A Succinct Way to Diagonalize the Translation Matrix in Three Dimensions †

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Abstract

The diagonalization of the translation matrix is crucial in reducing the solution time in the fast multipole method. The translation matrix can be related to the matrix representation of the translation operators in the translation group in group theory. Therefore, these matrices can be diagonalized with a proper choice of basis representation. Here, a different and succinct way to diagonalize the translation operator in three dimensions for Helmholtz equation involving a general number of multipoles is demonstrated. The derivation is concise, and can be related to a set of similarity transforms equivalent to the change of basis representation for the translation group. The result can be used for scattering calculations related to wave equation as found in electrodynamics, elastodynamics, and acoustics where the fast multipole method is used.

1. Introduction

The fast multipole method [1-6] is an effective way to expedite iterative solutions of integral equations for electrodynamic and elastodynamic problems. The matrices that arise from integral equations of these problems are always dense. One way to solve these matrix equations is via an iterative method. Iterative solutions, such as the conjugate gradient method, requires matrix vector multiplies, and for dense matrices, these matrix-vector multiplies constitute the predominant computational cost as well as memory requirement. Fast multipole method reduces the solution time by curtailing the number

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of operations needed to perform a matrix-vector multiply and the memory requirement of the algorithm.

The fast multipole method is based on the translation of multipoles from one coordinate system to another. This translation can be achieved by the use of translation matrices. However, the mere use of translation matrices does not reduce the computational cost nor the memory requirement for surface scatterers. The crucial step in the fast multipole method for dynamic problems, for instance, as in Helmholtz equation, is the diagonalization of the translation operators. For static problems, this diagonalization is not necessary to achieve reduced computational complexity, but for dynamic problems, it is imperative.

The diagonalization of the translation matrix from a monopole source point to a monopole receive point in three dimensions was first reported in [2]. The diagonalization of the translation operator has been formally performed by Rokhlin [7]. Later, Epton and Dembart [8] showed more details in the derivation of the diagonal translation operator. In this paper, we will show an alternative and also more succinct method to diagonalize the general translation matrix. This translation matrix translates from the general number of multipoles in one coordinate system to a general number of multipoles in another coordinate system. The result can be used to expedite the solution of the wave equation and related equations as found in electrodynamics and elastodynamics where multiple scattering involves multipoles. The derivation also shows that the diagonalization is achieved by the use of a plane-wave basis, and a series of similarity transforms.

A two level implementation of the dynamic fast multipole method results in an algorithm with $O(N^{1.5})$ complexity with the same complexity for memory requirement [1-3,6]. The use of the ray propagation approach [4,5] further reduces the complexity and memory requirement of the two-level algorithm to $O(N^{1.33})$. An electrodynamic multilevel implementation results in an algorithm with $O(N \log N)$ complexity for both computation and memory requirement [9,10]. For volumetric scatterers, the complexity can be reduced to $O(N)$ [11]. Other implementations of the multilevel fast multipole method have also been reported in [12,13].

2. Diagonalization

The addition theorem in three dimensions is [14,15, p. 594]

$$\Psi_L(k,\mathbf{r}) = \sum_{L'} \Re g \Psi_{L'}(k,\mathbf{r}')\alpha_{L',L}(k,\mathbf{r}''), \tag{1}$$

where $L = (l,m)$, $L' = (l',m')$ and $\mathbf{r} = \mathbf{r}' + \mathbf{r}''$, $\Psi_L(k,\mathbf{r})$ is a scalar wave function given by $h_l^{(1)}(kr)Y_{lm}(\theta,\phi)$, k is the wavenumber in Helmholtz equation, $h_l^{(1)}(x)$ is the spherical Hankel function of the first kind, and $Y_{lm}(\theta,\phi)$ is a normalized spherical harmonic function involving the Legendre polynomial $P_l(\cos\theta)$ and $\exp(im\phi)$. In Equation (1), $\Re g$ implies the "regular part" whereby a Hankel function is replaced by a Bessel function. In the domain L' of the above summation, $l' \geq 0$ and $-l' \leq m' \leq l'$ and similarly for the range L. Furthermore [15],

$$\alpha_{L',L}(\mathbf{r}'') = \sum_{L''} \Psi_{L''}(k, \mathbf{r}'') \int d\Omega_k Y_L(\Omega_k) Y^*_{L'}(\Omega_k) Y^*_{L''}(\Omega_k) 4\pi i^{(l'+l''-l)}, \tag{2}$$

where the k dependence of the $\alpha_{L',L}$ matrix is implied. Also, since the integral above is homomorphic to the addition of angular momentum in quantum mechanics, where l, l', and l'' are magnitudes of three angular momenta, the integral is nonzero only if $|l - l'| \leq l'' \leq l + l'$, viz., the triangular inequality [16].

