Solution of the Poisson equation for two dimensional periodic structures (slabs) in an overlapping localized site density scheme

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Bertaut’s equivalent electric density idea (E. F. Bertaut, Journal de Physique 39, 1331 (1978)) is applied to the case of two dimensional periodic continuous charge density distributions. The following derivation differs from what was introduced by Bertaut. The presented method solves the Poisson equation for the scheme of overlapping localized site densities with periodic boundary conditions in the \((x, y)\) plane and with the general finite voltage boundary condition in the perpendicular \(z\)-direction. As usual the long-range potential is calculated in the Fourier space. For the \(K_{\parallel} \neq 0\) case a Fourier transformation helps to calculate the solution in a three dimensional periodic sense, while for \(K_{\parallel} = 0\) the required charge neutrality is the starting point. For both cases suitable representations of the spherical harmonics are needed to arrive at expressions that are convenient for numerical implementation. In this localized density scheme an explicit relation can be derived between the finite voltage in \(z\)-direction and the \(z\)-component of the dipole density.

Keywords: slabs, Ewald summation, Poisson equation

I. INTRODUCTION

The solution of the Poisson equation for periodic structures has great practical importance in many areas of solid state physics, e.g. in band structure calculations or in molecular dynamics simulations. The Bertaut’s ‘equivalent electric density’ idea, realized in the pseudo-charge or multipole compensation method developed by Weinert is nowadays the standard approach in plane-wave implementations for three dimensional (3D) periodic problems. The Bertaut approach to sum up the long-range electrostatic interactions is based on the replacement of the point-like multipoles at every lattice sites by non overlapping charge distributions with equivalent multipoles. In the Weinert method every site might have several multipoles and the crystal is divided up into atomic site domains \(\Omega\) (muffin-tin sphere) and into an interstitial part. To calculate the electrostatic potential in the interstitial region (the long-range potential contribution) Weinert realizes Bertaut’s idea by introducing pseudo-charge densities confined to the atomic volumes \(\Omega\). Inside \(\Omega\) the Dirichlet problem for the original charge density is solved, using the potential value at the boundary of \(\Omega\), which result from the interstitial solution.

Dealing with 3D crystalline extended systems the periodic Born-von Kármán boundary conditions (PBC) in each direction are mandatory. For films or single slab geometries the PBC is applicable only to the extended \((x, y)\) (in-plane) directions. In the perpendicular \(z\)-direction the system has only finite extension and requires a different boundary condition. The most general physical situation allows for a finite voltage at infinity in \(z\)-direction, which would be the case for slabs without a in-plane mirror symmetry. This general finite voltage condition in the \(z\)-direction coincides with the physical picture of a charged capacitor.

A possible treatment of films is the super-cell (vacuum-film-vacuum) method with 3D periodicity, which describes the electrostatic potential inside the super-cell as a continuous function and thus excludes any step like discontinuities. The introducing of an artificial dipole layer in the vacuum region allows to model the finite voltage situation. However, there is still a possibility of spurious image interactions. Furthermore, an additional parameter, the vacuum thickness, has to be converged. The plane-wave based layer-FLAPW method\[6,7\] treats the single slab geometry as a real 2D periodic unit cell extending from \(-\infty\) to \(+\infty\) in \(z\)-direction with three different regions: the muffin-tin, the interstitial, and a vacuum (no charge) segment. The method is applicable to surface problems without any invocation of an artificial periodicity. In this method a finite voltage may occur between the two interstitial boundaries. It seems that this treatment of the potential step feature via plane-waves produces thicker interstitial regions than necessary.

This work presents the general solution of the Poisson equation for two dimensional periodic systems based on the multipole compensation method for a scheme of overlapping localized site densities. In the compact site density ansatz (see Refs.\[8,9\]) the total electronic charge density is written as a locally finite sum without any interstitial density. The presented derivation differs from what is given by Weinert\[2\] or Bertaut\[1\] for 3D periodic systems. The correct capacitor-like boundary condition is taken explicitly into account, which results in a direct relation between the finite voltage and the dipole of the slab as is expected from macroscopic electrostatics of a film geometry.

