SPLITTING OF THE COULOMB KERNEL IN THE MULTILEVEL FAST SUMMATION METHOD

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A family of Coulomb kernels smoothed with even order polynomials is studied in the framework of the multilevel approach to the calculation of the interaction energy between particles. It is shown that the Ewald decomposition of the Coulomb potential is close to the polynomial softening with the order $8 \div 12$. It follows from the multilevel estimation of the Madelung constant, that, for a small cut-off radius, the better accuracy can be attained by using polynomials of smaller order. Therefore, these polynomials are computationally inexpensive to evaluate in the fast summation methods.

Introduction

A general problem in the evaluation of the energy of a many-body system with the Coulomb interaction between particles is the calculation of a conditionally convergent sum. Conditional convergence means that the final result depends on the particular order of adding up the terms. From the physical point of view, this implies a special spatial arrangement of the charges in the system. In particular, such a situation is realized in ionic crystals [1]. The local electroneutrality condition implies a certain charge average ordering in liquid electrolytes [2, 3].

Nevertheless, even if the electrostatic energy of a charge system is defined, a straightforward naive summation of particle contributions is very slow and impracticable. The earliest effective methods, allowing to avoid this problem, had been worked up by Madelung [4] and Ewald [5] for the evaluation of the electrostatic energy of ionic crystals. The Ewald approach, it seems, is the most widely used in recent years. It is very close to the Kummer acceleration of the convergence of series [6] and consists of two successive stages. The Coulomb interaction potential is split into short-range singular and long-range smooth parts. Contributions to the electrostatic energy of the short-range interaction are directly calculated in the real space. The remaining sum of smooth potentials is evaluated in the reciprocal space using the Fourier transformation. The smoother the potential, the faster the convergence. A number of modifications to the standard Ewald method have been devised to ensure the efficient calculation of just this smooth contribution to the electrostatic energy (see, e.g. [7—9]).

A general multilevel approach to the calculation of integral transforms and particle interactions with a smooth kernel was developed in [10]. It was successfully applied to the evaluation of a smooth part of the electrostatic energy [11, 12]. At the same time, the accuracy and efficiency of such calculations depend on the splitting method of the Coulomb potential. Our goal is to study the family of smoothed kernels in the framework of the multilevel approach.

1. Splitting of the Coulomb Potential

In order to reduce the Coulomb potential $1/r$ of a point charge, it is necessary to surround it by a screening charge distribution of opposite sign. In case the charge distribution is spherical, the definition of the electric field E follows from the Gauss law [13]:

$$x^2 E = 1 - \int_0^x \rho(\tau)\tau^2 d\tau, \tag{1}$$

where $\rho(\tau)$ is the screening charge distribution and the integral depicts the charge inside the sphere of a radius x. Requirement of the electroneutrality leads to the following restriction on the charge distribution:

$$\int_0^\infty \rho(\tau)\tau^2 d\tau = 1. \tag{2}$$

In accordance with (1), the screened potential $\phi(r)$ at distance r from the point charge is defined by:

$$\phi(r) = \frac{1 - rG(r)}{r}, \tag{3}$$

where

$$G(r) = \int_r^\infty \frac{dx}{x^2} \int_0^x \rho(\tau)\tau^2 d\tau. \tag{4}$$

Screening of the Coulomb potential is described in (3) by the function

$$S(r) = 1 - rG(r) \tag{5}$$

which can be treated as the switch function.

One can see from (2) and (4) that potential (3) can approach zero faster than that in the case of a bare point charge. The proper choice of the charge distribution allows one to neglect its value (or make it exact zero) beyond some cut-off radius R_{cut}.

Thus, the Coulomb potential of a point charge can be split into two parts:

$$\frac{1}{r} = \phi(r) + G(r). \tag{6}$$

Its first singular term rapidly decays and the second one is the slow decaying non-singular long-range part.

For example, in the framework of the Ewald approach, the charge distribution is chosen in the form of spherical Gaussian:

$$\rho(x) = 4\frac{\alpha^3}{\pi^{1/2}} e^{-\alpha^2 x^2}, \tag{7}$$

where α is the free parameter which defines the shape of charge distribution curve. Evaluating (4) with substitution of (7) yields:

$$G(r) = \frac{\text{erf}(\alpha r)}{r}, \tag{8}$$

where $\text{erf}(x)$ is the error function.

