Results for the ground state energy of a finite system of dipoles in a one-dimensional crystal lattice

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We investigate the ground state energy of a finite classical system consisting of an arbitrary number of electric dipoles localized at the sites of a regular one-dimensional crystal lattice. The ground state energy per dipole can be exactly calculated in the thermodynamic limit but an exact analytical expression for the energy valid for an arbitrary finite number of dipoles is not possible. In this work we obtain an approximate analytical expression for the ground state energy that applies to any given finite number of dipoles. The approximate analytical expression that we report reproduces the exact numerically calculated values of the ground state energy with an astonishing accuracy.

Keywords: One-dimensional crystal lattice; Dipole-dipole interaction; Ground-state energy; Theory and modeling.

Understanding the interaction between electric dipoles or their magnetic counterparts is crucial to many scientific disciplines. Any electric or magnetic dipole posseses a given dipole moment, a vector quantity. Since the interaction potential energy between a pair of electric dipoles has the same mathematical form as that of magnetic dipoles (apart from irrelevant constants), from now on we specifically consider a system of electric dipoles. The electric dipole moment for a pair of opposite point charges, $\pm q$ is written as $\vec{p} = q\,\vec{l}$ where $q > 0$ is the magnitude of the charge and $\vec{l}$ is the separation vector between them. By convention, the direction of such a vector is taken from the negative towards the positive charge. In the point dipole limit, the electric dipole has a constant magnitude. The dipole-dipole interaction is the most important interaction among neutral particles. It gives rise to van der Waals forces [1–7] and is also crucial to understand living organisms. For example, every process of protein formation that involves protein folding is dependent on dipole-dipole interactions [8–12].

The potential energy possessed by two electric dipoles interacting with each other depends on the dipole moment of each particle, their separation distance and the orientation in space of the dipole moments. Therefore, unlike the Coulomb interaction between two point charges [13–16], the dipole-dipole interaction between two point dipoles is highly anisotropic. The anisotropy of the dipole-dipole interaction leads to nontrivial effects. For example, it is not at all easy to determine the ground state energy at zero temperature for a given system of dipoles placed on a two-dimensional (2D) or a three-dimensional (3D) lattice of a given type [17–27]. Under most general conditions, this can be done only via numerical methods. The exception is a system of dipoles placed in a regular one-dimensional (1D) crystal lattice where the ground state energy per dipole can be analytically calculated in the thermodynamic limit (when the number of dipoles goes to infinity). However, an exact analytical expression that applies to the ground state energy of an arbitrary finite number of dipoles is not possible. The purpose of this work is to report an approximate analytical expression for the ground state energy of an abitrary system with $N \geq 2$ dipoles on a regular 1D crystal lattice which reproduces with very high accuracy the exact ground state energy values obtained numerically.

The model under consideration is that of $N \geq 2$ electric dipoles localized on N sites of a regular 1D crystal lattice with lattice parameter, a. The potential energy of interaction between two dipoles i and j located at lattice sites $\vec{r}_i$ and $\vec{r}_j$ is written as:

$$U_{ij} = k\left[\frac{\vec{p}_i \cdot \vec{p}_j}{r_{ij}^3} - 3\,\frac{(\vec{p}_i \cdot \vec{r}_{ij})\,(\vec{p}_j \cdot \vec{r}_{ij})}{r_{ij}^5}\right] , \qquad (1)$$

where k is Coulomb's constant, $\vec{r}_{ij} = \vec{r}_j - \vec{r}_i$ is the interparticle separation vector and $r_{ij} = |\vec{r}_{ij}| = |\vec{r}_j - \vec{r}_i| \geq 0$ is the separation distance between the dipole moments $\vec{p}_i$ and $\vec{p}_j$ of equal magnitude p. The ground state energy of the pair of dipoles at zero temperature is obtained when $\vec{p}_i$ is parallel to $\vec{p}_j$ and both are parallel to the separation vector $\vec{r}_{ij}$.

This allows us to state that the ground state energy for a system with $N \geq 2$ dipoles is achieved when:

$$\vec{p}_i \parallel \vec{p}_j \parallel \vec{r}_{ij} \quad ; \quad i < j \ . \qquad (2)$$

The ground state energy configuration for such a case represents a linear chain of dipoles as shown schematically in Fig. 1 for a system of $N = 5$ dipoles. The total ground state energy of a finite system with an arbitrary number of dipoles localized in a regular 1D crystal lattice can be written as:

$$U(N) = -2\,E_0 \sum_{i<j}^{N} \frac{1}{(j-i)^3} \ , \qquad (3)$$

where

$$E_0 = \frac{k\,p^2}{a^3} \ , \qquad (4)$$

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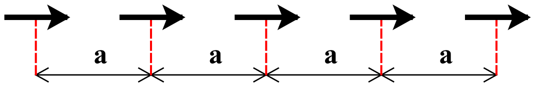

FIG. 1: Schematic view of the ground state energy configuration for a system of $N = 5$ electric dipoles located at the sites of a regular 1D crystal lattice. Dipoles are represented by short arrows and a is the lattice parameter (distance between two neighbouring sites).

is a suitable unit of energy. One can write the result is Eq.(3) as:

$$U(N) = -2\, E_0\, S_N \ , \tag{5}$$

where

$$S_N = \sum_{i<j}^{N} \frac{1}{(j-i)^3} = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \frac{1}{(j-i)^3} \ . \tag{6}$$

Calculation of $U(N)$ for an arbitrary number of $N \geq 2$ dipoles hinges upon the calculation of S_N which, for finite N, can be done only numerically.