In Appendix\[4\] we shortly sketch how our ideas apply to the 1D periodic problem, which differs in methodology from the treatments\[10,11,12\] presented elsewhere, however resulting in the same expressions.
II. THE MULTIPOLe COMPENSATION IN THE LOCALIZED SITE DENSITY SCHEME

For crystalline structures in the thermodynamic limit there is an infinite periodic adjustment of the finite number of sites in the unit cell \( \{ s_1, \ldots, s_d \} \), by the Bravais vectors \( \mathbf{R} \). In the case of film geometry the Bravais vectors \( \mathbf{R} \) span one of the 2D Bravais lattices. In other words, the slab geometry means a three dimensional object with two dimensional periodicity. The symmetry groups of this geometry are called layer groups \( \mathbf{R} \). According to the main assumption at any point \( \mathbf{r} \) in the extended solid only a finite number of site charges with compact support \( \Omega_{s_j}, j \in \{ 1, \ldots, d \} \) will overlap, as it is shown in Fig. 1. Each site domain may contain several neighboring unit cells.

![Schematic site charge (compact support) distribution are overlapping at the point \( \mathbf{r} \).](image)

**Fig. 1:** Schematic site charge (compact support) distribution are overlapping at the point \( \mathbf{r} \).

Using the local expansion ansatz
\[
|kn\rangle = \sum_{\mathbf{R}} \sum_{j} | R s_j \rangle L e^{ik s_j} e^{i \mathbf{k} (\mathbf{R} + \mathbf{s}_j)} \tag{1}
\]
for the Bloch state \( |kn\rangle \), where \( \mathbf{k} \) is the crystal momentum, \( n \) is the band index and \( L \) is a composite index for atomic orbitals containing the principal and the angular quantum numbers, a local expression can be derived for the total density \( \rho \)
\[
\rho(\mathbf{r}) = \sum_{\mathbf{k}, n} \langle kn | \mathbf{r} | kn \rangle = \sum_{\mathbf{R}} \sum_{j=1}^{d} \rho_j(\mathbf{r} - \mathbf{s}_j), \tag{2}
\]
which defines the site-density \( \rho_j \) and the corresponding domain \( \Omega_{s_j+\mathbf{R}} \), see Koepferl and Eschrig. The total charge density
\[
\rho(\mathbf{r}) = \sum_{\mathbf{R}, j} \sum_{\mathbf{R}+s_j} \rho_j(\mathbf{r} - \mathbf{R} - \mathbf{s}_j) = \sum_{\mathbf{R}, j} \sum_{L} \rho_j L (| \mathbf{r} - \mathbf{s}_j \rangle Y_L (\mathbf{r} - \mathbf{s}_j)), \tag{3}
\]
is accordingly a finite sum of site contributions and is written as a uniformly convergent sum of spherical harmonics \( Y_L, L = (\ell, m) \). The first line defines the total density by the site densities. The complicated restriction in the summation allows only such \( \mathbf{R} \) and \( j \) indices that the domain of the corresponding site density contains the point \( \mathbf{r} \). The lattice periodicity of the total electronic density \( \rho(\mathbf{r}) \) is not broken because of the \( \mathbf{r} \) dependence of the summation.

To calculate the electrostatic potential \( \phi(\mathbf{r}) \) of the system one needs to solve the Poisson equation
\[
\Delta \phi(\mathbf{r}) = \sum_{\mathbf{R}, j} \rho_j (\mathbf{r} - \mathbf{R} - \mathbf{s}_j) - \sum_{\mathbf{R}, j} Z_j \delta(\mathbf{r} - \mathbf{R} - \mathbf{s}_j) \tag{4}
\]
at any \( \mathbf{r} \in \mathbb{R}^3 \), where no restriction is used in the second Dirac delta summation. To get ‘bulk’ quantities PBC is used in the periodic directions (say \( x \) and \( y \)) while in the third direction the general finite voltage boundary condition is considered. Through the paper atomic units are used.