In Equation (1), $\alpha_{L',L}$ is the translation matrix that translates from a general number of multipoles in the $\mathbf{r}$ coordinate system to a general number of multipoles in the $\mathbf{r}'$ coordinate system. If the $\Psi_{L''}$ in (2) is replaced by $\Re g \Psi_{L''}$, then these translation matrices are actually the matrix representations of the translation group in group theory [16]. However, these representations are reducible, since the translation group has its simplest and irreducible representation under a plane-wave basis. Therefore, it hints that a simpler and diagonal form of these translation matrices exists. We will seek to derive a diagonal representation of this translation matrix.

In a fast algorithm, we need to compute [see 3 or 15 for this notation]

$$\overline{\boldsymbol{\alpha}}_{ij} = \overline{\boldsymbol{\beta}}_{i\lambda} \cdot \overline{\boldsymbol{\alpha}}_{\lambda\lambda'} \cdot \overline{\boldsymbol{\beta}}_{\lambda' j}, \tag{3}$$

or

$$\alpha_{L,L'}(\mathbf{r}_{ij}) = \sum_{L_1,L_2} \beta_{L,L_1}(\mathbf{r}_{i\lambda}) \alpha_{L_1,L_2}(\mathbf{r}_{\lambda\lambda'}) \beta_{L_2,L'}(\mathbf{r}_{\lambda' j}), \tag{3a}$$

where $\mathbf{r}_{ij}$ represents the translation direction of the origin of the pertinent coordinate systems. Furthermore,

$$\beta_{L',L}(\mathbf{r}'') = \sum_{L''} 4\pi i^{(l'+l''-l)} \Re g \Psi_{L''}(k, \mathbf{r}'') \int d\Omega_k Y_L(\Omega_k) Y^*_{L'}(\Omega_k) Y^*_{L''}(\Omega_k), \tag{4}$$

implying that $\beta_{L',L}$ is just the regular part of $\alpha_{L',L}$, and hence, the matrix representation of the translation group [16].

The factorization in (3) can be used to potentially reduce computational labor in a matrix vector multiplication since it allows the grouping of source points and receiving points [1-3]. Unfortunately, the $\overline{\boldsymbol{\alpha}}$ matrices are dense matrices. Hence, there is no reduction in computational cost if one factors the $\overline{\boldsymbol{\alpha}}$ matrices as indicated in Equation (3). However, if we diagonalize the $\overline{\boldsymbol{\alpha}}$ matrices, then the factorization in the manner of Equation (3) will reduce the computational cost. To this end, we will use the plane-wave representation as much as possible to achieve the diagonalization of the α matrix.

Since [15, p. 592, Eq. (D4),17]

$$e^{i\mathbf{k}\cdot\mathbf{r}''} = \sum_{L''} 4\pi i^{l''} Y^*_{L''}(\Omega_k) \Re g \Psi_{L''}(k, \mathbf{r}''), \tag{5}$$

we have

$$\beta_{L',L}(\mathbf{r}'') = i^{(l'-l)} \int d\Omega_k Y^*_{L'}(\Omega_k) Y_L(\Omega_k) e^{i\mathbf{k}\cdot\mathbf{r}''}. \tag{6}$$

The above is the statement that the β matrix is related to its plane-wave representation $\exp(i\mathbf{k}\cdot\mathbf{r}'')$ by a similarity transform. Hence, the diagonalization of the β matrices is already attained. We next use the representation of the β matrix from (6) into (3) to achieve the final diagonalization of the α matrix.

Using (6) in (3a), we have

$$\alpha_{L,L'}(\mathbf{r}_{ij}) = \sum_{L_1,L_2} i^{(l-l_1)} \int d\Omega_k Y^*_L(\Omega_k) Y_{L_1}(\Omega_k) e^{i\mathbf{k}\cdot\mathbf{r}_{i\lambda}} \alpha_{L_1,L_2}(\mathbf{r}_{\lambda\lambda'}) \\ i^{(l_2-l')} \int d\Omega'_k Y^*_{L_2}(\Omega'_k) Y_{L'}(\Omega'_k) e^{i\mathbf{k}'\cdot\mathbf{r}_{\lambda' j}}. \tag{7}$$

Exchanging the order of integrations and summations, we have

$$\alpha_{L,L'}(\mathbf{r}_{ij}) = \int d\Omega_k i^l Y^*_L(\Omega_k) e^{i\mathbf{k}\cdot\mathbf{r}_{i\lambda}} \int d\Omega'_k i^{-l'} Y_{L'}(\Omega'_k) e^{i\mathbf{k}'\cdot\mathbf{r}_{\lambda' j}} \\ \sum_{L_1,L_2} i^{l_2-l_1} Y_{L_1}(\Omega_k) \alpha_{L_1,L_2}(\mathbf{r}_{\lambda\lambda'}) Y^*_{L_2}(\Omega'_k). \tag{8}$$