In this work, we show that S_N can be approximated by an analytical function denoted as $f(N)$ that is so accurate in reproducing the numerical values of S_N that can be considered as exact for all practical purposes. Furthermore, it is noted that the accuracy of such an analytical description improves as the value of N increases. This is precisely the most desirable property when one must study interacting systems with a growing size.

The method that we use to obtain such an approximate analytical formula starts from the observation that one can write the finite series S_N in Eq.(6) as:

$$S_N = (N-1)\,\frac{1}{1^3} + (N-2)\,\frac{1}{2^3} + \ldots + \left[N-(N-1)\right]\frac{1}{(N-1)^3} \ . \tag{7}$$

By regrouping the terms in the series above one has:

$$\begin{aligned} S_N \ = \ & N \left[\frac{1}{1^3} + \frac{1}{2^3} + \ldots + \frac{1}{(N-1)^3}\right] \\ & - \left[\frac{1}{1^2} + \frac{1}{2^2} + \ldots + \frac{1}{(N-1)^2}\right] \ . \end{aligned} \tag{8}$$

At this juncture, one adds and substracts additional terms to the quantity in Eq.(8) to rewrite it as:

$$\begin{aligned} S_N \ = \ & N \left[\frac{1}{1^3} + \frac{1}{2^3} + \ldots + \frac{1}{(N-1)^3} + \frac{1}{N^3} + \ldots + \frac{1}{\infty^3} - \left(\frac{1}{N^3} + \ldots + \frac{1}{\infty^3}\right)\right] \\ & - \left[\frac{1}{1^2} + \frac{1}{2^2} + \ldots + \frac{1}{(N-1)^2} + \frac{1}{N^2} + \ldots + \frac{1}{\infty^2} - \left(\frac{1}{N^2} + \ldots + \frac{1}{\infty^2}\right)\right] \ . \end{aligned} \tag{9}$$

At this point one recognizes that the quantity in Eq.(9) is equivalent to:

$$\begin{aligned} S_N \ = \ & N\,\xi(3) - \xi(2) + \left[\frac{1}{N^2} + \ldots + \frac{1}{\infty^2}\right] \\ & -N \left[\frac{1}{N^3} + \ldots + \frac{1}{\infty^3}\right] \ , \end{aligned} \tag{10}$$

where

$$\xi(s) = \sum_{n=1}^{\infty} \frac{1}{n^s} \quad ; \quad s > 1 \ , \tag{11}$$

is the so-called Riemann zeta function. The next step is straightforward, approximate S_N with an analytic function $f(N)$ written as:

$$f(N) = N\,\xi(3) - \xi(2) + \int_N^{\infty} \frac{dx}{x^2} - N \int_N^{\infty} \frac{dx}{x^3} \ . \tag{12}$$

Simple calculations lead to the following final result:

$$f(N) = N\,\xi(3) - \xi(2) + \frac{1}{2\,N} \ . \tag{13}$$

As we will show, the analytic function $f(N)$ in Eq.(13) reproduces very accurately the exact values of S_N (calcu-

TABLE I: Numerically exact values of S_N and analytically obtained ones using the expression for $f(N)$ are compared for a given number of $N = 2, 3, \ldots, 20$ dipoles. The data have a numerical accuracy of five digits after the decimal point meaning that the fifth digit after the decimal point is rounded.

N	S_N	$f(N)$
2	1.00000	1.00918
3	2.12500	2.12790
4	3.28704	3.28829
5	4.46470	4.46535
6	5.65036	5.65074
7	6.84065	6.84089
8	8.03386	8.03402
9	9.22902	9.22913
10	10.42555	10.42563
11	11.62308	11.62315
12	12.82137	12.82142
13	14.02023	14.02023
14	15.21955	15.21958
15	16.41923	16.41925
16	17.61921	17.61923
17	18.81943	18.81945
18	20.01985	20.01987
19	21.22045	21.22046
20	22.42119	22.42120

lated numerically) for any arbitrary number $N = 2, 3, \ldots$ of dipoles.

Looking back at Eq.(10), one might be tempted to believe that a natural first step is to cancel out the first terms of the last two sums, i.e. $(1/N^2 - N/N^3)$ and then make the approximation of replacing the sums with integrals. We tried that, but we noticed that we would get a worse approximation than the one obtained in Eq.(12). Note that the expression for S_N in Eq.(10) contains the difference between two infinite sums. Replacing the sums with integrals as done in Eq.(12) will necessarily result in errors. It turns out that the errors introduced while approximating each of the two sums with an integral expression cancel out to a very large degree when the difference is calculated. This is the reason why the expression for $f(N)$ in Eq.(13) is such an accurate approximation to S_N in Eq.(10). One can pursue the matter in more depth and, perhaps, recalculate the finite sums in Eq.(6) differently. This may lead to an improved approximate expression for S_N that goes beyond the function $f(N)$ in Eq.(13). However, we expect that such an improvement of $f(N)$ would be quite small (of the order of $1/N^3$ as we estimate it later on).