We now introduce the generalized Ewald densities expanded by spherical harmonics
\[
\rho_j^E(\mathbf{r}) = \sum_{L} \rho_j^E(\mathbf{r}) Y_L (\mathbf{r}) \tag{5}
\]
\[
\rho_j^E(\mathbf{r}) = A_j L N_{\ell} p^{\ell} e^{-r^2 p^2}, \quad N_{\ell} = \frac{2 p^{2\ell+3}}{\Gamma(\ell + \frac{3}{2})} \tag{6}
\]
where \( p \) is the usual Ewald parameter and the multipole freedom is settled in \( A_j L \). With that normalization \( A_j L \) are not dimensionless quantities, but their dimensions are \([A_j L] \equiv \text{meter}^\ell\). The last line of Eq. (6) indicates the most reasonable coupling of terms what is used in the calculations below. By the additional multipole compensators (Ewald charges) a modified electrostatic problem is created with a new Poisson equation
\[
\Delta \tilde{\phi}(\mathbf{r}) = \tilde{\rho}(\mathbf{r}) \tag{7}
\]
\[
\tilde{\rho}(\mathbf{r}) = \sum_{\mathbf{R}, j} \rho_j (\mathbf{r} - \mathbf{R} - \mathbf{s}_j) - \sum_{\mathbf{R}, j} Z_j \delta(\mathbf{r} - \mathbf{R} - \mathbf{s}_j) + \sum_{\mathbf{R}, j} \rho_j^E (\mathbf{r} - \mathbf{R} - \mathbf{s}_j), \tag{8}
\]
where

\begin{align*}
\Delta \phi^E(\mathbf{r}) & = \sum_{\mathbf{R}, j} \rho_j^E (\mathbf{r} - \mathbf{R} - \mathbf{s}_j) = \rho^E(\mathbf{r}) \tag{9}
\end{align*}
is derived. Thus, the complicated original Poisson problem is subdivided into two simpler problems, $\phi(r) = \bar{\phi}(r) - \rho_{Ewald}(r)$. Before discussing the boundary conditions for the latter two equations the solutions of the multipole compensations are needed because they define the Ewald densities and thus the two Poisson equations Eqs. (6,7). Keeping the 2D periodicity in both subproblems is compatible with the original PBC.

A difficulty shows up in the solution of Eq. (6) by the non-restricted sum of overlapping non-compact Ewald densities. To get rid of this difficulty one can assume that the Ewald densities are negligible outside the site domains. This results the same finite number of terms in both subproblems as in the first sum. Using the approximate compactness of the Ewald densities the multipole compensation equations are written as integrals over the whole space

$$0 = \int_{\Omega} d^3r \, Y_\ell^m(r) r^\ell \left( \rho_j(r - R - s_j) - Z_j \delta(r - R - s_j) + \rho_{Ewald}^j(r - R - s_j) \right).$$

The introduced assumption simplifies the Poisson equation Eq. (6) into the form

$$\Delta \bar{\phi}(r) \approx \bar{\rho}(r),$$

where the r.h.s. is given as a r-dependent finite sum of site densities. This equation is referred below as the short-range Poisson equation. The accuracy of the approximation is measured by the localization of the applied Ewald densities.

The linearity of $\Delta$ allows one to look for the solution also in a finite sum

$$\bar{\phi}(r) = \sum_{R_j} \bar{\rho}_j(r - R - s_j),$$

at any point $r$, where $\bar{\rho}_j$ has the same compact support as the site density $\rho_j$. Accordingly on each site domain $\Omega_s$, a Dirichlet boundary problem is derived by the multipole compensations. Extrapolating these boundary conditions to the discussed equation Eq. (6) gives that $\bar{\rho}$ has to vanish at the boundary of a composite compact region. Of course, the in-plane periodicity is kept by means of the r-dependent summation. The solution of a site boundary problem with vanishing potential at the boundaries is not discussed in the paper because it corresponds with the 3D periodic case which is already published in Refs. 2,3.

Accordingly, the Ewald problem shows also the obvious infinite lattice periodicity and carries the finite voltage boundary condition in the surface normal direction. The infinite lattice periodicity allows one to use Fourier expansion for the functions

$$\rho_{Ewald}^j(r) = \sum_{K_{||}} e^{iK_{||} r} \rho_{Ewald}^j(K_{||}, z)$$

and the Ewald problem Eq. (7) is transformed into the reciprocal $K_{||}$ space

$$\frac{d^2}{dz^2} \phi_{Ewald}^j(K_{||}, z) - K_{||}^2 \phi_{Ewald}^j(K_{||}, z) = \rho_{Ewald}^j(K_{||}, z)$$

$$\rho_{Ewald}^j(K_{||}, z) = \frac{1}{U} \sum_{j=1}^d \int_{\mathbb{R}^2} d^2r \, \rho_{Ewald}^j(r - s_j) e^{-iK_{||} r},$$

where $U$ means the volume of the 2D unit cell and $d^2r$ denotes $dxdy$. The structure of the last equation dictates different treatment for $K_{||} = 0$ and $K_{||} \neq 0$. Since the $K_{||} = 0$ Fourier coefficient is a constant in-plane function on the r.h.s. value the $K_{||} = 0$ equation provides the required finite voltage boundary condition whereas all the $K_{||} \neq 0$ solutions vanish at $z = \pm \infty$.

