Efficient Recursion Method for Inverting Overlap Matrix

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Abstract

A new $O(N)$ algorithm based on a recursion method, in which the computational effort is proportional to the number of atoms $N$, is presented for calculating the inverse of an overlap matrix which is needed in electronic structure calculations with the the non-orthogonal localized basis set. This efficient inverting method can be incorporated in several $O(N)$ methods for diagonalization of a generalized secular equation. By studying convergence properties of the 1-norm of an error matrix for diamond and fcc Al, this method is compared to three other $O(N)$ methods (the divide method, Taylor expansion method, and Hotelling’s method) with regard to computational accuracy and efficiency within the density functional theory. The test calculations show that the new method is about one-hundred times faster than the divide method in computational time to achieve the same convergence for both diamond and fcc Al, while the Taylor expansion method and Hotelling’s method suffer from numerical instabilities in most cases.

The development of $O(N)$ methods and the revival of localized orbitals as a basis set have been made during the last decade in order to extend the applicability of the first-principles molecular dynamics (FPMD) simulations using the plane wave expansion...
and the Car-Parrinello method within density functional theories (DFT) [20]. However, only few applications of these $O(N)$ methods to large systems have been reported within the DFT calculations [18,21,22]. Although there are a lot of limitations of the method based on the localized description [22], one of the limitations is that several $O(N)$ methods require evaluating the inverse of the overlap matrix $S$ which comes from non-orthogonality among the localized orbitals.

In the generalized Fermi operator expansion (FOE) method [4] to the non-orthogonal basis we need to calculate the inverse of overlap matrix to construct the modified Hamiltonian $H' \equiv S^{-1}H$, while Stephan et al. have proposed solving a linear equation $SH' = H$ with the cutoff radii of $H$ instead of calculating the inverse of overlap matrix. In the density matrix (DM) method [8–10] which is a promising approach for materials with a wide gap, fortunately, the evaluation of the inverse is not required during the optimization of grand potentials, although we have to evaluate the inverse of the overlap matrix for a good initial guess of the density matrix [10]. The block bond-order potential (BOP) method [2], which has good convergence properties for both insulators and metals, also requires the evaluation of the modified Hamiltonian $H'$ as in method the FOE method. If the overlap matrix is sparse, the computational cost scales as the second power of the number of atoms $N$ in the inverse calculation. Therefore, an efficient $O(N)$ method for inverting the overlap matrix should be developed.

So far, several $O(N)$ inverting methods have been proposed. Gibson et al. used a simple method in which a linear equation $SH' = H$ constructed for a finite cluster is solved without explicit calculation of $S^{-1}$ [23]. Mauri et al. considered approximating the inverse of overlap matrix by the Taylor expansion [7]. The approach could be an $O(N)$ inverting method when the matrix elements in the $p$th moment $O^p$ of the overlap matrix $O$ are cut at a finite distance. Palser and Manolopoulos proposed to evaluate the inverse by Hotelling’s method which is similar to the iterative purification algorithm of the DM method [10]. The iterative calculation can be performed in $O(N)$ operations, provided that the cutoff of matrix elements at a finite distance is introduced in the product of two matrices. It is worth pointing out that
the ideas of these O(N) inverting methods are analogous to those of the O(N) methods for the diagonalization. The divide method by Gibson et al. [23], the Taylor expansion method [7], and Hotelling’s method [10] strategically and mathematically correspond to the divide and conquer method [5], the FOE method [3,4], and the DM method [8–10], respectively. Therefore, one may expect that these O(N) inverting methods may have the convergence properties for realistic materials similar to the O(N) methods for the diagonalization [24]. However, it remains to be seen whether the expectation is meaningful or not.

