

**Project Report**  
in the course  
“Methods of Molecular Simulation“  
during WiSe 21/22

**SummerOfSixtyNine**

—  
Implementation of the Ewald summation method for the  
sodium chloride crystal

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# 1 Introduction

This work is concerned with the implementation of the summation method that Paul Ewald published in 1921 and measuring it against a more naive implementation known as the direct sum for the sodium chloride crystal.[1] Both these methods attempt to calculate the electrostatic energy of the crystal's unit cell. From that, the Madelung constant can be determined, which is an important quantity in solid state physics and crystallography.[2] The python package that was developed to employ these methods was named SummerOfSixtyNine and will be abbreviated as SSN in the following. It was structured in accordance to the standards given in the *The Hitchhiker's Guide to Python*. [3]

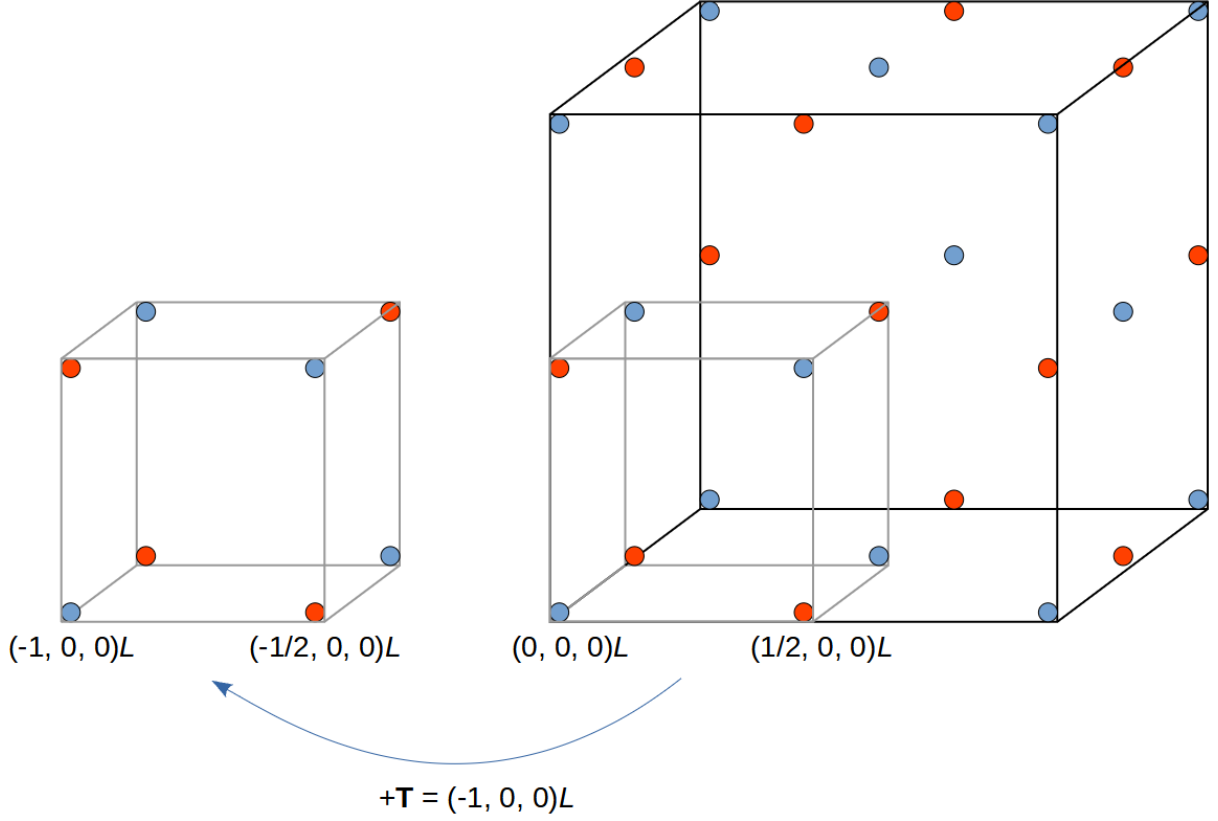
## 2 Theoretical background

Before taking a closer look into the realization, the theoretical concepts necessary to understand it shall be established. More detailed derivations of the formulae can be found in the appendix or the references given therein.

### 2.1 Periodic boundary conditions

Calculating the electrostatic energy for a macroscopic amount of substance, i.e. around  $n = 1$  mol, would imply a number of particles in the range of the Avogadro constant  $N = n \cdot N_A = 6.022 \cdot 10^{23}$ . This is obviously unfeasible for current generation computational devices and must thus be approximated.

One frequently employed method for solid state materials such as the sodium chloride crystal is the use of periodic boundary conditions. In this approach, the particles in the crystal may be described by their positions  $\mathbf{r}_i$  in the unit cell and an infinite set of translation vectors  $\mathbf{T}$  that create mirror images of the unit cell in all directions. This is depicted in figure 1. It can be seen in the figure that the unit cell of sodium chloride (black box) actually only contains eight distinct particles (grey box). By copying these with the translation vectors, the entire grid may be filled with particles eventually, one cubic shell at a time. This strategy is known as the cubic expansion and will be used throughout the reported work.



