Figure 3 shows the same for some close packed structures of the same atomic species.

The results are summarized in table 1. As expected both the range d and the strength α of the distortion has to be smaller for close packed structures than for single atoms. Since we use the simplified approach of transforming the APW to the ADPW basis set as in equation (11) through a Fourier transform, the ADPW II set is less adapted with its more structured distortion (equation (8)). Therefore, we have concentrated our present study on the ADPW I basis set for the denser structures.

For the s -metal K we may use the strongest distortion due to the open structure and small MT-sphere radius compared to the lattice parameter. The more close packed d -metals Cu and

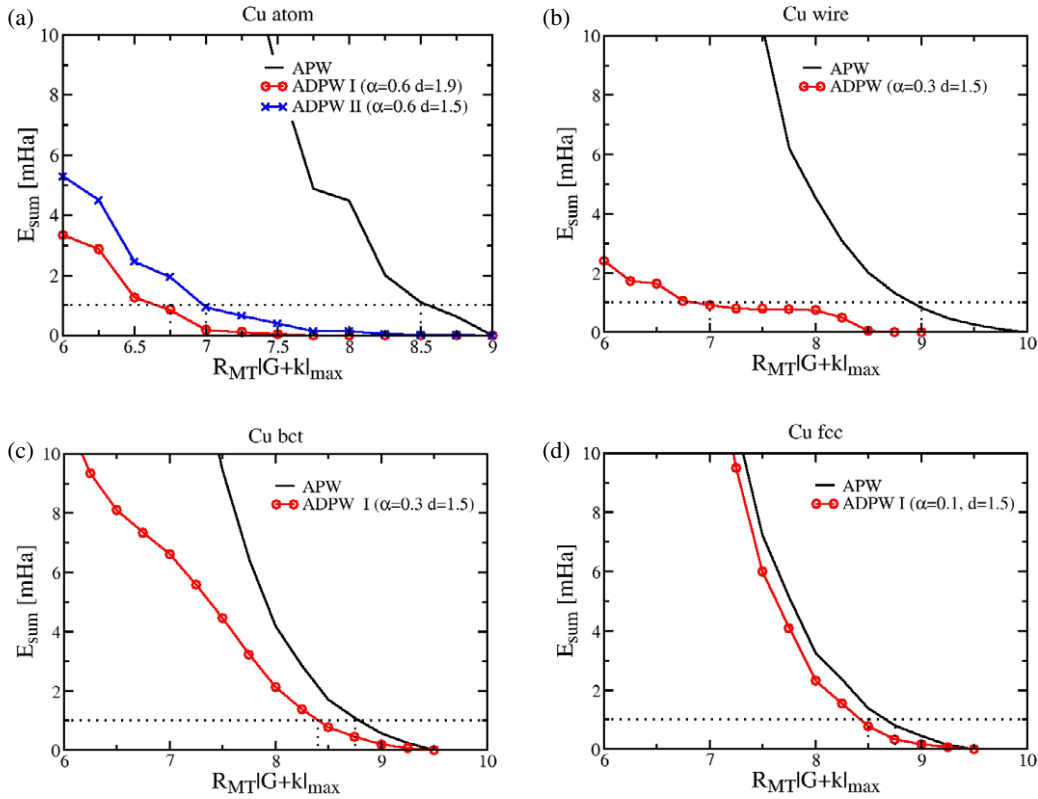


Figure 4. For open structures the ADPW-lo basis set converges considerably faster with respect to the number of basis functions than the APW-lo basis. In the case of bct and fcc structures the convergence is only slightly faster. The distortion parameters are chosen to give a reasonable convergence for both close packed and open structures.

Table 1. Optimal parameters for a small change ($\frac{M}{N} \approx 0.9$) in the number of basis functions for ADPW I and ADPW II (in parenthesis). The optimal values are always surrounded by a region of acceptable parameters that are close to optimal (see equation (18) and figures 2 and 3).