In this paper we propose a new O(N) method for calculating the inverse of the overlap matrix which is based on a resolvent and the block Lanczos algorithm. The new method is compared with the other three methods in terms of the computational accuracy and efficiency. Thus, our aim of this paper is to clarify the applicability of these four O(N) inverting methods for realistic materials. The paper is organized as follows. In Sec. II we present the theory of a new O(N) inverting method based on a recursion method, and also summarize the three other O(N) inverting methods. In Sec. III we discuss the convergence properties of these four O(N) inverting methods for the diamond and fcc Al within the DFT calculations using the 1-norm of an error matrix which will be related to the error in the eigenvalues in this section. In Sec. IV we conclude with clear characterization of the four O(N) inverse methods.

II. THEORY

A. Recursion method

It is assumed that one-particle wave functions are expanded by a localized orbital basis set (|iα⟩), where i is a site index and α is an orbital index. The localized orbitals could be Slater-type [12–14], Gaussian-type [15], and numerical orbitals [11,16] obtained by DFT calculations for atoms. In most cases, the orbitals are non-orthogonal between them, leading to an overlap matrix S defined by

\[ S_{i\alpha,j\beta} = \langle i\alpha | \hat{S} | j\beta \rangle, \]  (1)
where $\hat{S}$ is the overlap operator which is introduced as a matter of form in order to emphasize the similarity between the new inverting method and the block BOP method [2], although the overlap operator generally should be the identity operator $I$. The overlap integral exponentially decays in real space because of the localized nature of the orbitals, so that the overlap matrix $S$ is sparse. Here we introduce a resolvent $R(Z)$ for the matrix $S$ as follows:

$$ R(Z) = (S - ZI)^{-1}. $$

(2)

It is then easy to verify that

$$ S^{-1} = \text{Re} R(0). $$

(3)

Thus, we see that the real part of the resolvent for $Z = 0$ gives the inverse $S^{-1}$ of the overlap matrix. If the resolvent for $Z = 0$ has a finite value for the imaginary part, the basis set is not linearly independent. The resolvent can be evaluated by adopting the algorithm of the block BOP method [2] which is recently developed to simulate orthogonal tight-binding (TB) models in $O(N)$ operations. It is noted that the new inverting method is derived just by replacing the Hamiltonian $\hat{H}$ in the block BOP method within the orthogonal TB models with the overlap operator $\hat{S}$. The first step in this algorithm is to block-tridiagonalize the overlap matrix $S$ using the block Lanczos algorithm [25–28]. The central equations is

$$ \hat{S}|U_n\rangle = |U_n\rangle A_n + |U_{n-1}\rangle B_n + |U_{n+1}\rangle B_{n+1} $$

(4)

with

$$ |U_0\rangle = (|i1\rangle, |i2\rangle, \ldots, |iM_i\rangle) $$

(5)

as the starting state. $A_n$ and $B_n$ are recursion block coefficients with $M_i \times M_i$ in size, where $M_i$ is the number of localized orbitals on the starting atom $i$, and the underline indicates that the element is a block. In the block Lanczos algorithm, we need to start the recursion with Eq. (5) to make the recursion method accurate and efficient [2]. The Lanczos algorithm with a finite recursion transforms the overlap matrix $S$ into the block-tridiagonalized matrix $S^L$ which has the diagonal $A_n$ and the sub-diagonal block elements
$B_n$, where the index $L$ indicates the representation based on the Lanczos basis. Considering the resolvent $R_L(Z) \equiv (S^L - ZI)^{-1}$ for the block-tridiagonalized overlap matrix, the diagonal $R_{00}^L(Z)$ and off-diagonal block elements $R_{ln}^L(Z)$ can be easily derived along the same line as that described in the block BOP method [2]. For $Z = 0$, the elements are given by

$$R_{00}^L(0) = [A_0 - tB_1[A_1 - tB_2[\cdots]^{-1}B_2]^{-1}B_1]^{-1},$$

(6)

$$R_{ln}^L(0) = \left(\delta_{ln}I - R_{0n-1}(0)A_{n-1}ight)\left(-R_{0n-2}(0)^{tB_{n-1}}\right)(B_n)^{-1},$$