III. SOLUTION OF THE EW ALD PROBLEM

The Ewald boundary problem is defined in the previous section with two subproblems. As mentioned previously the $K_{||} = 0$ case differs notably from the ordinary $K_{||} \neq 0$ case and thus needs a different treatment. The $K_{||} \neq 0$ case contains a non-singular differential operator on the l.h.s. which ensures applicability of the Green function technique in the solution. On the other hand the $K_{||} = 0$ case can be solved by direct integration starting from the charge neutrality condition and using the given boundary conditions.

A. Solution of Eq. (12) for $K_{||} \neq 0$

This equation is a so called 1D modified Helmholtz equation and its Green function reads

$$G(z, \bar{z}) = -\frac{e^{-|z - \bar{z}|K_{||}}}{2K_{||}},$$

including the vanishing boundary conditions at $\pm \infty$, which results a complicated integral for the solution

$$\phi_{Ewald}^j(K_{||}, z) =$$

$$-\sum_j \frac{e^{-|s_j - \bar{r}|K_{||}}}{U} \int_{\mathbb{R}^3} d^3\bar{r} \left( \frac{e^{-|s_j - \bar{r}|K_{||}}}{2K_{||}} \right) \times \phi_{Ewald}^j(\bar{r}) e^{-iK_{||} \bar{r}}.$$  

The difficulty arises with the spherical harmonics expansion of $\phi_{Ewald}^j$, which is the most reasonable choice to have a straightforward solution of the short-range Poisson problem. Here this advantage turns into a troublesome disadvantage because the Green function and the exponential $e^{-iK_{||} \bar{r}}$ are preferably handled in a Cartesian coordinate system.
With the help of the Fourier transform of the Green function corresponding to the \( z - s_jz \) variable,
\[
- \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \ e^{i\omega (z-s_jz)} F(\omega, \bar{z}) = - e^{-\frac{1}{2} |z-s_jz|^2} K_{||},
\]
\[
F(\omega, \bar{z}) = \frac{e^{-i\omega \bar{z}}}{\sqrt{2\pi (\omega^2 + K_{||}^2)}} \quad (15)
\]
one can introduce an \( e^{-i\omega \bar{z}} \) function which can be coupled to the \( e^{-iK_{||} \hat{r}} \) function. The introduction of the new three dimensional vector
\[
K(\omega) = \left( \frac{K_{||}}{\omega} \right) \quad (16)
\]
allows one to make use of the Rayleigh relation
\[
e^{-iK(\omega) \hat{r}} = 4\pi \sum_{L'} (-i)^{\ell} Y_{L'}(K(\omega)) j_{\ell'}(K(\omega) \bar{r}) Y_{L'}^*(\bar{r}), \quad (17)
\]
where \( j_{\ell} \) are the spherical Bessel functions. In this way the problem is transformed into a form that is similar to the 3D periodic case with the only difference that now the third reciprocal direction \( \omega \) is continuous.

Interchanging the order of the Fourier \( \int d\omega \) and the real space integration \( \int d\bar{r} \hat{r} \) and doing a straightforward but lengthy calculation the following equation is resulted
\[
\phi^{\text{Ewald}}(K_{||}, \omega) = - \sum_{jL} \frac{e^{-iK_{||} s_j}}{U} (-i)^{\ell} \frac{K_{||}^2}{\omega} A_{jL} \ell^\ell \times 
\int_{\mathbb{R}} d\omega \frac{\pi Y_L(K_{||} / \omega)}{\Gamma(\ell + \frac{3}{2})} \frac{(K_{||}^2 + \omega^2)^{\ell \omega}^2}{(2\pi)^\ell} e^{-\omega^2 / (4\pi^2)} e^{i\omega (z-s_jz)}.
\quad (18)
\]

