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SINGLE LEVEL MULTIPOLE EXPANSIONS AND OPERATORS FOR POTENTIALS OF THE FORM $r^{-\lambda}$*

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Abstract. This paper presents the generalized multipole, local, and translation operators for three-dimensional static potentials of the form $r^{-\lambda}$, where λ is any real number. Addition theorems are developed using Gegenbauer polynomials. Multipole expansions and error bounds are presented in a manner similar to those for truncated classical multipole expansions. Numerical results showing error behavior versus number of terms, distance, and λ are presented.

Key words. FMM, Gegenbauer polynomials, van der Waals force

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1. Introduction.

The N-body three dimensional (3D) problem involving the Coulombic r^{-1} Green's function has been successfully accelerated using the FMM ($\mathcal{O}(N)$ method) by Greengard [1] and other related techniques [5, 7, 8]. These techniques improve drastically over the classical $\mathcal{O}(N^2)$ method by efficiently clustering sources and observers in a multilevel manner. Furthermore, the FMM is error-controllable; i.e., the truncation and approximation errors can be predicted in an a priori manner by choosing a specific number of terms in multipole and local expansions.

A related area of research has been the development of FMM-like methods based on plane-wave expansions and variations [6] for oscillatory kernels arising in dynamic electromagnetics and acoustics. Apart from the r^{-1} and dynamic oscillatory kernels, another class includes potential functions of the form $r^{-\lambda}$, where λ is a positive integer. For example, the van der Waals forces, Lennard-Jones potentials, and H-bonds have the forms r^{-6}, r^{-12}, and r^{-10} and have important applications in chemistry [10], molecular dynamics [11] and fluid mechanics [12]. Present computational approaches rely heavily on FMM or related methods for Coulombic interactions, but do not have the same approaches for the van der Waals forces, owing to a lack of exact multipole expansions. (Other approaches based on precorrected FFT on a uniform grid are topics of current research.) A generalized FMM technique for nonoscillatory kernels based on singular value decomposition has been presented in [9]. In this paper, to the best of our knowledge, for the first time analytic multipole expansions are developed for potential functions of the form $r^{-\lambda}$, for all real λ. In a manner analogous to the classical multipole expansions for electrostatic potentials, these expansions are error-controllable and enable efficient clustering of sources and observers. In the multipole method presented in [1] spherical harmonics are used. In this paper the well-known Gegenbauer polynomials are used instead to deduce the necessary addition theorems for source-clustering, observer-clustering, and cluster-cluster interactions. In doing so all the necessary operators for a single level FMM for functions of the form $r^{-\lambda}$ are obtained.

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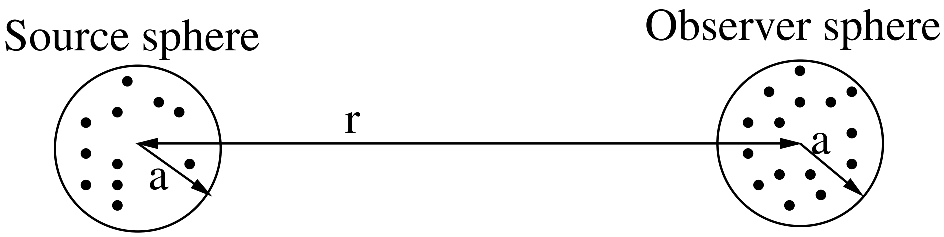

FIG. 1. *Two well-separated spheres ($r > 2a$) consisting of N source and N observation points.*

The organization of the paper is as follows: In section 2 the problem statement is made. Section 3 briefly discusses the previous treatment of the case $\lambda = 1$ as in [1]. In section 4 the required addition theorems for general λ, multipole operators, and error bounds are derived. In section 5 numerical results are stated. In section 6 conclusions are drawn and discussion about the scope of extending this research is given.

2. Statement of the problem. Consider a sphere containing N source points of strengths q_i, located at coordinates $(\rho_i, \alpha_i, \beta_i)$ and a sphere of N observation points located at (r_j, θ_j, ϕ_j), where $i, j = 1 \dots N$, as depicted in Figure 1. The two spheres are well separated so that they are nonoverlapping. The total potential at the jth observation point is given by $\sum_{i=1}^{N} G(\rho_\mathbf{i}, \mathbf{r_j})q_i$. This paper deals with potential functions of the form $G(\rho_\mathbf{i}, \mathbf{r_j}) = |\mathbf{r_j} - \rho_\mathbf{i}|^{-\lambda}$. The potentials at the N observation points can be represented in the matrix form $\Phi_{N\times 1} = \bar{\mathbf{G}}_{N\times N}\mathbf{q}_{N\times 1}$, where Φ and $\mathbf{q}$ are vectors containing the potentials and the charges at the N source and observation points. The (i, j)th entry of matrix $\bar{\mathbf{G}}$ is the potential function $G(\rho_\mathbf{i}, \mathbf{r_j})$. The brute force cost of forming $\bar{\mathbf{G}}$ and then of obtaining Φ by the matrix vector multiplication is $\mathcal{O}(N^2)$. The aim of this paper is to factorize the $\bar{\mathbf{G}}$ matrix into $\overline{\mathbf{L2P}}_{N\times c}$, $\overline{\mathbf{M2L}}_{c\times c}$ and $\overline{\mathbf{Q2M}}_{c\times N}$, c being a small constant number, independent of N and dependent on the desired accuracy. This reduces the cost of generation and multiplication into $\mathcal{O}(cN)$.

3. Classical FMM operators for r^{-1}. This section summarizes the results for the case $\lambda = 1$ as obtained in [1]. The geometry of the problem is described by Figure 2. The three vectors are $\mathbf{Q} = (\rho, \alpha, \beta)$, $\mathbf{P} = (r, \theta, \phi)$, and $\mathbf{P} - \mathbf{Q} = (r', \theta', \phi')$ in spherical coordinates. For this geometry $\phi' = \phi - \beta$, $\cos\gamma = \cos\alpha\cos\theta + \sin\alpha\sin\theta\cos\phi'$. It will be assumed hereafter that $r > \rho$.