(7)

where $\delta$ is Kronecker’s delta, and $R_{0n-1}(0) = tB_0 = 0$. Once the block diagonal element is calculated as the multiple inverse Eq. (6), the off-diagonal elements are evaluated from the recurrence relation Eq. (7) with $R_{00}^L(0)$ as the starting element. In order to truncate the multiple inverse in Eq. (6) without reducing the accuracy significantly, a square root terminator could be used, while there could be an infinite number of levels in the multiple inverse of diagonal Green’s function for an infinite system. In the test calculations of Sec. III we used the square root terminator for the truncation at a finite number of levels. The two Eqs. (6) and (7) provide the resolvent based on the Lanczos basis representation, so that we can obtain the original resolvent through the following inverse transformation:

$$R_{ij}(0) = \sum_n R_{0n}^L(0)^{tU_{nj}},$$

(8)

where $^{tU_{nj}}$ is defined by $^{tU_{nj}} = (U_n(|j1\rangle, |j2\rangle, \ldots, |jM_j\rangle)$. The inverse transformation Eq. (8) is significantly simplified because of the orthogonality in the Lanczos bases. Therefore, we only have to evaluate the 0th block line of the resolvent in the Lanczos basis representation. The resolvent exactly satisfies a sum rule $\sum_{ij} \text{tr}\{S^L_{ij}R_{ij}(0)\} = N_B$ which is derived from Eq. (2), where $N_B$ is the number of bases, and is constructed by up to $(q+1)$th moments $S^{q+1}$ [2], where $q$ is a final level for the recursion. Equation (8) gives a good approximation for the inverse of overlap matrix as the number of recursion levels increases. However, the approximated inverse is not strictly a symmetric matrix at a finite recursion.
If the approximated inverse is symmetric, eigenvalues of a generalized secular equation with
the overlap matrix are real numbers. Therefore, we evaluate the inverse of overlap matrix
by symmetrizing the resolvent in terms of simple arithmetic average:

\[ S_{ij}^{-1} = \frac{\text{Re} R_{ji}(0) + \text{Re} \imath R_{ij}(0)}{2}. \]  

(9)

The symmetrization preserves the above sum rule. The all elements of the inverse are
evaluated by applying the series of the algorithm repeatedly to each atom. The cluster over
which the hops are made in the Lanczos algorithm is determined by the logical truncation
method [2]. Thus, the computational cost of the recursion method is strictly proportional
to the number of atoms \( N \).

B. Divide method

In the case of the block BOP [2] and FOE methods [3,4], it is required to evaluate the
modified Hamiltonian \( H' = S^{-1}H \) rather than the inverse of overlap matrix. In such cases
we have an alternative way where a linear equation

\[ SH' = H \]  

(10)
is solved instead of calculating the inverse. In conventional ways of solving the linear equation
for a total system, the computational cost scales as the third power of the number of atoms
\( N \), while the scaling could be reduced to \( O(N^2) \), making use of the sparseness of the overlap
matrix. Therefore, Gibson et al. have proposed a solution of Eq. (10) with the cutoff radii
of \( H \) and \( S \) [23]. The linear equation Eq. (10) can be decomposed into \( N \) subspace linear
equations for \( N \) finite clusters under this constraint. One solves each of the subspace linear
equations for the finite clusters centered on atom \( i \) using a conventional method such as
the Cholesky factorization, which results in \( O(N) \) operations for the computational effort.
However, the divide method has redundancy in the calculation that one has to evaluate
all matrix elements of the modified Hamiltonian \( H' \) for each finite cluster compared to the
other \( O(N) \) inverting methods in which the elements in the inverse of the overlap matrix are
not doubly calculated. Thus, the prefactor of the $O(N)$ operations could be very large for highly coordinated structures such as fcc. The magnitude of the prefactor will be discussed in Sec. III. An iterative scheme such as the Gauss-Siedel method [24,29] which is commonly used for large-scale systems is also available for solving the linear equation Eq. (10). However, it has been recognized that the iterative scheme is computationally expensive [23], so that the iterative scheme was not investigated in this study. We used the logical truncation method to construct the subspace linear equation as well as the recursion method in the test calculations discussed in Sec. III in order to compare the computational performance.