Here, the prefactor in the first brackets is dimensionless and the \( \omega \)-integral shows the dimension of length. In the calculation of the \( \omega \)-integral a representation of the spherical harmonics by hypergeometric functions is used. An appropriate choice provides not only a simplified writing of the solution but also a representation that allows an accurate numerical implementation. It is worth to mention that taking any representation of \( Y_L \) in Eq. (18) the \( L = (0, 0) \) case will result the same integral, this case is come down from the Fourier transform of the Green function. According to the handy relations between the spherical angle-coordinates \((\theta, \varphi) = \hat{r}\) and the variables \( K_{||} \) and \( \omega \)

\[
\sin \theta = \frac{K_{||}}{\sqrt{K_{||}^2 + \omega^2}}, \quad \cot \theta = \frac{\omega}{K_{||}},
\]
\[
e^{i\varphi} = \frac{(K_{||} \sin \varphi + iK_{||} \cos \varphi)^m}{K_{||}^m} \quad (19)
\]

the most reasonable choice is given by
\[
-2^{\ell+1} \sqrt{\pi} Y_L(\hat{x}) = \frac{C(\ell, m)}{2^\ell} e^{im\varphi} (\sin \theta)^\ell \times 
\begin{cases}
2F_1 \left( -\frac{\ell - m}{2}, -\frac{\ell + m}{2}, -\frac{\ell - 1}{2}; \frac{1}{\sin \theta} \right) \\
\cot \theta F\left( -\frac{\ell + m}{2}, -\frac{\ell - m}{2}, -\frac{\ell - 1}{2}; \frac{1}{\sin \theta} \right)
\end{cases}
\quad (20)
\]

(see Varshalovich, page 137, Eq.(30)) with the real valued quantity
\[
C(\ell, m) = \frac{2^\ell (-1)^{\ell + m + 1}}{\sqrt{(l + m)!!(l - m)!!(2\ell + 1)}} \quad (21)
\]

where \([\cdots]\) indicates the greatest integer function or floor. \( 2F_1 \) is the hypergeometric function and \((\cdots)!!\) denotes the double factorial defined by
\[
n!! = \begin{cases}
\prod_{n=0}^{n-1} (n - 2) & \text{odd} \\
1 & \text{even}
\end{cases}
\quad (22)
\]

In Eq. (18) the \( A_{jL} \) quantities are calculated by means of the multipole compensation. Experience shows that the quantity \( A_{jL} \) decays quickly with higher \( \ell \) values. This fact enables one to apply a cut-off in the summation which usually has a value of \( \ell_{\text{max}} = 12 \).

For any finite \( \ell \) the hypergeometric functions above terminate after finite number of terms
\[
2\ell^2 e^{\ell}/o = \sum_{k=0}^{k_{\text{max}}(\ell, m)} a_k^{e/o}(\ell, m) K_{||}^{-2k} (K_{||}^2 + \omega^2)^k, \quad (23)
\]
because one of the first two arguments of \( F \) is always a non-positive integer, \( k > 0 \). Here the subscript \( e/o \) distinguishes the even and odd values of \( (\ell + m) \).

The expansion coefficients \( a_k^{e/o}(\ell, m) \) are real with alternating sign and \( k_{\text{max}}(\ell, m) \) is the \( \ell \) and \( m \) dependent termination value, see Table I.

| \( (\ell, m) \) | \( k_{\text{max}}(\ell, m) \) | \( k_{\text{max}}(\ell, m) \) | \( k_{\text{max}}(\ell, m) \) | \( k_{\text{max}}(\ell, m) \) |
|-------------|-----------------|-----------------|-----------------|-----------------|
| (0, 0)      | 0 (3, -3)       | 0 (4, -3)       | 1 (5, -3)       | 1 (5, -3)       |
| (1, -1)     | 0 (3, -2)       | 0 (4, -1)       | 1 (5, -2)       | 1 (5, -2)       |
| (1, 0)      | 0 (3, -1)       | 0 (4, 0)        | 2 (5, -1)       | 2 (5, -1)       |
| (1, 1)      | 0 (3, 0)        | 0 (4, 1)        | 1 (5, 0)        | 2 (5, 0)        |
| (2, -2)     | 0 (3, 1)        | 0 (4, 2)        | 1 (5, 1)        | 2 (5, 1)        |
| (2, -1)     | 0 (3, 2)        | 0 (4, 3)        | 0 (5, 2)        | 1 (5, 2)        |
| (2, 0)      | 0 (3, 3)        | 0 (4, 4)        | 0 (5, 3)        | 1 (5, 3)        |
| (2, 1)      | 0 (4, -4)       | 0 (5, -5)       | 0 (5, 4)        | 0 (5, 4)        |
| (2, 2)      | 0 (4, -3)       | 0 (5, -4)       | 0 (5, 5)        | 0 (5, 5)        |