**Figure 1:** Schematic representation of the NaCl unit cell and the periodic mirroring induced by the translation vector  $\mathbf{T}$ .

## 2.2 Direct sum

By virtue of the periodicity, each individual particle interacts with all other particles, including the ones in all mirrored cells. The electrostatic energy per unit cell can then be cast as

$$E_{direct} = \frac{1}{4\pi\epsilon_0} \frac{1}{2} \sum_{\mathbf{n}} \sum_{i=1}^N \sum_{j=1}^N ' \frac{q_i q_j}{|\mathbf{r}_{ij} + \mathbf{T}|}. \quad (1)$$

Here,  $|\mathbf{r}_{ij} + \mathbf{T}| = |\mathbf{r}_j - \mathbf{r}_i + \mathbf{T}|$  is the distance between the particles and  $\epsilon_0 \approx 8.854 \times 10^{-12} \text{ A sec/Vm}$  is the dielectric constant. The ' symbol indicates that the summand  $i = j$  and  $\mathbf{T} = (0, 0, 0)$  is set to 0 and the factor of  $\frac{1}{2}$  accounts for the sum counting each ion pair twice. For the cubic unit cell of sodium chloride with uniform length  $L$  along all

three Cartesian unit vectors  $\mathbf{x}, \mathbf{y}, \mathbf{z}$ , the translation vectors can be rephrased in terms of so-called repeat vectors  $\mathbf{n} = n_1(1, 0, 0) + n_2(0, 1, 0) + n_3(0, 0, 1)$  as

$$\begin{aligned}
\mathbf{T} &= n_1 \mathbf{T}_1 + n_2 \mathbf{T}_2 + n_3 \mathbf{T}_3 \\
&= n_1 \mathbf{x}L + n_2 \mathbf{y}L + n_3 \mathbf{z}L \\
&= n_1(1, 0, 0)L + n_2(0, 1, 0)L + n_3(0, 0, 1)L \\
&= (n_1(1, 0, 0) + n_2(0, 1, 0) + n_3(0, 0, 1))L \\
&= \mathbf{n}L,
\end{aligned} \tag{2}$$

over which the first sum in eq. 1 runs. In practical implementations, the set of repeat vectors is not actually infinite, but bounded by a user-defined cutoff value  $n_{cut}$  that represents the number of cubic shells around the unit cell taken into account in the calculation. The components are then given as

$$n_1, n_2, n_3 = -n_{cut}, -n_{cut} + 1, \dots, 0, \dots, n_{cut} - 1, n_{cut}. \tag{3}$$

Unfortunately, the series in eq. 1 is slowly and conditionally convergent, i.e. the order of the summation influences the convergence and one needs to choose high values of  $n_{cut}$ . Studies have shown, however, that the direct sum energy in the cubic expansion may eventually converge to the correct value.[4]

## 2.3 Ewald summation

A scheme that converges fast and also absolutely is the Ewald summation method. The idea here is to split the charge distribution  $\rho_i(\mathbf{r})$  of the particles, which so far has implicitly been assumed to be a delta function  $\rho_i(\mathbf{r}) = q_i \delta(\mathbf{r} - \mathbf{r}_i)$  located at the particle's position  $\mathbf{r}_i$ . The splitting is done by adding and subtracting a Gaussian function

$$g_\sigma(\mathbf{r}) = \frac{1}{(2\pi\sigma^2)^{3/2}} e^{-|\mathbf{r}-\mathbf{r}_i|/2\sigma^2} \tag{4}$$

with the Gaussian parameter  $\sigma$ . The charge distribution can then be reorganized into a short- and a long-range part. These give rise to different electrostatic potentials, which

in turn cause distinct short- and long-range contributions to the energy. The total electrostatic energy can thus be cast as

$$\begin{aligned}
E_{ewald} &= E^S + E^L - E^{self} \\
&= \frac{1}{4\pi\epsilon_0} \frac{1}{2} \sum_{\mathbf{n}} \sum_{i=1}^N \sum_{j=1}^N, \frac{q_i q_j}{|\mathbf{r}_{ij} + \mathbf{T}|} \operatorname{erfc} \left( \frac{|\mathbf{r}_{ij} + \mathbf{T}|}{\sqrt{2}\sigma} \right) \\
&\quad + \frac{1}{2L^3\epsilon_0} \sum_{\mathbf{k} \neq 0} \sum_{i=1}^N \sum_{j=1}^N \frac{q_i q_j}{G^2} e^{-i\mathbf{G} \cdot \mathbf{r}_{ij}} e^{-\sigma^2 G^2/2} \\
&\quad - \frac{1}{4\pi\epsilon_0} \frac{1}{\sqrt{2\pi}\sigma} \sum_{i=1}^N q_i^2.
\end{aligned} \tag{5}$$