The potential Φ_j at $\mathbf{P}$ due to a unit charge at $\mathbf{Q}$ is $1/r'$. $1/r'$ can be written in the following way using the generating function of the Legendre polynomials:

$$\frac{1}{r'} = \frac{1}{r\sqrt{1 - 2\frac{\rho}{r}\cos\gamma + \left(\frac{\rho}{r}\right)^2}} = \sum_{n=0}^{\infty} \frac{\rho^n}{r^{n+1}} P_n(\cos\gamma), \tag{1}$$

where $P_n(\cos\gamma)$ is the Legendre polynomial. The addition theorem for the Legendre polynomials is given by

$$P_n(\cos\gamma) = \sum_{m=-n}^{n} Y_n^{-m}(\theta, \phi) Y_n^m(\alpha, \beta), \tag{2}$$

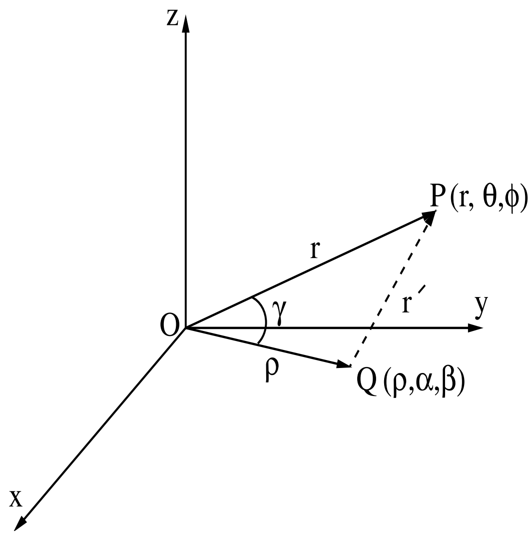

FIG. 2. *Geometry of the problem:* **P** *and* **Q** *are separated by* r' *and subtend an angle* γ *at the origin. Here* $\mathbf{P} - \mathbf{Q} = (r', \theta', \phi')$ *and* $r > \rho$.

where $Y_n^m(\theta, \phi) = \sqrt{\frac{n-|m|}{n+|m|}} P_n^{|m|}(\cos\theta) e^{im\phi}$ is the spherical harmonic and $P_n^m(\cos\theta)$ is the associated Legendre function [3].

Using (1) and (2), the potential at the jth observation point is converted into the following multipole expansion:

$$\phi_j = \sum_{n=0}^{p} \sum_{m=-n}^{n} \frac{M_n^m}{r_j^{n+1}} Y_n^m(\theta_j, \phi_j), \tag{3}$$

where the multipole expansion $M_n^m = \sum_{i=1}^N q_i \rho_i^n Y_n^{-m}(\alpha_i, \beta_i)$ and p is the number of terms, referred to as the number of harmonics, that is chosen during truncation of the infinite series in (1). Using (3) the potential at N points can thus be expressed in the matrix form $\Phi_{N\times 1} = \overline{\mathbf{M2P}}_{N\times(p+1)^2}\ \overline{\mathbf{Q2M}}_{(p+1)^2\times N}\ \mathbf{q}_{N\times 1}$, where

$$\begin{aligned} \overline{\mathbf{Q2M}}(k, j) &= \rho_j^n Y_n^{-m}(\alpha_j, \beta_j), \\ \overline{\mathbf{M2P}}(i, k) &= \frac{Y_n^m(\alpha_i, \beta_i)}{r_i^{n+1}}, \end{aligned} \tag{4}$$

where $i, j = 1, 2 \ldots N$, $k = 1 \ldots (p+1)^2$. Here the entries of $\overline{\mathbf{Q2M}}$ depend only on the source points and the entries of $\overline{\mathbf{M2P}}$ depend only on the observation points. To complete the formulation for single level FMM it is necessary that the $\overline{\mathbf{M2P}}$ matrix be factorized into $\overline{\mathbf{L2P}}\ \ \overline{\mathbf{M2L}}$, where the $\overline{\mathbf{M2L}}$ operator translates the multipole expansion to a local expansion at a local point in the observation sphere and the $\overline{\mathbf{L2P}}$ operator transfers the local expansion to the potentials at the observation points. In other words an addition theorem for the function $\frac{Y_n^m(\theta,\phi)}{r^{n+1}}$ is required. This addition theorem has been obtained in [1, Chapter 3] and is given by

$$\frac{Y_{n'}^{m'}}{r'^{n'+1}} = \sum_{n=0}^{p} \sum_{m=-n}^{n} \frac{J_m^{m'} A_n^m A_{n'}^{m'} \rho^n Y_n^{-m}}{A_{n+n'}^{m+m'}} \frac{Y_{n+n'}^{m+m'}}{r^{n+n'+1}}, \tag{5}$$

where

$$J_m^{m'} = \begin{cases} (-1)^{min(|m|,|m'|)} & \text{if } m.m' < 0, \\ 1 & \text{otherwise} \end{cases}$$

and $A_n^m = (-1)^n/\sqrt{(n-m)!(n+m)!}$. Using (5) a multipole expansion at $\mathbf{P}$ can be converted into a local expansion at the origin O in Figure 2. $\overline{\mathbf{M2P}}$ can be expressed as a product of two matrices $\overline{\mathbf{L2P}}_{N\times(p+1)^2}\ \overline{\mathbf{M2L}}_{(p+1)^2\times(p+1)^2}$ using (5) in a similar manner as in (4). The entries of $\overline{\mathbf{L2P}}$ depend on the observation points, and the entries of $\overline{\mathbf{M2L}}$ depend on the locations of the centers of the source and the observation spheres. Thus the factorization $\Phi = \overline{\mathbf{L2P}}\ \overline{\mathbf{M2L}}\ \overline{\mathbf{Q2Mq}}$ is complete. The rest of this paper will present an analogous approach using Gegenbauer polynomials instead of Legendre polynomials to solve the general problem for $r^{-\lambda}$.

4. Formulation for the function $r^{-\lambda}$. In this section Gegenbauer polynomials are introduced, which will be central to the treatment for general λ. These are orthogonal polynomials denoted by $C_n^\lambda(x)$, where n is an integer and $\lambda > -1/2$. These polynomials are also known as ultraspherical polynomials and arise as solutions to the Gegenbauer differential equation

$$(1-x^2)y'' - (2\lambda+1)xy' + n(n+2\lambda)y = 0.$$

They are computed by the following recurrence formula [2]:

$$\begin{aligned} &C_0^\lambda(x) = 1, \\ &C_1^\lambda(x) = 2\lambda x, \\ &nC_n^\lambda(x) = 2(n+\lambda-1)xC_{n-1}^\lambda(x) - (n+2\lambda-2)C_{n-2}^\lambda(x). \end{aligned}$$

The generating function for these polynomials [2] is given by

$$(1-2xz+z^2)^{-\lambda} = \sum_{n=0}^{\infty} C_n^\lambda(x)z^n, \quad \text{for } |z| < 1. \tag{6}$$

It is clear from (6) that the Legendre polynomial ($\lambda = 1/2$) is a special case of the Gegenbauer polynomial. This strongly suggests that there might be an extension of Greengard's method to general values of λ and lays the ground for this investigation.

4.1. Some properties of Gegenbauer polynomials.

NOTATION 1.