Letting

$$A_{\lambda\lambda'}(\Omega_k,\Omega'_k) = \sum_{L_1,L_2} i^{l_2-l_1} Y_{L_1}(\Omega_k) \alpha_{L_1,L_2}(\mathbf{r}_{\lambda\lambda'}) Y^*_{L_2}(\Omega'_k), \tag{9}$$

we seek to simplify $A_{\lambda\lambda'}(\Omega_k,\Omega'_k)$. Using (2) in (9), we have

$$A_{\lambda\lambda'}(\Omega_k,\Omega'_k) = \sum_{L''} \Psi_{L''}(k,\mathbf{r}_{\lambda\lambda'}) \int d\Omega''_k Y^*_{L''}(\Omega''_k) 4\pi i^{l''} \\ \sum_{L_1,L_2} Y_{L_1}(\Omega''_k) Y_{L_2}(\Omega'_k) Y^*_{L_1}(\Omega_k) Y^*_{L_2}(\Omega''_k). \tag{10}$$

Using the fact that

$$\delta(\Omega_k - \Omega'_k) = \sum_L Y_L(\Omega_k) Y^*_L(\Omega'_k), \tag{11}$$

we have

$$A_{\lambda\lambda'}(\Omega_k,\Omega'_k) = \sum_{L''} \Psi_{L''}(k,\mathbf{r}_{\lambda\lambda'}) 4\pi i^{l''} \delta(\Omega_k - \Omega'_k) Y_{L''}(\Omega'_k). \tag{12}$$

Consequently, (8) becomes

$$\alpha_{L,L'}(\mathbf{r}_{ij}) = \int d\Omega_k i^l Y^*_L(\Omega_k) e^{i\mathbf{k}\cdot\mathbf{r}_{i\lambda}} \tilde{\alpha}_{\lambda\lambda'}(\Omega_k) i^{-l'} Y_{L'}(\Omega_k) e^{i\mathbf{k}\cdot\mathbf{r}_{\lambda' j}}, \tag{13}$$

where

$$\tilde{\alpha}_{\lambda\lambda'}(\Omega_k) = \sum_{L''} \Psi_{L''}(k, \mathbf{r}_{\lambda\lambda'}) 4\pi(-1)^{l''} Y_{L''}(\Omega_k). \tag{14}$$

Equation (13) above represents the diagonal form of Equation (3) where the middle factor $\tilde{\alpha}_{\lambda\lambda'}$ is diagonal so that instead of a double summation as in (3a), Equation (13) has only one single integral. Notice that the calculation of $\alpha_{L,L'}(\mathbf{r}_{ij})$ via (13) is a lot more efficient than that via (3a).

It is to be noted that the summation in (14) is divergent if taken over an infinite range. The reason is that α_{L_1,L_2} becomes infinitely large when $|l_1 - l_2| \to \infty$. Therefore, the inner summation in (8) does not converge. To prevent this from happening, the summation in (2) should be truncated. In this case, $\alpha_{L_1,L_2} = 0$ when $|l_1 - l_2| > l''$. Therefore, when (2) is used for α_{L_1,L_2}, the summations over L'' in (10), and hence (14), are automatically truncated.

In Equation (14), the double summation inherent in the index $L'' = (l'', m'')$ can be removed if one selects the z axis to coincide with the direction of $\mathbf{r}_{\lambda\lambda'}$, viz.,

$$\tilde{\alpha}_{\lambda\lambda'}(\Omega_k) = \sum_{l=0}^{L_{max}} i^l (2l+1) h_l^{(1)}(k r_{\lambda\lambda'}) P_l(\hat{k} \cdot \hat{r}_{\lambda\lambda'}). \tag{15}$$

Notice that the above form is expressible in a coordinate independent form and the argument of the Legendre polynomial depends on the angle between $\hat{k}$ and $\hat{r}_{\lambda\lambda'}$. If $L = L' = 0$ in (13), the formula reduces to that given in [2].

3. Conclusions

The translation matrix in three dimensions for Helmholtz wave equation has been successfully diagonalized using an alternative and succinct method. The method reveals the relationship between the translation matrices and their representation of the translation group in group theory. A diagonalization is expected under a plane-wave basis for the representation since a plane-wave basis forms an irreducible representation for the translation group. Hence, the diagonalization of the translation matrices from the spherical harmonic representation can be viewed as a series of similarity transforms. In other words, the manipulation from (7) to (13) can be viewed as a series of similarity transforms equivalent to the change of basis. The result can be used for the fast multipole method and the multilevel fast multipole method where multiple scattering involves interaction between multipoles.

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