The reciprocal lattice vectors  $\mathbf{G}$  are given as

$$\begin{aligned}
\mathbf{G} &= k_1 \mathbf{G}_1 + k_2 \mathbf{G}_2 + k_3 \mathbf{G}_3 \\
&= (k_1 \mathbf{x} + k_2 \mathbf{y} + k_3 \mathbf{z}) \frac{2\pi}{L} \\
&= \mathbf{k} \frac{2\pi}{L}
\end{aligned} \tag{6}$$

and  $G^2 = |\mathbf{G}|^2$  is their square modulus. The reciprocal repeat vectors are  $\mathbf{k} = k_1(1, 0, 0) + k_2(0, 1, 0) + k_3(0, 0, 1)$  and their components are tied to a user-defined cutoff value  $k_{cut}$  as

$$k_1, k_2, k_3 = -k_{cut}, -k_{cut} + 1, \dots, 0, \dots, k_{cut} - 1, k_{cut}. \tag{7}$$

The first sum in the second term of eq. 5 runs over these  $\mathbf{k}$ -vectors. The specific  $\mathbf{k}$ -vector with modulus 0 would correspond to an infinite distance and is thus omitted. The last sum in eq. 5 accounts for a self-interaction error that is formally introduced by the long-range energy term. A more detailed derivation of eq. 5 can be found in the appendix or the textbook *Understanding molecular simulation: from algorithms to applications* written by Frenkel and Smit.[5]

## 2.4 Setting up the formula for the implementation

Naively implementing the Ewald summation formula as given in eq. 5, one could express the sums over particles and repeat vectors as a series of nested for loops, which would suffer from a terrible performance in python. Additionally, handling the complex exponential in the long-range term could be done with python's native complex algebra, further complicating the code. Consequently, the formula was reorganized to a more convenient form. After taking the steps elaborated in the appendix and introducing the charge number

$c_i = q_i/e$  with the elementary charge  $e$ , one obtains the following expression for the total electrostatic energy:

$$E_{ewald} = \frac{e^2}{8\pi\epsilon_0} \sum_{i=1}^N \sum_{j=1}^N c_i c_j \left( \sum_{\mathbf{n}}' \frac{\text{erfc}\left(\frac{|\mathbf{r}_{ij} + \mathbf{n}L|}{\sqrt{2}\sigma}\right)}{|\mathbf{r}_{ij} + \mathbf{n}L|} + \frac{4\pi}{L^3} \sum_{\mathbf{k} \neq 0} \cos(\mathbf{G} \cdot \mathbf{r}_{ij}) \frac{e^{-\sigma^2 G^2/2}}{G^2} - \frac{\sqrt{2}}{\sqrt{\pi}\sigma} \delta_{ij} \right) \quad (8)$$

In this formula, it is apparent that quick convergence of the short-range part is ensured by the complementary error function and the long-range part converges due to the exponential decay. Thus, the total Ewald sum is quickly and absolutely convergent, as was claimed at the start of the section.

## 2.5 Madelung constant

To measure the accuracy of the presented methods, one may calculate the Madelung constant  $M$  from the electrostatic energy, as it can be taken as a reference from the literature.[2] This dimensionless factor is defined as the ratio between the average bond energy of a single ion in the crystal and the average bond energy of an ion in an isolated ion pair. For sodium chloride, it can be expressed in terms of already known quantities as

$$M = E \frac{4\pi\epsilon_0}{8e^2}, \quad (9)$$

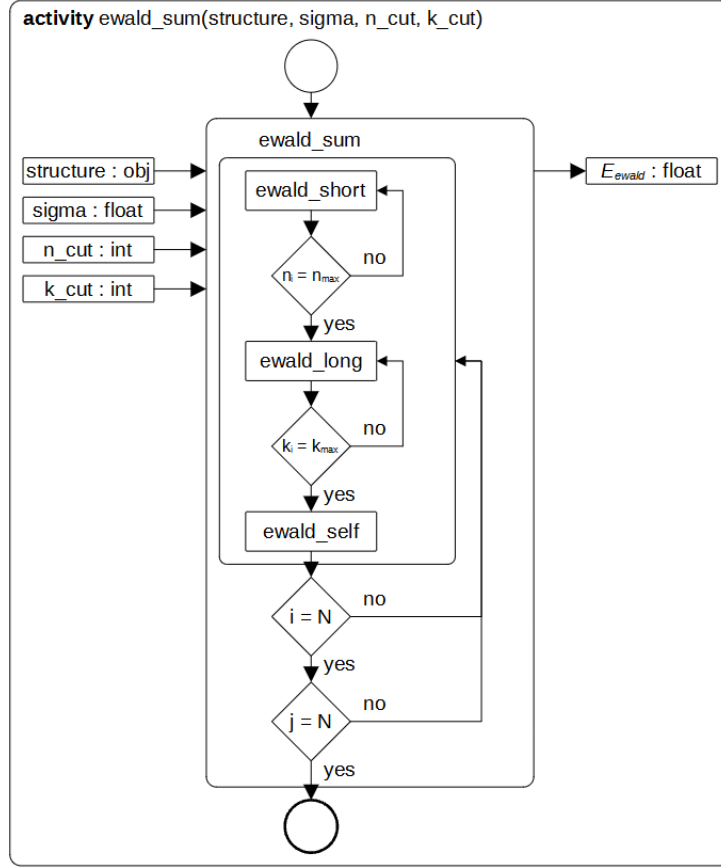
where  $E$  is the electrostatic energy per unit cell calculated with the direct sum or Ewald summation.