1. $\left(\frac{\partial}{\partial x} \pm i\frac{\partial}{\partial y}\right) = \partial_\pm$,
2. $\partial_{x,y,z} = \frac{\partial}{\partial(x,y,z)}$,
3. $(\lambda)_m = \lambda(\lambda+1)\ldots(\lambda+m-1) = \frac{\Gamma(\lambda+m)}{\Gamma(\lambda)}$,
4. $A(n,m,\lambda) = (-1)^n(n-m)!2^m\left(\frac{\lambda}{2}\right)_m$,
5. $T(m,k,\lambda) = (-1)^{m+k}(\lambda-1)_{2k}\binom{m}{k}$,
6. $P(r,\theta,\pm\phi,n,m,\lambda) = \frac{\sin^m\theta}{r^{n+\lambda}}e^{\pm im\phi}C_{n-m}^{\lambda/2+m}(\cos\theta)$.

The following properties of Gegenbauer polynomials are stated in [2] and will be used later in this paper:

$$C_n^\lambda(\cos\alpha) = \sum_{m=0}^{n} \frac{(\lambda)_m(\lambda)_{n-m}}{m!(n-m)!}\cos(n-2m)\alpha, \tag{7}$$

$$C_n^\lambda(x) = \sum_{m=0}^{[n/2]} (-1)^m \frac{\lambda_{n-m}}{m!(n-2m)!}(2x)^{n-2m}, \tag{8}$$

$$\frac{d^m}{dx^m} C_n^\lambda(x) = 2^m (\lambda)_m C_{n-m}^{\lambda+m}(x), \tag{9}$$

$$C_n^\lambda(-x) = (-1)^n C_n^\lambda(x), \tag{10}$$

$$C_n^\lambda(1) = \frac{(2\lambda)_n}{n!}. \tag{11}$$

The following theorem appears to be new and is important in the subsequent development, so the proof is discussed here.

THEOREM 1. *Let* $\mathbf{P} = (r, \theta, \phi) \in R^3$. *Then*

$$\frac{\partial^{n-m}}{\partial z^{n-m}} \left(\frac{\partial}{\partial x} \pm i \frac{\partial}{\partial y} \right)^m \frac{1}{r^\lambda} = \frac{\sin^m \theta}{r^{n+\lambda}} e^{\pm im\phi} (-1)^n (n-m)! 2^m \left(\frac{\lambda}{2}\right)_m C_{n-m}^{\lambda/2+m}(\cos\theta).$$

Proof. The following theorem is stated in Hobson [3]:

$$\begin{aligned} &f_n(\partial_x, \partial_y, \partial_z) F(x^2+y^2+z^2) \\ &= \left(2^n \frac{d^n F}{d(r^2)^n} + \frac{2^{n-2}}{1!} \frac{d^{n-1}F}{d(r^2)^{n-1}} \nabla^2 + \cdots + \frac{2^{n-2t}}{t!} \frac{d^{n-t}F}{d(r^2)^{n-t}} \nabla^{2t} + \cdots \right) f_n(x,y,z), \end{aligned} \tag{12}$$

where $r^2 = x^2+y^2+z^2$. Put $F(r^2) = \frac{1}{r^\lambda}$. Let $r^2 = r_1$, so $F(r_1) = \frac{1}{r_1^{\lambda/2}}$.

Putting $f_n(\partial_x, \partial_y, \partial_z), = \partial_z^{n-m} \partial_\pm^m$,

$$\begin{aligned} \partial_z^{n-m} \partial_\pm^m \frac{1}{r^\lambda} &= \left(2^n (-1)^n \left(\frac{\lambda}{2}\right)_n \frac{1}{r^{2n+\lambda}} + \frac{2^{n-2}}{1!} (-1)^{n-1} \left(\frac{\lambda}{2}\right)_{n-1} \frac{r^2}{r^{2n+\lambda}} \nabla^2 + \cdots \right. \\ &\quad \left. + \frac{2^{n-2t}}{t!} (-1)^{n-t} \left(\frac{\lambda}{2}\right)_{n-t} \frac{r^{2t}}{r^{2n+\lambda}} \nabla^{2t} + \cdots \right) z^{n-m} (x \pm iy)^m \\ &= (x \pm iy)^m \left(2^n (-1)^n \left(\frac{\lambda}{2}\right)_n \frac{1}{r^{2n+\lambda}} + \frac{2^{n-2}}{1!} (-1)^{n-1} \left(\frac{\lambda}{2}\right)_{n-1} \frac{r^2}{r^{2n+\lambda}} \frac{d^2}{dz^2} + \cdots \right. \\ &\quad \left. + \frac{2^{n-2t}}{t!} (-1)^{n-t} \left(\frac{\lambda}{2}\right)_{n-t} \frac{r^{2t}}{r^{2n+\lambda}} \frac{d^{2t}}{dz^{2t}} + \cdots \right) z^{n-m} \\ &= r^m \sin^m \theta e^{\pm im\phi} \frac{(-1)^n}{r^{2n+\lambda}} \sum_{t=0}^{[\frac{n-m}{2}]} (-1)^t \frac{2^{n-2t}}{t!} \left(\frac{\lambda}{2}\right)_{n-t} \frac{(n-m)!}{(n-m-2t)!} r^{2t} z^{n-m-2t} \end{aligned}$$

$$= \sin^m \theta e^{\pm im\phi} \frac{(-1)^n}{r^{n+\lambda}}(n-m)! \sum_{t=0}^{[\frac{n-m}{2}]} (-1)^t \frac{2^{n-2t}}{t!} \left(\frac{\lambda}{2}\right)_{n-t} \frac{\mu^{n-m-2t}}{(n-m-2t)!}$$
$$\left(\text{where } \mu = \frac{z}{r} = \cos\theta\right)$$

$$= \sin^m \theta e^{\pm im\phi} \frac{(-1)^n}{r^{n+\lambda}}(n-m)! \frac{d^m}{d\mu^m} \sum_{t=0}^{[\frac{n}{2}]} \frac{(-1)^t}{t!} \left(\frac{\lambda}{2}\right)_{n-t} \frac{(2\mu)^{n-2t}}{(n-2t)!}$$

$$= \sin^m \theta e^{\pm im\phi} \frac{(-1)^n}{r^{n+\lambda}}(n-m)! 2^m \left(\frac{\lambda}{2}\right)_m C_{n-m}^{\lambda/2+m}(\cos\theta)$$

using (8) and (9). □

The following identity is known for $\lambda = 1$ [2, 3]:

$$\partial_\pm^m \partial_z^{n-m} \left(\frac{1}{r}\right) = (-1)^{n-m}(n-m)! \frac{P_n^m(\cos\theta)}{r^{n+1}} e^{\pm im\phi}.$$