C. Taylor expansion method

Mauri et al. have proposed to approximate the inverse of the overlap matrix using the Taylor expansion in their $O(N)$ unconstrained minimization method [7]. The overlap matrix $S$ is expressed as a sum of the identity $I$ and an $O$-matrix $O$ which is the overlap matrix between the different orbitals:

$$S = I + O,$$  \hspace{1cm} (11)

then we can expand the inverse of $S$ in respect to the $O$-matrix as follows:

$$S^{-1} = \sum_{n=0}^{\infty} (-1)^n O^n = I - O + O^2 - O^3 + \ldots$$  \hspace{1cm} (12)

The computational accuracy and efficiency of the approximation by the Taylor series depend on the convergence for the summation of Eq. (12). The summation in Eq. (12) does not converge, but diverges, when the spectrum radius of the $O$-matrix exceeds 1.0. Even if the $O$-matrix has no eigenvalues which are and below -1.0, indicating the basis set is linearly independent, the eigenvalues of the $O$-matrix exceed 1.0 in most cases as shown in Sec. III. In such cases, the Taylor expansion method cannot be applied. The matrix $O^n$ is calculated as the product of the perfect but highly sparse $O$-matrix, and $O^{n-1}$ with the cutoff radii for the elements, so that the summation to a finite order in Eq. (12) can be performed with $O(N)$ operations.
D. Hotelling’s method

Palser and Manolopoulos [10] have suggested evaluating the inverse $S^{-1}$ using Hotelling’s method [30,31]. The method has an iterative algorithm very similar to the purification algorithm [10] in the DM method. The convergence rate in Hotelling’s method is also quadratic as with the DM method. The purification of an approximate inverse is achieved using the following iterative relation:

$$S^{-1}_{n+1} = 2S^{-1}_n - S^{-1}_n S S^{-1}_n.$$  \hspace{1cm} (13)

In case of $S^{-1}_0 = I$, Hotelling’s method is equivalent to the Taylor expansion method to a finite order described in the previous subsection (C). It is easy to verify that $S_1$ and $S_2$ are the Taylor series to the first and third orders of the $O$-matrix, respectively:

$$S^{-1}_1 = 2S^{-1}_0 - S^{-1}_0 S S^{-1}_0,$$

$$= I - O,$$  \hspace{1cm} (14)

$$S^{-1}_2 = 2S^{-1}_1 - S^{-1}_1 S S^{-1}_1,$$

$$= I - O + O^2 - O^3.$$  \hspace{1cm} (15)

From Eqs. (14) and (15), we see that Hotelling’s method converges quadratically compared to the linear convergence of Taylor expansion method. Thus, if Eq. (12) is a convergent series, Hotelling’s method should be more efficient rather than the Taylor expansion method. When the spectrum radius of the $O$-matrix exceeds 1.0, the identity $I$ cannot be used as the initial guess for the inverse $S^{-1}$. In such cases, although it is very difficult to estimate a good initial matrix $S_0^{-1}$ for the iteration Eq. (13), in this study, we use the overlap $S$ with a small prefactor $\sigma$ derived by Pan and Reif [31] as the initial guess:

$$S_0^{-1} = \sigma S$$  \hspace{1cm} (16)

with
\[ \sigma = \frac{1}{\left( \max_{i \alpha} \sum_{j \beta} |S_{i \alpha, j \beta}| \right)^{\frac{1}{2}}} . \]  

(17)

It is noted that Hotelling’s method possesses an advantage that the inverse at the previous MD step could be a good guess of \( S^{-1}_0 \) at the current MD step, while any information at the previous MD step cannot be made use of in the other methods; the recursion method, the divide method, and the Taylor expansion method. In the iteration Eq. (13), the elements of \( S^{-1}_n \) are cut at a finite distance. As a result of this truncation, the computational effort of Hotelling’s method scales linearly with the system size. In test calculations of Sec. III, we used the logical truncation method for the cutoff of the elements as in the other inverting O(\( N \)) methods.