## 3 Implementation

Due to the considerable efforts made on the theoretical side, the implementation of the two presented methods in python is straightforward.

### 3.1 Ewald sum implementation

The double sum over all particles in eq. 8 was implemented as a double for loop which would call three lower-level functions for the short-range, the long-range and the self-energy in each instance. Each of these would get the user parameter  $\sigma$  as input. The calculation of the short-range part was done with a for loop over the set of repeat vectors  $\mathbf{n}$  determined with the user-defined parameter  $n_{cut}$ , as is given in eq. 3. The long-range energy contribution was calculated accordingly by looping over the set of reciprocal repeat vectors  $\mathbf{k}$  with the user parameter  $k_{cut}$ .



**Figure 2:** UML activity diagram of the implemented Ewald summation function.

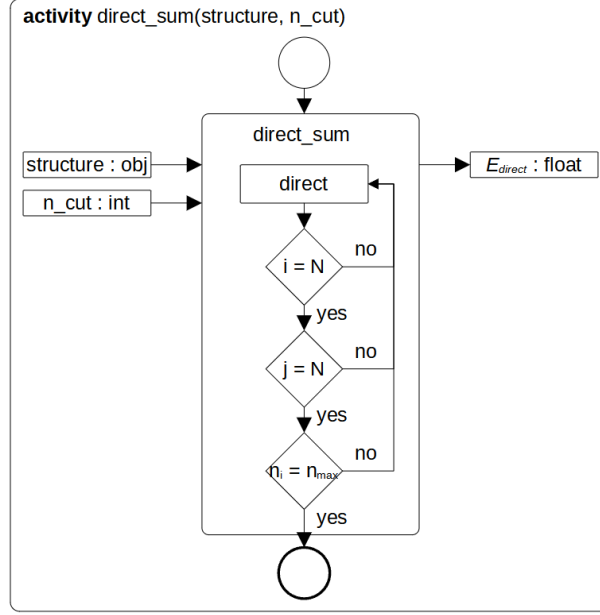
The number  $\pi$ , the vacuum permittivity  $\epsilon_0$  and the elementary charge  $e$  were taken from the `scipy.constants` subpackage and the functions `erfc`, `sin` and `cos` were taken from `scipy.special`. The exponential function and the dot and cross products were carried out with numpy functions and all vectors were represented as numpy arrays. A schematic representation of the Ewald summation function can be seen in figure 2.

All structural properties such as positions, charges, repeat vectors, etc. were handled by the newly implemented `Structure` class, which would be instantiated by the user in advance to calling the Ewald summation function.

### 3.2 Direct sum implementation

The implementation of the direct sum was done for later comparison and closely resembles the formula given in eq. 1. In analogy to the UML activity diagram given above, its functionality can be seen in figure 3. Since this is essentially also a triple-nested for loop, it is expected to exhibit similar scaling to the implementation of the Ewald sum.