Thus putting $\lambda = 1$ gives the following identity documented in [2], which describes the relation between the Gegenbauer polynomials and the associated Legendre functions:

$$(-2)^m \sin^m\theta \left(\frac{1}{2}\right)_m C_{n-m}^{1/2+m}(\cos\theta) = P_n^m(\cos\theta). \qquad \square$$

LEMMA 1.

$$(\partial_+\partial_-)^m \left(\frac{1}{r^\lambda}\right) = (-1)^m \sum_{k=0}^{m} (-1)^k \binom{m}{k} (\lambda-1)_{2k} (\partial_z^2)^{m-k} \frac{1}{r^{2k+\lambda}}.$$

Proof. From $r = (x^2+y^2+z^2)^{1/2}$ it may be verified that

$$\nabla^2 \frac{1}{r^\lambda} = \frac{-3\lambda + \lambda(\lambda+2)}{r^{\lambda+2}} = \frac{\lambda(\lambda-1)}{r^{\lambda+2}}$$

$$\Rightarrow \partial_+\partial_- \left(\frac{1}{r^\lambda}\right) = -\partial_z^2 \frac{1}{r^\lambda} + \frac{\lambda(\lambda-1)}{r^{\lambda+2}}$$
$$\Rightarrow (\partial_+\partial_-)^2 \frac{1}{r^\lambda} = \partial_z^4 \frac{1}{r^\lambda} - 2\lambda(\lambda-1)\partial_z^2 \frac{1}{r^{\lambda+2}} + \frac{(\lambda+2)(\lambda+1)\lambda(\lambda-1)}{r^{\lambda+4}}.$$

By induction the proof is completed as follows:

$$(\partial_+\partial_-)^m \frac{1}{r^\lambda} = (-1)^m \sum_{k=0}^{m} (-1)^k (\lambda-1)_{2k} \binom{m}{k} (\partial_z^2)^{m-k} \frac{1}{r^{\lambda+2k}}. \qquad \square$$

COROLLARY 1.

$$\partial_z^{n-a} \partial_+^b \partial_-^{a-b} \left(\frac{1}{r^\lambda}\right)$$
$$= \sum_{k=0}^{m} T(m,k,\lambda) A(n-2k, |a-2b|, \lambda+2k) P(r,\theta,\operatorname{sgn}(2b-a)\phi, n-2k, |a-2b|, \lambda+2k),$$

where $m = \min(b, a-b)$, $\operatorname{sgn}(2b-a)$ *gives the sign of* $2b-a$.

Proof. Let $b = \min(b, a-b)$. Then,

$$\begin{aligned}
\partial_z^{n-a}\partial_+^b\partial_-^{a-b}\left(\frac{1}{r^\lambda}\right) &= \partial_z^{n-a}\partial_-^{a-2b}(\partial_+\partial_-)^b\left(\frac{1}{r^\lambda}\right) \\
&= \partial_z^{n-a}\partial_-^{a-2b}\sum_{k=0}^{b} T(b,k,\lambda)(\partial_z^2)^{b-k}\left(\frac{1}{r^{\lambda+2k}}\right) \text{ (from Lemma 1)} \\
&= \sum_{k=0}^{b} T(b,k,\lambda)\partial_z^{n-a+2b-2k}\partial_-^{a-2b}\left(\frac{1}{r^{\lambda+2k}}\right) \\
&= \sum_{k=0}^{b} T(b,k,\lambda)A(a-2k, a-2b, \lambda+2k) \\
&\qquad \times P(r,\theta,-\phi,n-2k,a-2b,\lambda+2k) \text{ (by Theorem 1).}
\end{aligned}$$

Similarly when $a-b = \min(b, a-b)$ it can be shown that $a-2b$ in the above identity will be replaced by $2b-a$. ∎

Next the results obtained so far are used to derive the necessary addition theorems required to perform the single level FMM on the potential function $r^{-\lambda}$.

4.2. Addition theorems. From (6) the following can be written for the given geometry (see Figure 2):

$$\frac{1}{r'^\lambda} = \sum_{n=0}^{\infty}\frac{\rho^n}{r^{n+\lambda}}C_n^{\lambda/2}(\cos\gamma). \tag{13}$$

One may be tempted to use the following addition theorem for the Gegenbauer polynomials which is well known [2, 4]:

$$\begin{aligned}
C_n^\lambda(\cos\gamma) = \sum_{m=0}^{n} 4^m(2\lambda+2m-1)(n-m)!\frac{[(\lambda)_m]^2}{(2\lambda-1)_{n+m+1}}(\sin\alpha)^m C_{n-m}^{\lambda+m}(\cos\alpha) \\
\times(\sin\theta)^m C_{n-m}^{\lambda+m}(\cos\theta)C_m^{\lambda-1/2}(\cos(\phi-\beta)),
\end{aligned}$$

where γ, α, β, θ, and ϕ are angles as shown in Figure 2. However, unlike (2) the above equation is not in a completely separated form because of the last term $C_m^{\lambda-1/2}(\cos(\phi-\beta))$, making it difficult to represent the multipole, translation, and local operators elegantly. So alternative addition theorems are developed to aid in elegant and readily applicable formulation of the required operators.

THEOREM 2. *For any two vectors* $\mathbf{Q} = (x', y', z') \in R^3$ *and* $\mathbf{P} = (x, y, z) \in R^3$ *as shown in Figure* 2*,*

$$\left(\frac{x'}{\rho}\partial_x + \frac{y'}{\rho}\partial_y + \frac{z'}{\rho}\partial_z\right)^n\frac{1}{r^\lambda} = (-1)^n n!\frac{C_n^{\lambda/2}(\cos\gamma)}{r^{n+\lambda}},$$

where $\rho = ||\mathbf{Q}||$*,*$r = ||\mathbf{P}||$*,*γ *is the angle between the vectors* $\mathbf{P}$ *and* $\mathbf{Q}$*.*

Proof. Consider that

$$\frac{1}{(r^2 - 2r\rho\cos\gamma + \rho^2)^{\lambda/2}} = \frac{1}{((x-x')^2 + (y-y')^2 + (z-z')^2)^{\lambda/2}}.$$

Taylor's series expansion of the left-hand side gives (13). One may expand the right-hand side by Taylor's theorem in powers of either x, y, z or x', y', z'. Because the nth power terms are the same on both sides, the relationship

$$(r\rho)^n C_n^{\lambda/2}(\cos\gamma) = r^{2n+1} \sum\sum\sum \frac{(-1)^n}{n!} \frac{x'^a y'^b z'^c}{a!b!c!} \frac{\partial^{a+b+c}}{\partial x^a \partial y^a \partial z^c} \frac{1}{(x^2+y^2+z^2)^{\lambda/2}}$$
$$= \rho^{2n+1} \sum\sum\sum \frac{(-1)^n}{n!} \frac{x^a y^b z^c}{a!b!c!} \frac{\partial^{a+b+c}}{\partial x'^a \partial y'^a \partial z'^c} \frac{1}{(x'^2+y'^2+z'^2)^{\lambda/2}}$$

is obtained, the summation being taken for all integral values of a, b, c which are such that $a + b + c = n$. ∎