Species/structure	$R_{\text{MT}} (a_0)$	d	α
Carbon	1.45		
Atom		2.5 (1.7)	0.7 (0.6)
Graphite		2.1	0.2
Diamond		1.9	0.1
Copper	2.0		
Atom		1.9 (1.5)	0.5 (0.6)
fcc		1.5	0.1
Iron	2.0		
bcc		1.5	0.1
Potassium	2.2		
Atom		1.9 (1.9)	0.7 (0.9)
bcc		1.3	0.2

Fe are, however, more sensitive to large distorting parameters α and d .

In figures 4 and 5 convergence tests with respect to basis set sizes, as described by the dimensionless parameter $R_{\text{MT}}^{(\text{min})}|\mathbf{G}+\mathbf{k}|_{\text{max}}$, are displayed for Cu and K atoms in different geometries. With the same convergence criterion, 1 mHa, it is clear that for the most open systems a large gain in basis set sizes is obtained for the ADPW + lo basis compared to the APW + lo basis. This gain is smaller when the MT spheres

start to fill up a larger part of the volume and is marginal for close packed fcc Cu.

For larger differences in size of the basis sets, the range of usable parameters is increased. In general the method works better when the number of planewaves needed to converge the APW calculation is large, for open systems where lattice parameters are large and/or where the MT-sphere radii are small. This is expected since the relative size of the interstitial region, where the new basis functions matters, is larger in these cases. A summary of the potential computational gain is shown in table 2. The two different distorting functions give similar results, although the atom centered distorting function (ADPW I) generates smoother basis functions which in some cases leads to faster convergence of eigenvalues with respect to number of basis functions. This is probably a numerical artifact due to the expansion of the new basis functions in a limited number of planewaves in equation (10).

In a full implementation both distorting functions would probably lead to basis sets that behave similarly and converge faster than undistorted functions, with respect to the number of basis functions used. In such an implementation the matrix elements of the Hamiltonian and overlap matrices are calculated in the new basis directly, which would be much more efficient than the work-around presented in this paper. However, special efforts have to be made to treat the MT geometry. In the distorted space the MT spheres get deformed. Then it is not so straightforward to get the augmentation