### III. CONVERGENCE PROPERTIES

#### A. Error analysis

In order to compare the four O(\( N \)) inverse methods presented in the Sec. II in terms of computational accuracy and efficiency, we first relate the 1-norm of an error matrix \( E \) with the error of eigenvalues \( \epsilon_\nu \) of a secular equation by using an error analysis theory \[32,33\]. The generalized secular equation with the overlap matrix \( S \) is derived from the variational principle within DFT using a non-orthogonal basis set.

\[ S^{-1}HC_\nu = \epsilon_\nu C_\nu, \]  

(18)

where \( H_{i \alpha, j \beta} \equiv \langle i \alpha | \hat{H} | j \beta \rangle \) and \( C_{i \alpha, \nu} \) is an expansion coefficient \( C_{i \alpha, \nu} \equiv \langle i \alpha | \phi_\nu \rangle \) in a one-particle wave function \( | \phi_\nu \rangle \). Let us consider substituting the exact inverse \( S^{-1} \) with an approximate inverse \( S'^{-1} \) in Eq. (18), then the difference between \( S^{-1} \) and \( S'^{-1} \) is

\[ S'^{-1} - S^{-1} = \Delta S^{-1} . \]  

(19)

For the approximate inverse \( S'^{-1} \) the secular equation \( S'^{-1}HC'_\nu = \epsilon'_\nu C'_\nu \) is satisfied with approximate eigenvalues \( \epsilon'_\nu \) and eigenvectors \( C'_\nu \). According to the error analysis theory \[32,33\], the difference between the exact and the approximate eigenvalues is given by
\[ |\epsilon'_\nu - \epsilon_\nu| = O(\lambda) \]  

(20)

with \( \lambda \), which is the 1-norm of a matrix \( \Delta S^{-1}H \), defined by

\[
\lambda = \max_{j\beta} \sum_{i\alpha} \left| \sum_{k\gamma} \Delta S^{-1}_{i\alpha,k\gamma} H_{k\gamma,j\beta} \right|. 
\]  

(21)

Therefore, we see that the error in eigenvalue is proportional to the 1-norm of \( \Delta S^{-1}H \) for the approximation of the overlap matrix. Equation (20) apparently connects the error of the overlap matrix to that of the eigenvalue. However, it is not possible to calculate the exact inverse for infinite or periodic systems, so that we introduce an error matrix \( E \), which is easily evaluated, defined as the difference between a matrix \( SS'^{-1}H \) and the original Hamiltonian \( H \):

\[
E \equiv SS'^{-1}H - H = S\Delta S^{-1}H. 
\]  

(22)

The 1-norm \( \eta \) of the error matrix \( E \) can be related to that \( \lambda \) of the matrix \( \Delta S^{-1}H \) as follows:

\[
\eta = \max_{j\beta} \sum_{k'\gamma'} \sum_{i\alpha} S_{k'\gamma', i\alpha} \Delta S^{-1}_{i\alpha,k\gamma} H_{k\gamma,j\beta} \\
\leq \max_{j\beta} \sum_{k'\gamma'} \sum_{i\alpha} \left( S_{k'\gamma', i\alpha} \right) \Delta S^{-1}_{i\alpha,k\gamma} H_{k\gamma,j\beta} \\
\leq N_{av} \left( \max_{j\beta} \sum_{i\alpha} \mid \Delta S^{-1}_{i\alpha,k\gamma} H_{k\gamma,j\beta} \right) \\
= N_{av} \lambda, 
\]  