THEOREM 3 (first addition theorem). *For the geometry shown in Figure 2 let the vectors $\mathbf{P} = (x, y, z)$, $\mathbf{Q} = (x', y', z')$, and $||\mathbf{P} - \mathbf{Q}|| = r'$ in the Cartesian coordinate system. Then*

$$\frac{1}{r'^{\lambda}} = \sum_{n=0}^{\infty}\sum_{a=0}^{n}\sum_{b=0}^{a} \frac{(-1)^n \binom{n}{a}\binom{a}{b}}{2^a n!} (z')^{n-a}(\eta')^b(\xi')^{a-b} \partial_z^{n-a}\partial_+^b\partial_-^{a-b}\left(\frac{1}{r^{\lambda}}\right), \tag{14}$$

where $\eta' = x' - iy'$, $\xi' = x' + iy'$, and $\partial_z^{n-a}\partial_+^b\partial_-^{a-b}\left(\frac{1}{r^\lambda}\right)$ is given by Corollary 1.

Proof. Let $\eta' = x' - iy'$, $\xi' = x' + iy'$. Then

$$(xx' + yy' + zz')^n = \left(\frac{\eta'\xi}{2} + \frac{\xi'\eta}{2} + zz'\right)^n$$
$$= \sum_{a=0}^{n}\sum_{b=0}^{a} \frac{\binom{n}{a}\binom{a}{b}}{2^a} (zz')^{n-a}(\eta'\xi)^b(\eta\xi')^{a-b}.$$

Using (12), one can replace (x, y, z) by $(\partial_x, \partial_y, \partial_z)$, and then dividing both sides by ρ^n and letting both sides operate on $\frac{1}{r^\lambda}$ it follows from Theorem 2 that

$$\frac{C_n^{\lambda/2}(\cos\gamma)}{r^{n+\lambda}} = \frac{(-1)^n}{n!} \sum_{a=0}^{n}\sum_{b=0}^{a} \frac{\binom{n}{a}\binom{a}{b}}{2^a \rho^n} (z')^{n-a}(\eta')^b(\xi')^{a-b} \partial_z^{n-a}\partial_+^b\partial_-^{a-b}\left(\frac{1}{r^{\lambda}}\right).$$

By substituting $\frac{C_n^{\lambda/2}(\cos\gamma)}{r^{n+\lambda}}$ by the above result in (13), the proof is completed. ∎

THEOREM 4 (second addition theorem).

$$\partial_z^{n'-a'}\partial_+^{b'}\partial_-^{a'-b'}\left(\frac{1}{r'^{\lambda}}\right) = \sum_{n=0}^{\infty}\sum_{a=0}^{n}\sum_{b=0}^{a} \frac{(-1)^n \binom{n}{a}\binom{a}{b}}{2^a n!} (z')^{n-a}(\eta')^b(\xi')^{a-b}$$
$$\times \partial_z^{n+n'-a-a'}\partial_+^{b+b'}\partial_-^{a+a'-b-b'}\left(\frac{1}{r^{\lambda}}\right). \tag{15}$$

Proof. By operating both sides of (14) by $\partial_z^{n'-a'}\partial_+^{b'}\partial_-^{a'-b'}$, the proof is completed. ∎

Now it is a simple matter to obtain the multipole expansions and obtain the translation operators required for performing a single level FMM on the function $r^{-\lambda}$.

4.3. Multipole expansions. In this section, the operators to assist in efficient clustering and cluster-cluster interaction computation will be derived, in a manner similar to that done by the classical multipole expansion for the restricted case of $\lambda = 1$.

Consider Figure 1. A total N number of charges of strength q_i, $i = 1, 2 \ldots N$ are placed in the source sphere. The radius of both source and observation spheres is a. The distance between the sphere centers is $r > a$. The total potential due to the potential function $r^{-\lambda}$ at each of the N observation points is given by

$$\phi_j = \sum_{i=0}^{N} \frac{q_i}{r_{ij}^{\lambda}}, \quad j = 1, 2 \ldots N.$$

Now pth-order expansions for this configuration are obtained.

1. *Multipole Expansion* (Q2M, M2P) *for* Q2M2P. The order p multipole expansion for the jth observation point is obtained from Theorem 3 and is given by

$$\phi_j = \sum_{n=0}^{p} \sum_{a=0}^{n} \sum_{b=0}^{a} M_n^{a,b} \frac{(-1)^n \binom{n}{a} \binom{a}{b}}{2^a n!} \partial_z^{n-a} \partial_+^b \partial_-^{a-b} \left(\frac{1}{r_j^{\lambda}} \right), \tag{16}$$

where $M_n^{a,b} = \sum_{i=0}^{N} q_i (z_i)^{n-a} (\eta_i)^b (\xi_i)^{a-b}$. The center of the source sphere (multipole center) is taken as the origin. The **Q2M** operator has N columns. It can be verified that for the jth observation point, number of columns of the **M2P** matrix = number of rows of the **Q2M** matrix = $\frac{(p+1)(p+2)(p+3)}{6}$.

2. *Local Expansion* (Q2L, L2P) *for* Q2L2P. The order p local expansion for the jth observation point is obtained similarly:

$$\phi_j = \sum_{n=0}^{p} \sum_{a=0}^{n} \sum_{b=0}^{a} L_n^{a,b} (z_j)^{n-a} (\eta_j)^b (\xi_j)^{a-b}, \tag{17}$$

where $L_n^{a,b} = \frac{(-1)^n \binom{n}{a} \binom{a}{b}}{2^a n!} \partial_z^{n-a} \partial_+^b \partial_-^{a-b} \left(\frac{1}{r_i^{\lambda}} \right)$. The center of the observation (local center) sphere is taken as the origin. The **Q2L** matrix has $\frac{(p+1)(p+2)(p+3)}{6}$ rows and N columns, while the **L2P** operator has $\frac{(p+1)(p+2)(p+3)}{6}$ columns for the jth charge.