The trivial, in the case of a lonely point charge, decomposition (6) is very useful if one intends to find the electrostatic potential $u(\vec{r}_i)$ produced by the system of N charges:

$$u(\vec{r}_i) = \sum_{j\neq i, \quad |\vec{r}_i - \vec{r}_j| < R_{\text{cut}}} q_j \phi(|\vec{r}_i - \vec{r}_j|) + \\ + \sum_{j\neq i}^{N} q_j G(|\vec{r}_i - \vec{r}_j|), \tag{9}$$

here q_j is a point charge and $\vec{r}_j$ is a radius-vector of this point. The first sum in (9) can be calculated directly and this operation is not computationally expensive. The last sum concerns *all charges* and represents the potential of their compensative charge distributions. On the other hand, (6) can be treated as the result of the splitting of the potential instead of the charge density. Therefore, one can consider the long-range contribution in (9) as a transformation with smooth kernel. The problem is how to evaluate this sum taking into account the smoothness property of the kernel.

2. Outline of the Multilevel Summation Method

In order to evaluate the smooth part of potential (9), we start with the arrangement of charges along a line, in which case that part is given by:

$$u_{\text{smooth}}(x_i) = \sum_{j\neq i} G(|x_i - x_j|) q_j, \tag{10}$$

where charges $q_j = \pm 1$ are, in general, arbitrarily located.

In the framework of the multilevel approach [10], the space is covered by a uniform grid which is defined by a set of gridpoints X_i, the meshsize being H. Assuming the kernel $G(|x_i - x_j|)$ is a smooth function of its arguments, it is possible to use the polynomial interpolation from that grid with $\mathcal{O}(\epsilon)$ error:

$$G(|x_i - x_j|) = \sum_{k=0}^{p} L_k^p(x_j) G(|x_i - X_k|) + \mathcal{O}(\epsilon). \tag{11}$$

Here the interpolating Lagrange polynomials of order p are defined by

$$L_k^p(x) = \prod_{i=0,\ i\neq k}^{p} \frac{x - X_i}{X_k - X_i}. \tag{12}$$

Substitution of (12) in (10) yields:

$$u_{\text{smooth}}(x_i) = \sum_{k=0}^{p} G(|x_i - X_k|) Q_k + \mathcal{O}(\epsilon), \tag{13}$$

where $\{Q_k\}$ is the set of charges at gridpoints:

$$Q_k = \sum_{j\neq i} L_k^p(x_j) q_j. \tag{14}$$

In contrast to the interpolation from the grid, operation (14) is the coarsening of the charges to the grid and is called adjoint interpolation, or anterpolation [10].

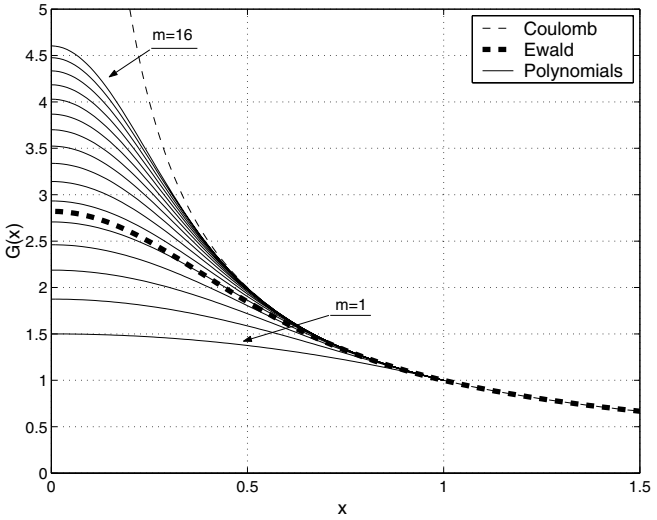

Fig. 1. Long-range smooth part of the Coulomb kernel for different polynomial orders. Comparison is made to the Ewald splitting (8) with $\alpha = 2.5$

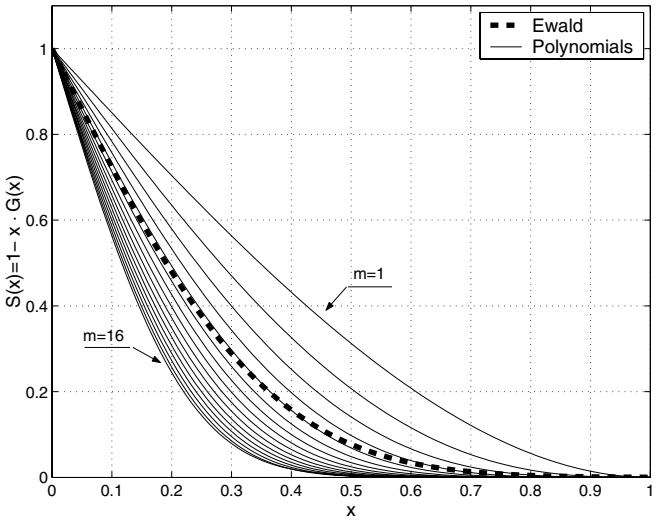

Fig. 2. Switch functions. For the Ewald splitting, $S(x) = \mathrm{erf}c(\alpha x)$