**Figure 3:** UML activity diagram of the implemented direct summation function.

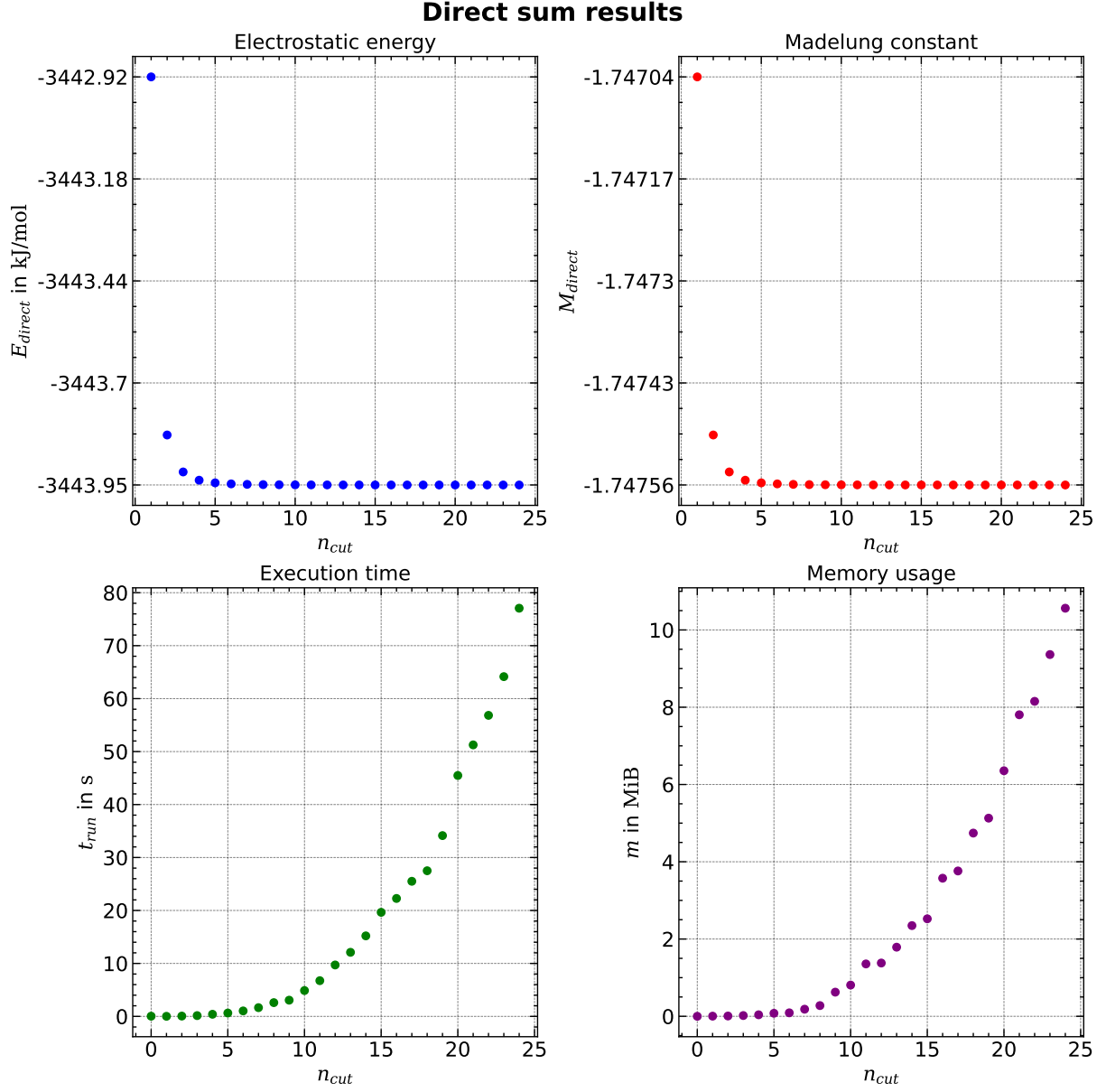
## 4 Results

Now that all necessary concepts in theory and implementation have been established, the SSN program shall be tested regarding its accuracy and performance. The values for the unit cell energy of  $E_{ref}^{NaCl} = 3443.95 \text{ kJ mol}^{-1}$  and the Madelung constant of  $M_{ref}^{NaCl} = 1,74756$  of sodium chloride are taken from the textbook *Festkörperphysik* written by Gross and Marx.[6] For a first measure, the results of the direct sum module are presented.

### 4.1 Direct sum results

As has been commented on before, the direct summation method is conditionally convergent and may converge to the correct value when using the cubic expansion. Its convergence behaviour depending on the chosen cutoff value was investigated and is shown in figure 4.

It can be seen that both the energy and the Madelung constant do indeed approach  $\lim_{n_{cut} \rightarrow \infty} E_{direct}^{NaCl}(n_{cut}) = 3443.95 \text{ kJ mol}^{-1}$  and  $\lim_{n_{cut} \rightarrow \infty} M_{direct}^{NaCl}(n_{cut}) = 1,74756$ . The values become satisfyingly close for cutoff values of  $n_{cut} = 5, \dots, 10$ , for which the performance is still very good with execution times of under 5 s and memory usage of less than 1 MiB. For greater cutoff values, no significant improvement in accuracy can be observed and the highly non-linear scaling in both time and memory usage renders the calculation prohibitive. In order to contextualize these measurements, the next section will deal with the results of the Ewald summation module.



**Figure 4:** Results of the direct sum implementation for different cutoff values. *Upper left:* Electrostatic energies vs. cutoff values; *Upper right:* Madelung constants vs. cutoff values; *Lower left:* Execution times vs. cutoff values; *Lower right:* Memory usages vs. cutoff values.

## 4.2 Ewald summation results

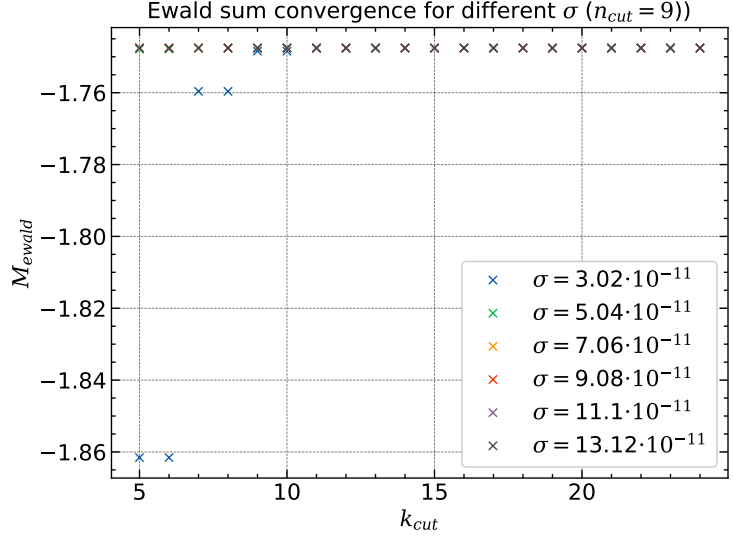
An extensive study of possible parameter combinations  $\sigma$ ,  $k_{cut}$  and  $n_{cut}$  has been carried out.