3. *Translation operator* (M2L) *for* Q2M2L2P. An order p multipole expansion at the multipole center can be converted into a local expansion at the local center using the second addition theorem

$$\phi_j = \sum_{n'=0}^{p} \sum_{a'=0}^{n'} \sum_{b'=0}^{a'} N_{n'}^{a',b'} (z_j)^{n'-a'} (\eta_j)^{b} (\xi_j)^{a'-b'}, \tag{18}$$

where

$$N_{n'}^{a',b'} = \frac{(-1)^{n'} \binom{n'}{a'} \binom{a'}{b'}}{2^{a'} n'!} \sum_{n=0}^{p} \sum_{a=0}^{n} \sum_{b=0}^{a} M_n^{a,b} \frac{(-1)^n \binom{n}{a} \binom{a}{b}}{2^a n!} \times \partial_z^{n+n'-a-a'} \partial_+^{b+b'} \partial_-^{a+a'-b-b'} \left(\frac{1}{r^{\lambda}} \right).$$

Thus the factorization $\Phi = \overline{\mathbf{L2P}}\ \overline{\mathbf{M2L}}\ \overline{\mathbf{Q2Mq}}$ is complete. To summarize, given an N point source sphere and an N point observation sphere, each of radius a and separated by a distance $r > 2a$ as depicted in Figure 1, first construct the $\overline{\mathbf{Q2M}}$ matrix of dimension $\frac{(p+1)(p+2)(p+3)}{6} \times N$, placing the origin at the center of the source sphere (multipole center). The matrix $\overline{\mathbf{Q2M}}$ is a function of only the source points. Then construct the $\overline{\mathbf{M2L}}$ matrix of dimension $\frac{(p+1)(p+2)(p+3)}{6} \times \frac{(p+1)(p+2)(p+3)}{6}$ as a function of the multipole center and the center of the observer sphere (local center). This operation transfers the multipole expansion into a local expansion. Next construct the **L2P** matrix of dimension $N \times \frac{(p+1)(p+2)(p+3)}{6}$ by placing the origin at the local center, which transfers the local expansion to the total potential at each observation point. Thus $\overline{\mathbf{L2P}}$ is a function only of the observation points. Finally compute $\overline{\mathbf{L2P}}\ \overline{\mathbf{M2L}}\ \overline{\mathbf{Q2M}}\mathbf{q}$. The total cost of this process is $\mathcal{O}(p^3N)$.

4.4. Error bounds.

LEMMA 2. $|C_n^\lambda(x)| \leq C_n^\lambda(1)$ *for* $|x| \leq 1$.

Proof. This is obvious from (7). The maximum value is attained by putting $\theta = 0$. ∎

THEOREM 5. *Let a charge of unit strength be placed at the* **Q** *(Figure* 2*), let the total potential at* **P** *be* ϕ_A*, and let* ϕ_A^p *be the multipole expansion of the pth order. Then the error is given by*

$$|\phi_A - \phi_A^p| \leq \frac{1}{r^\lambda}\left(\frac{\rho}{r}\right)^{p+1} (\lambda)_{p+1} \frac{1}{(1-\frac{\rho}{r})^{\lambda+p+1}}.$$

Proof.

$$\begin{aligned}
|\phi_A - \phi_A^p| &= \left|\frac{1}{r'^\lambda} - \sum_{n=0}^{p} \frac{\rho^n}{r^{n+\lambda}} C_n^{\lambda/2}(\cos\gamma)\right| \\
&= \left|\sum_{n=p+1}^{\infty} \frac{\rho^n}{r^{n+\lambda}} C_n^{\lambda/2}(\cos\gamma)\right| \\
&\leq \frac{1}{r^\lambda}\left(\frac{\rho}{r}\right)^{p+1} \sum_{n=0}^{\infty} \left(\frac{\rho}{r}\right)^n |C_{n+p+1}^{\lambda/2}(1)| \quad \text{(from Lemma 2)} \\
&= \frac{1}{r^\lambda}\left(\frac{\rho}{r}\right)^{p+1} \sum_{n=0}^{\infty} \left(\frac{\rho}{r}\right)^n \frac{(\lambda)_{n+p+1}}{(n+p+1)!} \quad \text{(from (11))} \\
&\leq \frac{1}{r^\lambda}\left(\frac{\rho}{r}\right)^{p+1} (\lambda)_{p+1} \sum_{n=0}^{\infty} \left(\frac{\rho}{r}\right)^n \frac{(\lambda+p+1)_n}{(n)!} \\
&= \frac{1}{r^\lambda}\left(\frac{\rho}{r}\right)^{p+1} (\lambda)_{p+1} \sum_{n=0}^{\infty} \left(\frac{\rho}{r}\right)^n C_n^{(\lambda+p+1)/2}(1) \\
&= \frac{1}{r^\lambda}\left(\frac{\rho}{r}\right)^{p+1} (\lambda)_{p+1} \frac{1}{\left(1-\frac{\rho}{r}\right)^{\lambda+p+1}}.
\end{aligned}$$

∎

Now it is straightforward to find the total error due to N charges.

COROLLARY 2. *Let there be* N *charges of strengths* $q_1, q_2 \ldots q_N$ *within a radius* a*. Then the total error due to multipole expansion of order* p *at a point* j *at a distance* $r > a$ *from the center of the sphere is given by*

$$|\phi_j - \phi_j^p| \leq A\frac{1}{r^\lambda}\left(\frac{a}{r}\right)^{p+1} (\lambda)_{p+1} \frac{1}{(1-\frac{a}{r})^{\lambda+p+1}},$$

where $A = \sum_{i=0}^{N} |q_i|$.

This gives the error bound for the computations.

5. Numerical results. In this section error behavior and computational requirements are discussed. The operators developed in this paper have been tested on an AMD Athlon 1500 platform. Following are the results of the simulation:

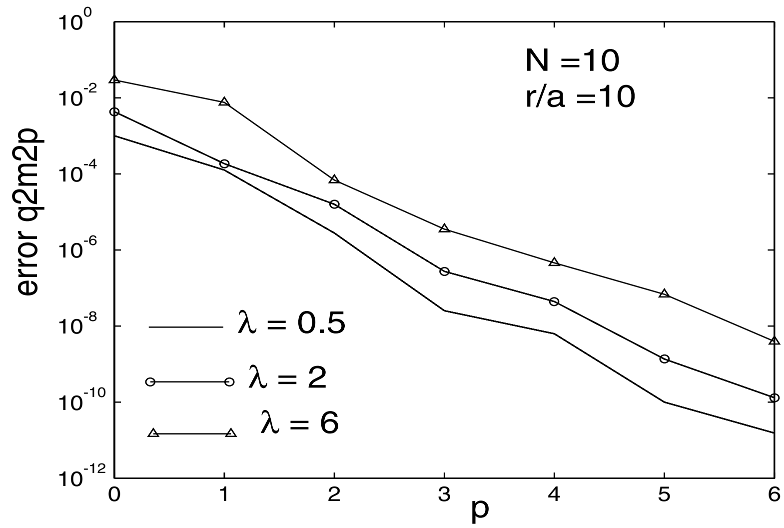

FIG. 3. *Error for* Q2M2P *operation versus* p *for positive* λ.