**TABLE I:** The \( k_{\text{max}}(\ell, m) \) values for \( \ell \in \{1, \ldots, 5\} \). Henceforth the even and odd contributions are treated
separately. The $\omega$-integrals from Eq. (18) with the third
bracketed prefactor are written as

$$I^*= C(\ell, m) e^{i\varphi} P_{lm} K_|| \int d\omega \frac{2 F_k e^{-\omega^2/(4p^2)}}{p^2 + \omega^2} e^{i\omega(z-s_{jz})},$$

$$I^o = C(\ell, m) e^{i\varphi} P_{lm} \int d\omega \frac{2 F_k e^{-\omega^2/(4p^2)}}{p^2 + \omega^2} e^{i\omega(z-s_{jz})},$$

$$P_{lm} = \frac{e^{-K_||^2/(4p^2)}}{2p^2} \left( \frac{K_||}{2p^2} \right)^{\ell-1} (A_j \ell \ell^j). \quad (24)$$

Inserting Eq. (23) into the above integrals results the finite
series

$$2 F_k e^{-\omega^2/(4p^2)} = \frac{e^{-\omega^2/(4p^2)}}{p^2 + \omega^2} + \sum_{n=0}^{k_{max}(\ell, m)-1} K_||^{-2n} \omega^{2n} e^{-\omega^2/(4p^2)} G_e^{o/n}(\ell, m, n) \quad (25)$$

in the integrands, where the $n$-summation comes from the
binomial expansion of $(p^2 + \omega^2)^k$ with $n \geq 0$ and

$$G_e^{o/n}(\ell, m, n) = \sum_{k=0}^{k_{max}(\ell, m)-1} e^{iK_||^2/2p^2} \left( \frac{K_||}{2p^2} \right)^{\ell-1} (A_j \ell \ell^j) \quad (26)$$

To derive Eq. (25) the order of the finite $k$ and $n$
summations is interchanged. After substituting the last two
equations into Eq. (24) a convenient handling,

$$I^* = C(\ell, m) e^{i\varphi} P_{lm} \times \left( I_3(z, j, K_||) + \sum_{n=0}^{k_{max}(\ell, m)-1} \tilde{I}_{2n} G_e^{o/n}(n, L) \right)$$

$$I^o = C(\ell, m) e^{i\varphi} P_{lm} \times \left( I_4(z, j, K_||) + \sum_{n=0}^{k_{max}(\ell, m)-1} \tilde{I}_{2n+1} G_e^{o/n}(n, L) \right) \quad (27)$$

is achieved for the lengthy expressions by introducing
three integrals $I_3, I_4$ and $I_\gamma$, where $\gamma$ can be even or
odd. Taking the values of $k_{max}$ from Table II it turns out
that in the cases of $k_{max}(\ell, m) = 0$ only $I_3$ and $I_4$
provide contributions. These two integrals are defined as

$$I_3(z, j, K_||) = \int d\omega \frac{e^{-K_||^2 z^2/(4p^2)}}{1 + x^2} e^{iK_||^2/(z-s_{jz})} x,$$

$$I_4(z, j, K_||) = \int d\omega \frac{e^{-K_||^2 z^2/(4p^2)}}{1 + x^2} e^{iK_||^2/(z-s_{jz})} x,$$

$$I_\gamma(z, j, K_||) = 2^{\gamma+1} \int d\gamma \gamma! e^{-(K_||^2 y^2/2p^2) + 2iK_||^(z-s_{jz})} y =$$

$$i^\gamma \left( \frac{2p}{K_||} \right)^{\gamma+1} \sum_{t=0}^{\gamma} \left( \begin{array}{c} \gamma \\ t \end{array} \right) (\frac{\gamma}{2t}) \Gamma(t + \frac{1}{2}) (1-t)^{\gamma-2t} \times$$