It was found that for values of  $\sigma > 10^{-9}$ , the long-range part does not contribute to the total energy at all and the convergence behaviour is similar to the one shown for the direct sum method. This can be explained by the strong dependence of the damping exponential term (eq. 8) on the reciprocal lattice vectors. Since these are divided by the unit cell length of  $L = 5.64 \times 10^{-10} \text{ \AA}$  and squared, they need to be compensated by

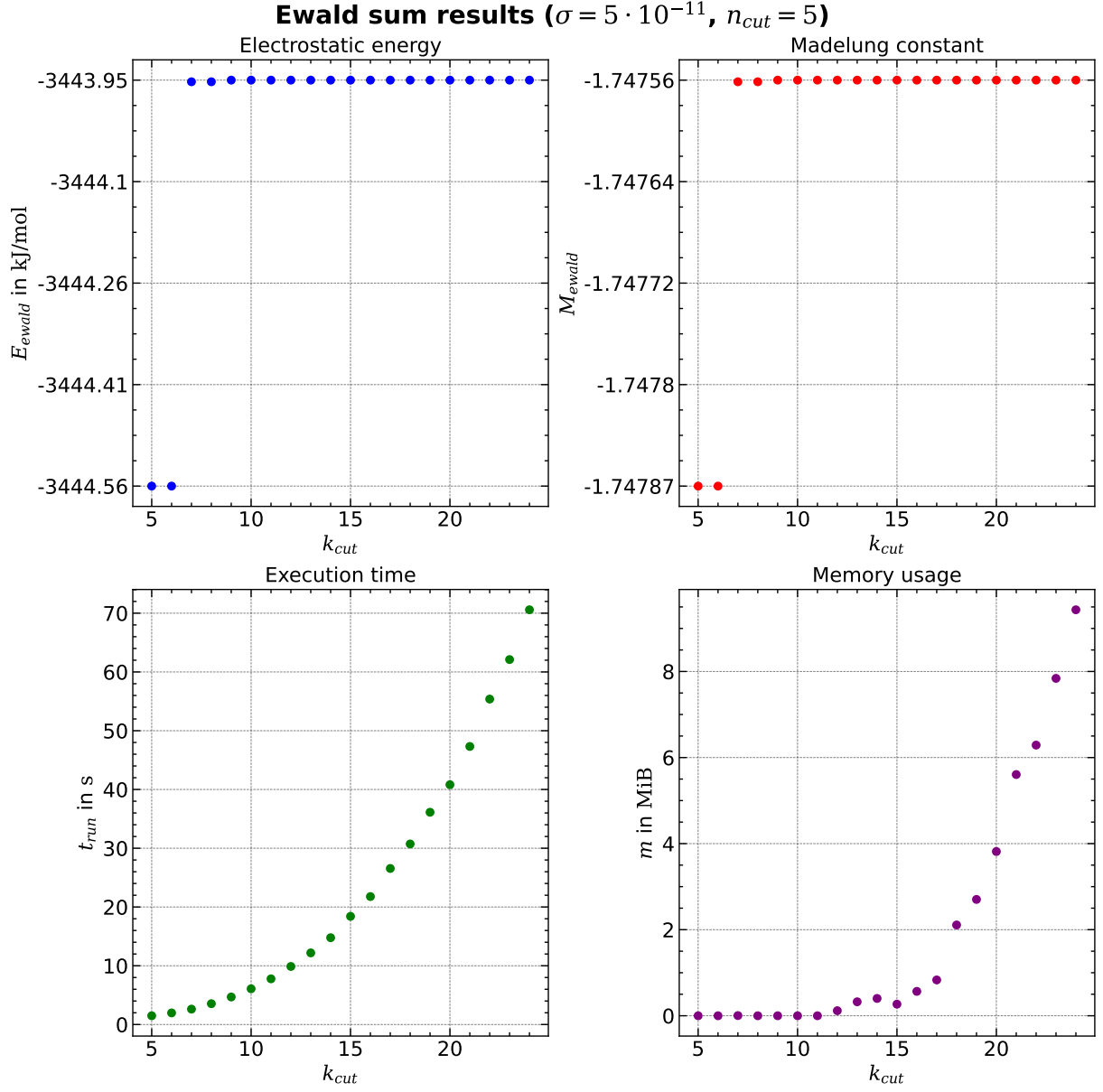
$\sigma$  values in the same order of magnitude to prevent the term from going to zero instantaneously. For  $\sigma < 10^{-9}$ , the convergence was found to also depend on  $k_{cut}$ . When using  $\sigma < 1e-11$ , however, the energy and Madelung constants converged very slowly with increasing  $k_{cut}$ . The right choice of parameters was thus found to be crucial for quick and clean convergence. The influence of the Gaussian parameter on the convergence with the reciprocal cutoff is shown in figure 5.

A particularly sufficient value for the Gaussian parameter was  $\sigma = 5e-11$ , for which the dependence of the four previously considered quantities on  $k_{cut}$  is shown in 6. The value of  $n_{cut} = 5$  was used based on the fast real-space convergence of the damping complementary error function.