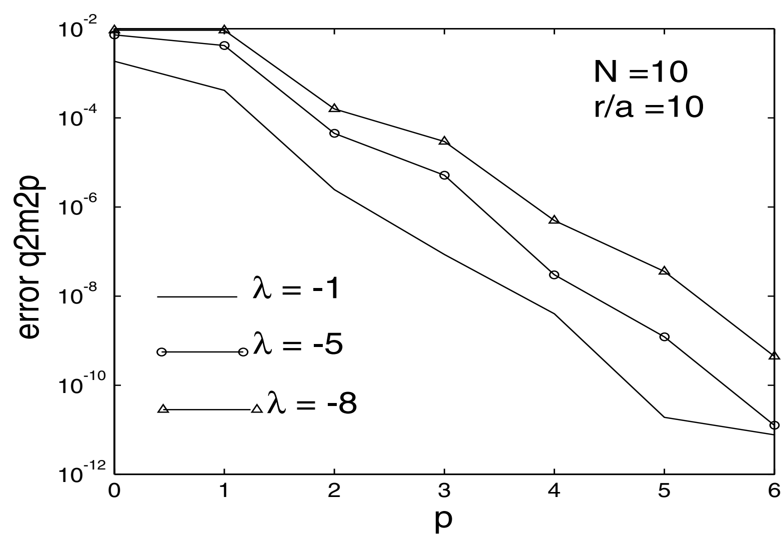

FIG. 4. *Error for* Q2M2P *operation versus* p *for negative* λ.

1. *Error behavior.* Figures 3–6 plot the relative errors versus the number of multipoles (p) used to compute the potential. The relative error is given by $||C_1 - C_2||/||C_1||$, where C_1 is the potential computed by the direct method and C_2 is the potential computed by the multipole method developed in this work. The error shows an exponential falloff with the increase in the number of multipoles while there is a slight worsening of the error with increase in λ. The significant point to note here is that the scheme works for all real λ, although the Gegenbauer polynomial is defined only for $\lambda > -1/2$. (This condition ensures a real and integrable weight function for the orthogonal polynomial; see [2]). The explanation for this is as follows: Although

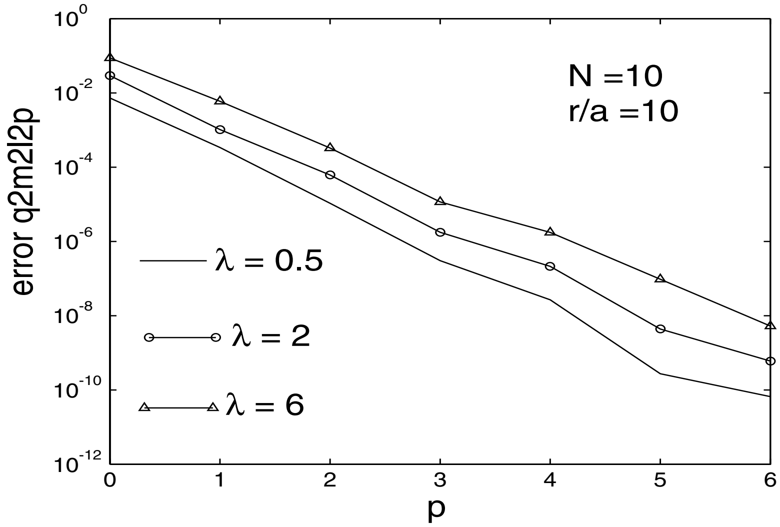

FIG. 5. *Error for* Q2M2L2P *operation versus* p *for positive* λ.

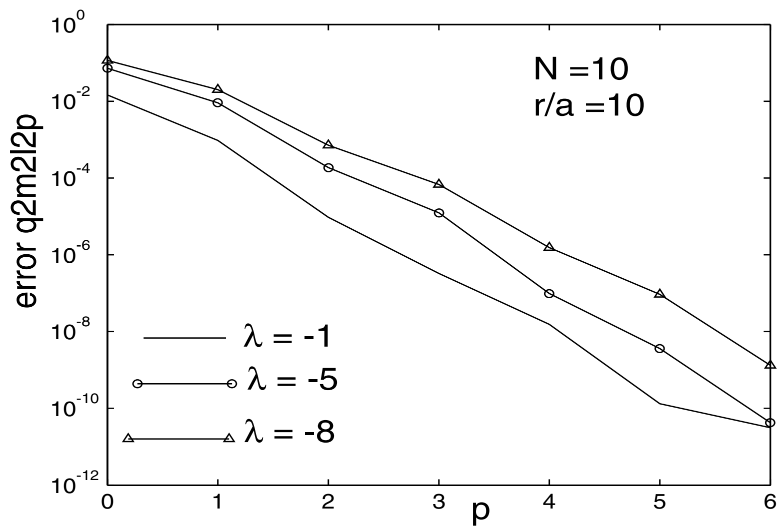

FIG. 6. *Error for* Q2M2L2P *operation versus* p *for negative* λ.

Gegenbauer polynomials are not defined for $\lambda < -1/2$, the identity (6) holds true for all λ because it is simply a Taylor series expansion as long as the polynomial is defined by identity (8). Theorem 1 is a consequence of identity (8), and hence it also holds true for all λ. All the subsequent addition theorems (i.e., Theorems 2–4) follow from Taylor's series expansions and Theorem 1. Thus they all *numerically* hold true for all λ. These polynomials cannot be called Gegenbauer polynomials when $\lambda < -1/2$, but one can still use them for the numerical method given in this paper as the theorems discussed here hold true for all $\lambda \in R$. Hence, although the Gegenbauer polynomials are *not* defined for $\lambda < -1/2$, the scheme still appears to work numerically. Figure 7

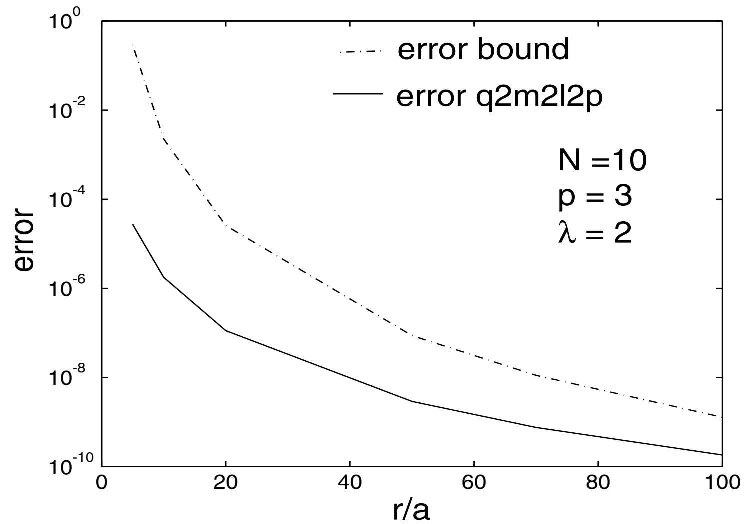

FIG. 7. *Error versus r/a and comparison with the error bound as in Corollary* 2.