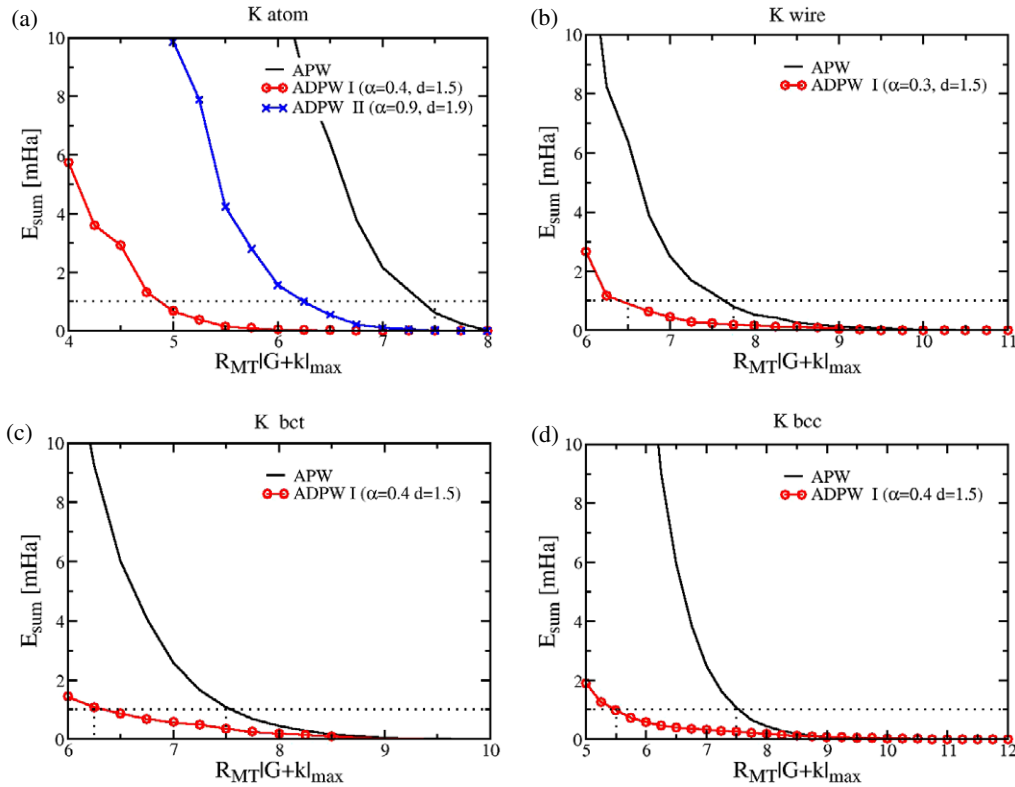


Figure 5. Sum of eigenvalues minus the sum of eigenvalues for the converged solution with maximum $R_{MT}|G + \mathbf{k}|_{max}$. Potassium has a large lattice parameter, compared to the MT radius, and all the investigated structures are relatively open.

Table 2. Computational gain for the distortion ADPW I.

Species/structure	M	N	Speed up of diagonalization estimated as $t(N)/t(M) = (N/M)^3$
Carbon			
Single atom	485	1503	29.8
Graphite	230	296	2.13
Diamond	125	138	1.35
Copper			
Single atom	619	1309	9.46
Wire	795	1687	9.55
bct	437	482	1.34
fcc	113	125	1.35
Iron			
bcc	92	116	2.00
Potassium			
Single atom	691	2301	36.9
Wire	467	815	5.31
bct	405	695	5.05
bcc	141	370	18.1

coefficients, to calculate the surface contribution to the kinetic energy or to solve Poisson’s equation. One approach to achieve this could be, for example, by allowing the MT spheres to be non-spherical in real space so that they are spheres in distorted space; another would be to do all the augmentations by numerical means. The charge density may still be expressed

as an expansion on a large Fourier mesh, as is usually done in the APW method [7].

4. Conclusions

A new set of basis functions, ADPW + lo, has been investigated. It is found that it has the capacity for faster convergence, since fewer basis functions are needed to accurately describe the wavefunction in the interstitial region and the matching at the MT boundary. In the present paper we have shown that with a simplified implementation it is possible for a range of different atomic species and crystal structures to reduce the size of the secular matrix. The distortion of space allowed for reduction in the basis set by up to a factor of three for open structures, while giving the same eigenvalues within fractions of mHa. The diagonalization is done using the LAPACK 3.0 routine zhpgvx, which scales as matrix size cubed (execution time $t \propto N^3$). This means a speed up of the diagonalization of the secular matrix by up to a factor of 30. It is worthwhile noting that in our simplified implementation the variational principle does not allow ADPW + lo to give lower energies than the APW + lo basis set which we expand our basis functions in. With a larger planewave expansion the accuracy of the ADPW + lo basis will improve.

The range of the distortion d could be put to 1.5 for most of the investigated realistic systems without losing any precision in the calculations. If a very small MT-sphere radius is used, this value might have to be increased (as in the case of carbon). The optimal strength of the distortion α varies between 0.5

and 1 for single atoms and down towards 0.1 for close packed systems. Further investigations are needed to see if there is any systematic way of choosing the distorting strength of different atomic species. It will also be desirable to investigate other choices of distorting function to determine whether it is possible to effectively exploit the fact that the variational freedom in the interior of the spheres is not needed. A full implementation that eliminates artifacts due to the truncation of the planewave expansion of the basis functions might find a 'universal' distorting strength that works well for all systems.

We conclude that our results justify further studies in order to determine how far this can be taken. Although a full implementation of the method might increase the efficiency of the method beyond the limit of the truncated planewave expansion, this simple approach already has some uses, especially for open structures where the gain in basis set sizes is largest. More studies are needed until it is definite that a full implementation of the ADPW + lo method, that works in the distorted space both in the set-up of the secular matrices and in the calculation of the charge density, is worthwhile.

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