$$e^{-p^2(z-s_{jz})^2/(p^2 z^2)} (z-s_{jz})^{\gamma-2t}, \quad (29)$$

where $\omega = K_|| x$ is used. They look like a Fourier
transformation which suggests the use of the convolution theorem
of Fourier transformations. The final results of the
integrals are presented in Appendix A. The $I_{2n}$ and $I_{2n+1}$
integrals are treated together by introducing the dimensionless
new variable $y$

$$I_\gamma(z, j, K_||) =$$

From the numerical numerical point of view in the
above sums the the quickly vanishing $A_j$ functions goes ahead and the same upper limits can be
used in the summations,

$$I^o = C(\ell, m) e^{i\varphi} P_{lm} \times$$

$$\sum_{n=0}^{k_{max}(\ell, m)-1} (-1)^n e^{-p^2(z-s_{jz})^2/(p^2 z^2)} \sum_{t=0}^{\gamma-2t} (\frac{2p}{K_||})^{2t+1} \left( \begin{array}{c} \gamma \\ 2t \end{array} \right) \Gamma(t - n + \frac{1}{2}) G_e^{o}(t, L);$$

$$I^o = C(\ell, m) e^{i\varphi} P_{lm} \times$$

$$iC(\ell, m) e^{i\varphi} P_{lm} \times$$

$$\sum_{n=0}^{k_{max}(\ell, m)-1} (-1)^n e^{-p^2(z-s_{jz})^2/(p^2 z^2)} \sum_{t=0}^{\gamma-2t} (\frac{2p}{K_||})^{2t+2} \left( \begin{array}{c} \gamma \\ 2t+1 \end{array} \right) \Gamma(t - n + \frac{1}{2}) G_e^{o}(t, L). \quad (30)$$
The final real valued $K_{||} \neq 0$ Ewald potential can be easily derived from the result
\[
\phi_{Ewald}^{em}(r) = \sum_{j} \sum_{K_{||}} \left( e^{iK_{||}(r-s_j)} \right) e^{-i\pi/2} e^{i\alpha \varphi} \times \]
\[
C(\ell, m) \frac{P_{\ell m}}{U\sqrt{\pi}} \left\{ \begin{array}{ll}
(\phi_3 + \sum_{\alpha} \phi_2 \alpha) & \ell + m \text{ even} \\
(-i\phi_4 - i\sum_{\alpha} \phi_2 \alpha) & \ell + m \text{ odd}
\end{array} \right.
\]
where the two dimensional column vector denotes the real and imaginary components of an arbitrary complex number.

Simpler expressions can be found for the special cases if $(z - s_j) = 0$. It is easily established by symmetry reasons that only for even $\gamma$ gives the integral $\phi_3$ (see Eq. (29)) a non-zero result
\[
\phi_3(z = s_j) = \left( \frac{K_{||}}{2p} \right)^{-\gamma-1} \frac{\Gamma(\frac{\gamma + 1}{2})}{4}.
\]
For the other two integrals $(\phi_3, \phi_4)$ the results can be calculated by using the general expressions given in the Appendix A (see also Gradshteyn, 3.466/1.)
\[
\phi_3(z = s_j) = \pi e^{K_{||}^2/(4p^2)} \operatorname{Erfc} \left( \frac{K_{||}}{2p} \right),
\]
\[
\phi_4(z = s_j) = 0,
\]
which tells that only the even ($\ell + m$) terms contribute.

Easy to check that all the integral results vanish at the boundaries $z = \pm\infty$ which ensures that the final formula fulfills the required boundary conditions.