Next, the value of the kernel in (13) at the point x_i can be interpolated from the grid

$$G(\mid x_i - X_k \mid) = \sum_{l=0}^{p} L_l^p(x_i) G(\mid X_l - X_k \mid) + \mathcal{O}(\epsilon). \quad (15)$$

Applying (15) to the kernel in (13), one obtains that

$$u_{\mathrm{smooth}}(x_i) = \sum_{l=0}^{p} L_l^p(x_i) \Phi(X_l) + \mathcal{O}(\epsilon), \quad (16)$$

where the following potential is introduced:

$$\Phi(X_l) = \sum_k G(\mid X_l - X_k \mid) Q_k. \quad (17)$$

Definition of potential (17) is close to (10). It fixes the potential at a gridpoint produced by anterpolated charges at *all* gridpoints.

The entire algorithm for the calculation of the long-range smooth part of the potential consists of following steps:

(i) Anterpolation of *all* charges (for the simplicity of calculations with the term $i = j$) to the coarse-level grid using (14). The erroneous contribution of the self-interaction caused by the charge q_i should be removed at the last step.

(ii) Calculation of the potential at coarse-level gridpoints defined by the lattice sum (17).

(iii) Interpolation of the potential from the coarse-level grid to the particle position (16). In order to correct the obtained value of the potential, the single charge q_i is anterpolated to the coarse-level grid, then the potential at gridpoints is evaluated, and the result of the interpolation to the finer level is subtracted from the former result corresponding to the contribution of all charges.

If charges are arranged on the plane or in the three-dimensional space without restrictions, the anterpolation and the interpolation are performed by the one-dimensional operation at a time.

The important feature of the multilevel fast summation method is the possibility to calculate potential (17) at the step (ii) by recursion. A number of coarser grids with the increasing meshsize are introduced. At each level, the potential is split into the short-range part and the long-range part which is smooth on the scale of the meshsize. Short-range contributions are calculated directly at the given level, the long-range part of the potential is interpolated from the coarser level. The recursion is performed until such a coarse grid is reached that calculation of potential (17) with its use needs a small amount of the computational work or the coarsest level potential is so smooth that the difference between values at gridpoints can be neglected.

3. Softening of the Coulomb Potential

As follows from (2) and (4), the smooth part of the Coulomb potential can be defined in different ways. In general, in order to remove the singularity of the potential, it is enough to soften it in the vicinity of

the origin only. This means that a screening charge distribution should be located inside a sphere of some radius $R_{\rm cut}$. In this case, the smooth long-range part of potential (4) is written as follows:

$$G(r) = \begin{cases} G_L(r), & r \le R_{\rm cut}, \\ 1/r, & r > R_{\rm cut}. \end{cases} \qquad (18)$$

If the softened potential is chosen in such a form, the screened potential (3) is exact zero outside the sphere of the radius $R_{\rm cut}$ and is really the short-range potential.

It is convenient to consider an arbitrary function $G_L(r)$ as the polynomial of order $2m$:

$$G_L^m(x) = \sum_{i=0}^{m} a_i^m x^{2i}, \qquad (19)$$

where $x = r/R_{\rm cut}$ is the dimensionless variable.

Coefficients a_i are determined so that kernel (18) and its m derivatives are continuous functions at the point $r = R_{\rm cut}$ ($x = 1$). Coefficients for the first polynomials of family (19) derived under these conditions are presented in the Table.

The Coulomb potential softened in accordance with (18) for different orders of polynomials (19) is shown in Fig.1. Smooth part of the Ewald splitting (8) as the function of the dimensionless variable is plotted for $\alpha = 2.5$. One can see from Fig.1 that, in this case, the behavior of (8) is close to (18).

Switch functions in cases of the Ewald splitting and the polynomial softening (19) are shown in Fig.2. Charge distributions corresponding to the screened potentials (3) can be restored in accordance with (1) and (4). The result is presented in Fig.3.

One can see from these pictures that the Ewald decomposition of the Coulomb potential is close to the polynomial softening with the polynomial order $2m = 8 \div 12$. At the same time, the larger m the smaller the contribution to the short-range part of the energy from charges placed near $R_{\rm cut}$ (see Fig.2). This means that the softening with polynomials of low orders can be more effective for the calculation of the short-range interaction energy. Therefore, the polynomial order in (19) serves as the additional degree of freedom comparatively with the Ewald splitting procedure, and the optimal softening of the Coulomb potential should be studied on the numerical examples of charge systems.