It is apparent that the energy and Madelung constant very rapidly converge to the correct values. The seemingly strange behaviour for  $k_{cut} = 5, 6$  was systematic to all Ewald sum calculations: Changes in energy would only be made after every two steps of  $k_{cut}$ . That aside, the results presented in figure 6 do suggest that using Ewald summation is superior to the direct sum method.



**Figure 5:** Convergence behaviour of the Ewald summation method for different values of  $\sigma$ .



**Figure 6:** Results of the Ewald sum implementation for different reciprocal cutoff values. *Upper left:* Electrostatic energies vs. reciprocal cutoff values; *Upper right:* Madelung constants vs. reciprocal cutoff values; *Lower left:* Execution times vs. reciprocal cutoff values; *Lower right:* Memory usages vs. reciprocal cutoff values.

## 5 Conclusion and perspective

The Ewald summation method was implemented alongside a direct summation method for cubic expansion of the sodium chloride unit cell. It could be shown that both methods converge, but it was found that the Ewald summation is the preferable choice if a suitable Gaussian parameter  $\sigma$  is known, as it converges very quickly with the real and reciprocal space cutoffs.

As a next step, it could be interesting to test the code against other crystal types, for which reference data is available - e.g. cesium chloride. This should be a straightforward task, as the SSN package was implemented with detailed documentation and the Structure class may serve as a template for such an extension.

## References

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## 6 Appendix

### 6.1 Electrostatic energy

Two classical point charges  $q_i$  and  $q_j$  in the vacuum that reside at positions  $\mathbf{r}_i$  and  $\mathbf{r}_j$  exhibit a potential on one another given by Coulombs law, which results in the electrostatic interaction energy

$$E_{ij} = \frac{1}{4\pi\epsilon_0} \frac{q_i q_j}{|\mathbf{r}_{ij}|}. \quad (10)$$

Here,  $|\mathbf{r}_{ij}| = |\mathbf{r}_j - \mathbf{r}_i|$  is the distance between the particles, and  $\epsilon_0 \approx 8.854 \times 10^{-12}$  A sec/Vm is the dielectric constant. This may be generalized to any number of particles  $N$  by summation over all pairwise interactions as

$$E_N = \frac{1}{4\pi\epsilon_0} \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N, \frac{q_i q_j}{|\mathbf{r}_{ij}|}. \quad (11)$$

### 6.2 Derivation of the Ewald summation formula

With the Gaussian distribution given in eq. 4. The charge distribution  $\rho_i(\mathbf{r})$  can be reorganized into

$$\begin{aligned} \rho_i(\mathbf{r}) &= q_i \delta(\mathbf{r} - \mathbf{r}_i) - q_i g_\sigma(\mathbf{r}) + q_i g_\sigma(\mathbf{r}) \\ &= \rho_i^S(\mathbf{r}) + \rho_i^L(\mathbf{r}). \end{aligned} \quad (12)$$

The term  $\rho_i^S(\mathbf{r}) = q_i \delta(\mathbf{r} - \mathbf{r}_i) - q_i g_\sigma(\mathbf{r})$  represents the short-ranged part of the charge distribution and  $\rho_i^L(\mathbf{r}) = q_i g_\sigma(\mathbf{r})$  is the long-range part. Applying the Poisson equation

$$\nabla^2 \phi(\mathbf{r}) = -\frac{\rho(\mathbf{r})}{\epsilon_0} \quad (13)$$

to the short-range distribution, one can obtain the corresponding electrostatic potential  $\phi^S$ , which leads to the following short-range contribution to the total electrostatic energy:

$$E^S = \frac{1}{4\pi\epsilon_0} \frac{1}{2} \sum_{\mathbf{n}} \sum_{i=1}^N \sum_{j=1}^N, \frac{q_i q_j}{|\mathbf{r}_{ij} + \mathbf{n}L|} \text{erfc} \left( \frac{|\mathbf{r}_{ij} + \mathbf{n}L|}{\sqrt{2}\sigma} \right). \quad (14)$$

The Poisson equation for the long-range charge distribution can be solved in Fourier space and when transformed back, the corresponding long-range potential  $\phi^L(\mathbf{r})$  gives rise to an energy contribution

$$E^L = \frac{1}{2V\epsilon_0} \sum_{\mathbf{k} \neq 0} \sum_{i=1}^N \sum_{j=1}^N \frac{q_i q_j}{G^2} e^{-i\mathbf{G} \cdot \mathbf{r}_{ij}} e^{-\sigma^2 G^2 / 2}, \quad (15)$$

where  $V$  is the volume of the unit cell defined as

$$\begin{aligned} V &= |\mathbf{T}_1 \cdot (\mathbf{T}_2 \times \mathbf{T}_3)| \\ &= |\mathbf{x}L \cdot (\mathbf{y}L \times \mathbf{z}L)| \\ &= L^3 \end{aligned} \quad (16)$$