TABLE 1
Memory requirements and average CPU times for computations. $\lambda = 2$, $r/a = 10$, *and* $p = 3$.

N	T_1	t_1	M_1	T_2	t_2	M_2	Rel. error
100	1.24e-02	2.13e-03	10000	1.04e-02	8.66e-04	8800	4.98e-06
300	1.12e-01	2.23e-02	90000	2.72e-02	2.73e-03	24800	5.47e-06
500	3.15e-01	6.21e-02	250000	4.39e-02	5.06-03	40800	4.82e-06
700	6.15e-01	1.23e-01	490000	6.00e-02	8.00e-03	56800	4.56e-06
1000	1.25e+00	2.54e-01	1000000	8.50e-02	1.10e-02	80800	4.84e-06
2000	5.15e+00	9.95e-01	4000000	1.68e-01	2.00e-02	160800	4.67e-06
3000	1.17e+01	2.29e+00	9000000	2.50e-01	3.00e-02	240800	4.82e-06

depicts the error falloff with increasing distance r/a. A comparison with the error bound (Corollary 2) is also shown. It can be seen that the error bound derived here is rather loose.

2. *Computational time and memory requirements.* Table 1 compares the memory requirements and average CPU times for the direct method (Q2P) and the multipole method (Q2M2L2P). N is the total number of source and observation points, T_1 is the average CPU time for setup for Q2P, t_1 is the average matrix vector product CPU time for Q2P, T_2 is the average CPU time for setup for Q2M2L2P, t_2 is the average matrix vector product CPU time for Q2M2L2P, M_1 is the total number of double precision numbers stored during Q2P, and M_2 is the total number of double precision numbers stored during Q2M2L2P $(4N(p+1)(p+2)(p+3)/6 + 2\,((p+1)(p+2)(p+3)/6)^2)$. Note that each element of the matrices **Q2M, M2L,** and **L2P** requires two double precision numbers, one for the real part and the other for the imaginary part, while each element of matrix **Q2P** is a real number and hence requires a single double precision number.

3. *Comparison with the standard FMM for* $\lambda = 1$. Figure 8 shows that the accuracy and error behavior for the case $\lambda = 1$ in this formulation is comparable to the standard method [1]. However, the memory and time requirements in the standard method is of order $\mathcal{O}(p^2N)$, while this formulation is of $\mathcal{O}(p^3N)$.

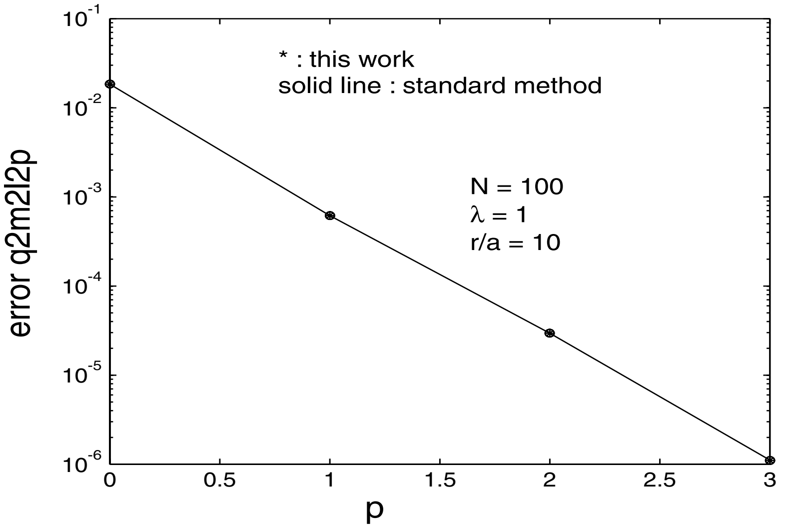

FIG. 8. *Comparison with the standard method for the case* $\lambda = 1$.

6. Conclusion. The formulation for performing single level FMM of arbitrary λ has been developed. This work can be viewed as a generalization of the well-known particular case of $\lambda = 1$. This work can be extended to multilevel FMM following the same method as the factorization of **M2P** into **L2P, M2L**. This will find applications to static problems which have potential function $r^{-\lambda}$, particularly in fast evaluation of van der Waals's forces and Lennard Jones's potentials in computational chemistry.

REFERENCES

[1] L. GREENGARD, *The Rapid Evaluation of Potential Fields in Particle Systems*, MIT Press, Cambridge, MA, 1988.

[2] H. BATEMAN, *Higher Transcendental Functions, Vol.* 2, McGraw–Hill, New York, 1953.

[3] E. W. HOBSON, *Theory of Spherical and Ellipsoidal Harmonics*, Cambridge University Press, Cambridge, UK, 1931.

[4] L. DURAND, P. M. FISHBANE, AND L. M. SIMMONS, *Expansion formulas and addition theorems for Gegenbauer polynomials*, J. Math. Phys., 17 (1976), pp. 1933–2121.

[5] W. APPEL, *An efficient program for many-body simulation*, SIAM J. Sci. Statist. Comput., 6 (1985), pp. 85–103.

[6] V. ROKHLIN, W. D. MURPHY, N. ENGHETA, AND M. S. VASSILIOU, *The FMM for electromagnetic scattering problems*, IEEE Trans. Antennas and Propagation, 40 (1992), pp. 634–641.

[7] J. BARNES AND P. HUT, *A hierarchical* $\mathcal{O}(N \log N)$ *force calculation algorithm*, Nature, 324 (1986), pp. 446–449.

[8] C. R. ANDERSON, *An implementation of the fast multipole method without multipoles*, SIAM J. Sci. Statist. Comput., 13 (1992), pp. 923–947.

[9] Z. GIMBUTAS AND V. ROKHLIN, *A generalized fast multipole method for nonoscillatory kernels*, SIAM J. Sci. Comput., 24 (2002), pp. 796–817.

[10] G. H. KO AND W. H. FINK, *Rapidly converging lattice sums for nanoelectronic interactions*, J. Comput. Chem., 23 (2001), pp. 477–483.

[11] Y. KOMEIJI, M. UEBAYASI, R. TAKATA, A. SHIMIZU, K. ITSUKAHI, AND M. TAIJI, *Fast and accurate molecular dynamics simulation of a protein using a special-purpose computer*, J. Comput. Chem., 18 (1997), pp. 1546–1563.

[12] X. B. NEI, S. Y. CHEN, W. N. E AND M. O. ROBBINS, *A continuum and molecular dynamics hybrid method for micro- and nano-fluid flow*, J. Fluid. Mech., 500 (2004), pp. 55–64.