4. Multilevel Estimation of the Madelung Constant

An ionic crystal is the simple example of a many-body system with the Coulomb interaction. The potential

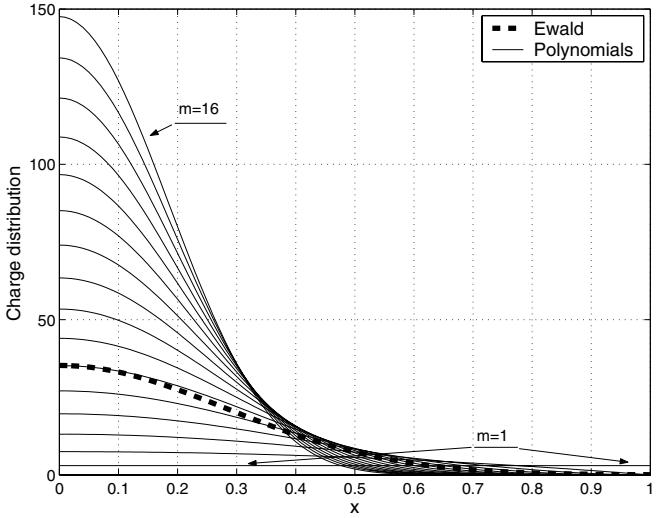

Fig. 3. Screening charge distributions

electrostatic energy per ion created in an infinite lattice by point charges $q_i = \pm e$ may be defined by [1]:

$$u_{\rm ion} = -\frac{e^2}{h} Z_{\rm M}, \qquad (20)$$

where h is the minimum distance between unlike charges and $Z_{\rm M}$ is the Madelung constant.

If the meshsize of the coarser-level grid equals the length of the unit cell in the same direction, anterpolation (14) of *all* lattice point charges results in the electroneutral coarse-level gridpoints [12]. This inference doesn't depend on the anterpolation order and the position of the coarse-level grid. Therefore, it is convenient to shift the coarse-level grid in order to simplify calculations. The reasonable disposition of the coarse-level grid is as follows: a gridpoint is placed above the ion i, for which the energy is to be calculated. Defini-

Coefficients of polynomials (19)

m	1	2	3	4	5	6
a_0	$\frac{3}{2}$	$\frac{15}{8}$	$\frac{35}{16}$	$\frac{315}{128}$	$\frac{693}{256}$	$\frac{3003}{1024}$
a_1	$-\frac{1}{2}$	$-\frac{5}{4}$	$-\frac{35}{16}$	$-\frac{105}{32}$	$-\frac{1155}{256}$	$-\frac{3003}{512}$
a_2		$\frac{3}{8}$	$\frac{21}{16}$	$\frac{189}{64}$	$\frac{693}{128}$	$\frac{9009}{1024}$
a_3			$-\frac{5}{16}$	$-\frac{45}{32}$	$-\frac{495}{128}$	$-\frac{2145}{256}$
a_4				$\frac{35}{128}$	$\frac{385}{256}$	$\frac{5005}{1024}$
a_5					$-\frac{63}{256}$	$-\frac{819}{512}$
a_6						$\frac{231}{1024}$

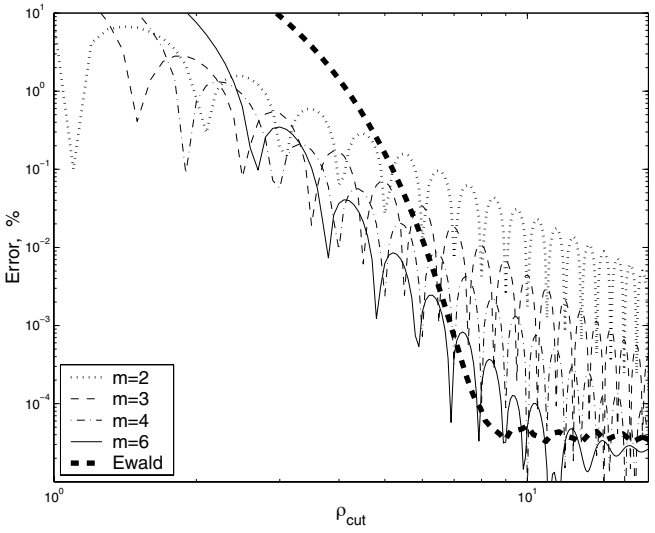

Fig. 4. Percentage error for the Madelung constant $Z_M(\rho_{\rm cut})$ versus $\rho_{\rm cut} = R_{\rm cut}/h$ for the polynomial softening of the long-range part of the Coulomb potential (19) and the Ewald splitting (8)