The primitive reciprocal lattice vectors  $\mathbf{G}_1$ ,  $\mathbf{G}_2$  and  $\mathbf{G}_3$  can be obtained from the primitive translation vectors with the equation

$$\mathbf{G}_i \cdot \mathbf{T}_j = 2\pi\delta_{ij}. \quad (17)$$

With eq. 2 and 16, this becomes

$$\mathbf{G}_i = \frac{2\pi}{L^3} \delta_{ij} (\mathbf{T}_k \times \mathbf{T}_l) \quad (18)$$

$$\begin{aligned} \Rightarrow \mathbf{G}_1 &= \frac{2\pi}{L^3} (\mathbf{T}_2 \times \mathbf{T}_3) = \frac{2\pi}{L^3} (L(0, 1, 0) \times L(0, 0, 1)) \\ &= \frac{2\pi}{L^3} L^2(1, 0, 0) = \frac{2\pi}{L} \mathbf{x} \end{aligned} \quad (19)$$

$$\Rightarrow \mathbf{G}_2 = \frac{2\pi}{L} \mathbf{y} \quad (20)$$

$$\Rightarrow \mathbf{G}_3 = \frac{2\pi}{L} \mathbf{z} \quad (21)$$

The long-range energy term introduces a self-interaction error

$$E^{self} = \frac{1}{4\pi\epsilon_0} \frac{1}{\sqrt{2\pi}\sigma} \sum_{i=1}^N q_i^2 \quad (22)$$

that needs to be subtracted for the calculation of the total electrostatic energy per unit cell.



### 6.3 Derivation of the set-up formula

If one defines a structure factor

$$S(\mathbf{k}) = \sum_{i=1}^N q_i e^{i\mathbf{G} \cdot \mathbf{r}_i} \quad (23)$$

as is done in [7], one can rephrase eq. 15 as

$$E^L = \frac{1}{2V\epsilon_0} \sum_{\mathbf{k} \neq 0} \frac{e^{-\sigma^2 G^2/2}}{G^2} |S(\mathbf{k})|^2. \quad (24)$$

The square modulus of the structure factor may be simplified with Euler's identity as

$$\begin{aligned} |S(\mathbf{k})|^2 &= S(\mathbf{k}) \cdot S^*(\mathbf{k}) \\ &= \left[ \sum_{i=1}^N q_i e^{i\mathbf{G} \cdot \mathbf{r}_i} \right] \cdot \left[ \sum_{j=1}^N q_j e^{-i\mathbf{G} \cdot \mathbf{r}_j} \right] \\ &= \left[ \sum_{i=1}^N q_i (\cos(\mathbf{G} \cdot \mathbf{r}_i) + i \sin(\mathbf{G} \cdot \mathbf{r}_i)) \right] \cdot \left[ \sum_{j=1}^N q_j (\cos(\mathbf{G} \cdot \mathbf{r}_j) - i \sin(\mathbf{G} \cdot \mathbf{r}_j)) \right] \\ &= \left[ \sum_{i=1}^N q_i \cos(\mathbf{G} \cdot \mathbf{r}_i) + i \sum_{i=1}^N q_i \sin(\mathbf{G} \cdot \mathbf{r}_i) \right] \cdot \left[ \sum_{j=1}^N q_j \cos(\mathbf{G} \cdot \mathbf{r}_j) - i \sum_{j=1}^N q_j \sin(\mathbf{G} \cdot \mathbf{r}_j) \right] \\ &= \sum_{i=1}^N \sum_{j=1}^N q_i q_j \cos(\mathbf{G} \cdot \mathbf{r}_i) \cos(\mathbf{G} \cdot \mathbf{r}_j) + \sum_{i=1}^N \sum_{j=1}^N q_i q_j \sin(\mathbf{G} \cdot \mathbf{r}_i) \sin(\mathbf{G} \cdot \mathbf{r}_j) \\ &= \sum_{i=1}^N \sum_{j=1}^N \cos(\mathbf{G} \cdot (\mathbf{r}_j - \mathbf{r}_i)) \\ &= \sum_{i=1}^N \sum_{j=1}^N \cos(\mathbf{G} \cdot \mathbf{r}_{ij}). \end{aligned} \quad (25)$$

The equality from the third last to the second last line holds due to the trigonometric identity  $\cos \alpha \cos \beta + \sin \alpha \sin \beta = \cos(\alpha - \beta)$ . Inserting this back into eq. 24 and reordering the sums yields

$$E^L = \frac{1}{2V\epsilon_0} \sum_{i=1}^N \sum_{j=1}^N q_i q_j \sum_{\mathbf{k} \neq 0} \cos(\mathbf{G} \cdot \mathbf{r}_{ij}) \frac{e^{-\sigma^2 G^2/2}}{G^2}. \quad (26)$$

In doing the same to eq. 14 to get

$$E^S = \frac{1}{4\pi\epsilon_0} \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N q_i q_j \sum_{\mathbf{n}}' \frac{\text{erfc}\left(\frac{|\mathbf{r}_{ij} + \mathbf{n}L|}{\sqrt{2}\sigma}\right)}{|\mathbf{r}_{ij} + \mathbf{n}L|}, \quad (27)$$

and expressing the sum in eq. 22 as

$$E^{self} = \frac{1}{4\pi\epsilon_0} \frac{1}{\sqrt{2\pi\sigma}} \sum_{i=1}^N \sum_{j=1}^N q_i q_j \delta_{ij}, \quad (28)$$

one arrives at a form for the electrostatic energy as given in eq. 8.