(23)

where \( N_{av} \) is the average number of the non-zero elements in the overlap matrix for an orbital \( \mid i\alpha \rangle \). The third relation in Eq. (23) is derived by substituting the non-zero overlap integrals \( |S_{k'\gamma', i\alpha}| \) to 1 with the variables \( i\alpha \) fixed in the second relation. Considering Eqs. (21) and (23), we can relate the 1-norm of the error matrix to the error of the eigenvalue:

\[ |\epsilon'_\nu - \epsilon_\nu| = O(\eta). \]  

(24)

Therefore, we will compare the four O(\( N \)) inverse methods using the 1-norm \( \eta \), which is easily evaluated, instead of \( \lambda \).
B. Numerical tests

We numerically studied convergence properties of the four inverse $O(N)$ methods using 1-norm $\eta$ for diamond and fcc Al within DFT proposed by Sankey and Niklewski [11]. In this DFT calculations we used numerical localized orbitals, fireball bases by Sankey and Niklewski [11], as a minimal basis set for valence electrons. The radii of the radial-wave function confinement are 2.1 and 3.7 Å for carbon and aluminum atoms, respectively. The minimal basis sets give 1.253 (1.244) and 2.515 (2.466) Å as an equilibrium bond length of dimer for carbon and aluminum, respectively, where the values in the parentheses are experimental results.

In Fig. (1) we show the density of states for eigenvalues of $O$-matrix, which is defined by Eq. (11), in diamond and fcc Al. In both cases the $O$-matrices have no eigenvalues smaller than -1.0, so that the basis sets are linearly independent for the structures. However, the density of states possess finite values for the eigenvalues larger than or equal to 1.0 in both cases. In other words the spectrum radius of the $O$-matrix exceeds 1.0. This means that the summation in Eq. (12) for the Taylor expansion method diverges for diamond and fcc Al. In addition to the above cases, we confirmed that the spectrum radii of the $O$-matrix also exceed 1.0 for the graphite and poly(ethylene), so that the applicability of the Taylor expansion method is strictly restricted. Therefore, we do not provide the convergence properties of the Taylor expansion method in this paper.

Figure 2 shows the convergence properties of the 1-norm $\eta$ of the error matrix for diamond calculated by the recursion, divide, and Hotelling’s methods. In the recursion method the 1-norm exponentially decays for each shell cluster as a function of the number of recursion levels, and finally converges to the value of the 1-norm calculated by the divide method for the corresponding cluster. In the divide method the 1-norm almost exponentially diminishes as a function of number of shells. For the seven-shell cluster the 1-norm is only $3.1 \times 10^{-5}$ eV. The identity matrix I cannot be used as an initial guess $S_0^{-1}$ in Hotelling’s method because the spectrum radii of the $O$-matrix exceed 1.0. Thus, we gave the initial guess $S_0^{-1}$ by
Eq. (16), where $\sigma$ is 0.021 for diamond. In Hotelling’s method the convergence properties are not monotonic compared to the other two methods. For three-, five-, and seven-shell clusters, the 1-norm is gradually reduced for smaller number of iterations. However, the 1-norm increases after reaching at the minimum, and finally we have a numerical instability that the 1-norm diverges as iteration proceeds. The smallest 1-norm for each shell-cluster is slightly larger than that calculated by the divide method for the same cluster. Therefore, we see that Hotelling’s method cannot reach the perfect convergence for diamond due to the numerical instability. For Hotelling’s method we also examined the convergence properties of the 1-norm $\eta$ for carbon in the diamond structure with 3.9 Å of a lattice constant in which the spectrum radius of the $O$-matrix is within 1.0, while the result is not shown in this paper. In this system the 1-norm very quickly converges to the corresponding value calculated by the divide method for the same cluster. Thus, we heuristically find that Hotelling’s method gives convergent results for systems with the spectrum radii smaller than 1.0.