tion of the Madelung constant, estimated in the framework of the multilevel summation method, results from (9), (17), and (20) [12]:

$$Z_{\rm M}(\rho_{\rm cut}) = \sum_{i\neq j,\ \rho_{ij}\leq\rho_{\rm cut}} \left(\frac{s_j}{\rho_{ij}} - G(\rho_{ij})\right) + G(0), \qquad (21)$$

where $\rho = r/h$ is the dimensionless distance.

A one-dimensional ionic lattice consists of alternating positive and negative point charges with the distance h ($\rho = 1$) between unlike charges and the distance $2h$ ($\rho = 2$, the meshsize of the coarser-level grid is set to this value) between like charges. In this case, the Madelung constant is defined by (20):

$$Z_{\rm M} = -2\sum_{i=1}^{\infty} \frac{(-1)^i}{i}. \qquad (22)$$

The sum in (22) can be calculated analytically, the exact value of the Madelung constant is $Z_{\rm M} = 2\ln 2$. Therefore it is reasonable to test the softening of the Coulomb potential with the use of (21) for the one-dimensional ionic lattice. Calculation errors are presented in Fig.4. One can see that for sufficiently large values of $\rho_{\rm cut}$ the polynomial softening (19) with $m = 4 \div 6$ and Ewald splitting of the long-range part of the Coulomb potential (8) give the estimation of the Madelung constant with compatible high accuracy. At the same time, the reasonable accuracy can be attained at smaller $\rho_{\rm cut}$ (and less computational work in the calculation of the short-range contribution in (21)) by using polynomials of smaller order in (19).

Conclusion

Fast summation methods yield the energy for systems with long-range (Coulomb or gravitational) interaction between particles in computational work that scales linearly with a number of particles. At the same time, the cost of the calculation per particle depends on the splitting of the interaction kernel (6). Though the common Ewald approach defines the very smooth long-range part of potential (8), it is computationally expensive, moreover, the short-range part (3) is not finite-range (the error of the short-range energy calculation depends on the value of the parameter α).

The polynomial softening (19) yields the truly short-range part of the potential and reproduces the Ewald splitting when the polynomial order is relatively small. This means that function (8) possesses "superfluous" smoothness properties. Estimation of the Madelung constant in the framework of the multilevel fast summation method shows that the splitting of the Coulomb potential considered in this work is computationally efficient. Such a method with the polynomial softening of the interaction potential can be easily incorporated into the Monte Carlo method (ordinary [14] or multilevel [15] approach) where the energy calculation should be as fast as possible at reasonable accuracy.

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РОЗКЛАДАННЯ ЯДРА КУЛОНІВСЬКОЇ ВЗАЄМОДІЇ У БАГАТОРІВНЕВОМУ МЕТОДІ ШВИДКОГО ПІДСУМОВУВАННЯ

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Р е з ю м е

У межах багаторівневого підходу до розрахунку енергії взаємодії між частинками вивчено сімейство ядер кулонівської взаємодії, згладжених із використанням многочленів парних степенів. Показано, що розкладання Евальда кулонівського потенціалу дає результати, схожі з поліноміальним згладжуванням степеня 8—12. З оцінки сталої Маделунга за допомогою багаторівневого методу випливає, що для малих радіусів обрізання підвищення точності можна досягти, використовуючи многочлени нижчих степенів. Таким чином, ці многочлени є ефективними з обчислювальної точки зору при застосуванні у методах швидкого підсумовування.

РАЗЛОЖЕНИЕ ЯДРА КУЛОНОВСКОГО ВЗАИМОДЕЙСТВИЯ В МНОГОУРОВНЕВОМ МЕТОДЕ БЫСТРОГО СУММИРОВАНИЯ

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Р е з ю м е

В рамках многоуровневого подхода к расчету энергии взаимодействия между частицами изучено семейство ядер кулоновского взаимодействия, сглаженных с использованием многочленов четных степеней. Показано, что разложение Эвальда кулоновского потенциала дает сходные результаты с полиномиальным сглаживанием степени 8—12. Из оценки постоянной Маделунга при помощи многоуровневого метода следует, что для малых радиусов обрезания повышения точности можно достичь, используя многочлены более низких степеней. Таким образом, эти многочлены эффективны с вычислительной точки зрения применительно к методам быстрого суммирования.