Results for S_N and $f(N)$ for systems with $2 \le N \le 20$ dipoles are shown in Table. I. The difference $f(N) - S_N$ for a system of $2 \le N \le 10$ dipoles is shown in

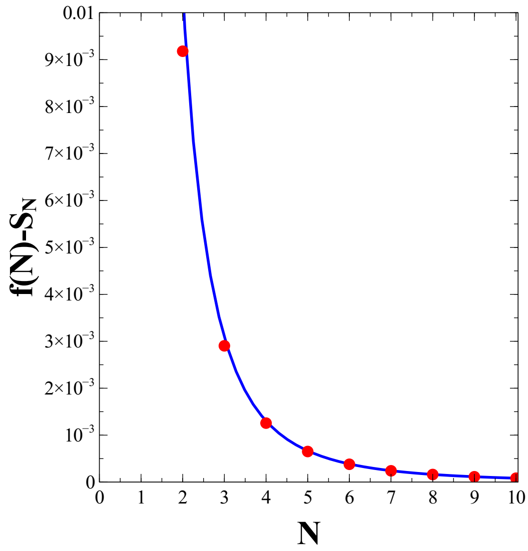

FIG. 2: Difference $f(N) - S_N$ between the analytical function, $f(N) = N\,\xi(3) - \xi(2) + \frac{1}{2\,N}$ and the numerically exact series, $S_N = \sum_{i<j}^{N} \frac{1}{(j-i)^3}$ calculated for values $2 \le N \le 10$ (filled circles). The deviation $f(N) - S_N$ is fitted quite well by the function $\frac{1}{12\,N^3}$ represented as a solid line.

Fig. 2 as filled circles. We used several simple functions to find a good fit for the data points in Fig. 2 (the filled circles). We found out that the deviation $f(N) - S_N$ can be approximated quite well by the function $\frac{1}{12\,N^3}$ which is shown as a solid line in Fig. 2. This result suggests that the difference $f(N) - S_N$ decreases approximately as $1/(12\,N^3)$ with increasing N.

The numerical results in Table. I indicate that the difference $f(N) - S_N$ decreases from $\sim 9 \times 10^{-3}$ (the largest discrepancy for $N = 2$) to $\sim 8 \times 10^{-5}$ (for $N = 10$). This difference becomes practically zero when the size of the system grows further. Note that $S_N \approx N\,\xi(3)$ for large N. This means that S_N/N is convergent. In fact, it is straightforward to verify that:

$$\lim_{N\to\infty} \frac{S_N}{N} = \lim_{N\to\infty} \frac{f(N)}{N} = \xi(3) \approx 1.20206\ . \tag{14}$$

This leads to the correct value for the ground state energy per dipole in the thermodynamic limit:

$$\lim_{N\to\infty} \frac{U(N)}{N} = -2\,\xi(3)\,E_0 \approx -2.40412\,E_0\ , \tag{15}$$

where E_0 is the unit of energy defined in Eq.(4).

At this juncture, it worth commenting that one might find attractive of using similar techniques to obtain approximations for the ground state energy of finite systems of dipoles in higher dimensional 2D or 3D crystal lattices. The ground state configuration for a system of arbitrary N dipoles placed at the sites of a 2D or 3D crystal lattice is highly non-trivial. It may be possible that approximate analytical expressions may be found in the $N \to \infty$ limit by using similar techniques. However, it is unlikely that highly accurate expressions can be obtained in such a simple way when considering a finite system with an arbitrary number of $N \geq 2$ dipoles in a 2D or 3D crystal lattice.

To conclude, in this work we investigated the ground state energy of a finite system with an arbitrary number $N \geq 2$ of electric dipoles localized at the sites of a regular 1D crystal lattice. We derived an analytic expression for the ground state energy of the system at any given number $N \geq 2$ of dipoles. The analytic formula that we obtained gives results that are extremely accurate. The energy obtained from the analytic formula differs from the numerically exact values by a very small amount (for example, the difference is $\sim 8 \times 10^{-5}$ for a system with $N = 10$ dipoles). The results are practically indistinguishable as the size of the system grows further (for example, the difference becomes $\sim 8 \times 10^{-8}$ for a system with $N = 100$ dipoles). Based on these considerations, we can conclude that, for any arbitrary system of N dipoles in a regular 1D crystal lattice, there is no practical difference between the energy $-2\,E_0\,f(N)$ and the numerically calculated ground state energy, $U(N) = -2\,E_0\,S_N$ since it was verified that $f(N)$ approximates the numerically exact values of S_N with an astonishing accuracy that only increases as N increases. This result is very appealing due to its simplicity and appears to be an attractive feature of this particular regular 1D crystal lattice model.

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