As with Fig. 2, the convergence properties of the 1-norm are shown in Fig. 3 for fcc Al. The magnitude of the 1-norm is 1~2 order larger than that of diamond, while the behavior of the 1-norm is very similar to that of diamond. In the recursion method the converged values of the 1-norm are consistent with those of the divide method for four- and six-shell clusters, respectively. In Hotelling’s method we used Eq. (16) with $\sigma = 0.0098$ as $S_0^{-1}$, since the spectrum radius of the $O$-matrix exceed 1.0 for fcc Al. The 1-norms for the four- and six-shell clusters finally diverge without achieving the full convergence like for diamond. Although we tested the convergence properties using several values for $\sigma$ in both diamond and fcc Al, we could not obtain converged results and moreover could not avoid the numerical instability.

Figures 4(a) and 4(b) show the relation between the magnitude of the 1-norm $\eta$ of the error matrix and the computational time per atom to evaluate the inverse of the overlap matrix for diamond and fcc Al, respectively. The comparison clearly indicates that the computational efficiency increases in the order of the divide < Hotelling’s < the recursion methods for both diamond and fcc Al. The recursion method is about one-hundred times
faster than the divide method in computational time to achieve the same convergence for diamond and fcc Al.

**IV. CONCLUSIONS**

We presented a new $O(N)$ algorithm for calculating the inverse of the overlap matrix $S$. It is based on the recursion method with the block Lanczos algorithm. The problem of evaluating $S^{-1}$ is mapped to the block BOP method for an orthogonal TB model just by replacing the Hamiltonian with the overlap operator. In addition, we briefly described the other known-methods for calculating the inverse in $O(N)$ operations: the divide, the Taylor expansion, and Hotelling’s methods. We examined the computational accuracy and efficiency of these $O(N)$ inverting methods using the 1-norm of the error matrix for diamond and fcc Al in DFT calculations with the minimal basis set for valence electrons. The spectrum radius of the $O$-matrix given by $(S-I)$ exceeds 1.0 for many real materials in the DFT calculations based on the localized bases, which means that the applicability of the Taylor expansion method is significantly restricted. In the recursion method the 1-norm of the error matrix exponentially converges to the value calculated by the divide method for the same cluster in both diamond and fcc Al with numerical stability. On the other hand, Hotelling’s method cannot reach the converged results due to the numerical instability in both cases. The comparison of computational time shows that the recursion method is the most efficient algorithm among the four $O(N)$ inverting methods in diamond and fcc Al. The recursion method is about one-hundred times faster than the divide method. Thus, the new method for the evaluation of the inverse is a practical algorithm and can be incorporated in several $O(N)$ methods for total energy calculations using localized orbital basis.

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FIGURES

FIG. 1. The density of states for eigenvalues of the $O$-matrix for diamond and fcc Al, where carbon and aluminum atoms have minimal numerical basis sets for valence electrons which were obtained by DFT calculations for the atomic states. The experimental values, 3.57 and 4.05 Å, were used as the lattice constants of diamond and fcc Al, respectively.

FIG. 2. The 1-norm of the error matrix for diamond calculated by the (a) recursion, (b) divide, and (c) Hotelling’s methods. In both the recursion and Hotelling’s methods, the 1-norms were calculated for three-, five-, and seven-shell clusters as a function of number of recursion levels and iterations, respectively.

FIG. 3. The 1-norm of the error matrix for fcc Al calculated by the (a) recursion, (b) divide, and (c) Hotelling’s methods. In both the recursion and Hotelling’s methods, the 1-norms were calculated for four- and six-shell clusters as a function of number of recursion levels and iterations, respectively.

FIG. 4. The 1-norm of the error matrix for (a) diamond and (b) fcc Al against the computational time taken per atom calculated by three $O(N)$ inverting methods. The calculations were performed using single processor on a compaq ES40 workstation.
Diamond
Al (fcc)