### B. Solution of Eq. (12) for $K_{||} = 0$

In this section the solution of the boundary problem
\[
\frac{d^2}{dz^2} \phi_{Ewald}(0, z) = \rho_{Ewald}(0, z),
\]
\[
\phi_{Ewald}(0, \pm\infty) = \phi_{Ewald}(0, \mp\infty) = C_2
\]
is looked for, where the Ewald densities are defined through the multipole compensation and $C_2$ refers to the already introduced finite voltage. Taking only the monopole equation
\[
\int_{\mathbb{R}^3} d^3r \left( \rho_j(r - s_j - R) + \rho_{j_{Ewald}}(r - s_j - R) \right) - Z_j = 0
\]

(35)

with the charge neutrality equation
\[
\sum_j \int_{-\infty}^{+\infty} dz \int_{\mathbb{R}^3} dxdy \rho_j(r - s_j - R) - \sum_j Z_j = 0
\]

(36)

the well-known fact of the neutrality of the Ewald density lattice can be derived
\[
\sum_j \int_{\mathbb{R}^3} d^3r \rho_{j_{Ewald}}(r - s_j) = \sqrt{\frac{1}{4\pi}} \sum_j A_{j(0,0)} = 0. \quad (37)
\]

For a 2D periodic system Eq. (37) has the consequence
\[
\int_{-\infty}^{+\infty} dz \rho_{Ewald}(K_{||} = 0, z) = 0, \quad \alpha \in \mathbb{R} \setminus \{0\}
\]

(38)

which can accurately be approximated by a bounded integration range $[D_{low}, D_{up}]$ for well localized Ewald charges. In words, one uses the bounded region where the Ewald charge distribution is non-zero. Integrating Eq. (31) and applying the previous equation results
\[
\int_{D_{low}}^{D_{up}} dx \alpha \left( \frac{dE(z)}{dz} \phi_{Ewald}(0, z) \right) \approx 0. \quad (39)
\]

which yields the boundary behavior of the negative electric field component $E(z) = d\phi_{Ewald}(0, z)/dz$
\[
\int_{D_{low}}^{D_{up}} dx \alpha \left( \int_{D_{low}}^{D_{up}} dz \alpha \frac{dE(z)}{dz} \phi_{Ewald}(0, z) \right) \approx 0.
\]

(40)

Applying the Gauss law outside of this bounded region results the boundary problem for $E$
\[
\frac{dE(z)}{dz} = \rho_{Ewald}(0, z), \quad E(z \leq D_{low}) = \text{const.},
\]
\[
E(z \geq D_{up}) = \text{const.},
\]

(41)

which defines another first order boundary problem for the $K_{||} = 0$ Ewald potential
\[
\frac{d\phi_{Ewald}(0, z)}{dz} = E(z), \quad \phi_{Ewald}(0, z \geq D_{low}) = 0, \quad \phi_{Ewald}(0, z \geq D_{up}) = C_2.
\]

(42)

The finite values at the potential boundaries dictate the $\text{const.}=0$ conditions for $E$. It is worth to mention that applying non-zero constant boundary conditions for $E$ contradicts with the constant behavior of the potential outside of the bounded range $[D_{low}, D_{up}]$.

Both problems can be solved by simple integration which results the final expression
\[
\phi_{Ewald}(0, z) = \frac{1}{2} \left( \int_{D_{low}}^{D_{up}} dz' E(z') - \int_{D_{low}}^{D_{up}} dz' E(z') \right) + C_2
\]

(43)

with explicit inclusion of the potential difference $C_2$.

### C. Evaluation of Eq. (41)

Integrating the boundary problem in Eq. (41) results
\[
E(z') = \frac{1}{U} \sum_{j} \frac{1}{2} \left( \int_{-D}^{D} dz'' \int_{-D}^{D} dz'' \right) \times
\]
\[
\int_{\mathbb{R}^2} dxdy \rho_{j_{Ewald}}(r') Y_L(r')
\]

(44)
with a common $D$, for which $D \to \infty$, and $E$ will satisfy the requirement given by Eq. (33). Unlike in the $K_{||} \neq 0$ case the above integral allows one to use cylindrical coordinates $(\varphi, z^\prime)$. Using the representation of the spherical harmonics (see Varshalovich, page 137, Eq.(33)),

$$Y_L(\hat{r}) = \zeta_{m0} e^{i m \varphi} \sqrt{\frac{2\ell + 1}{4\pi} \frac{(\ell + |m|)!}{(|m|)!}} |m|^{12m} \right] (\tan \theta)^{|m|}$$

$$\cdot \left[ (\cos \theta)^{\ell} F(\text{cosec} \delta) \left] \right] \right]$$

immediately results $2\pi \delta_{m,0}$ for the $\varphi$-integral and simplifies the expression for $E$ to

$$E(z') = \frac{2\pi}{U} \sum_{j \ell} N_LA_j(\ell,0) \sqrt{\frac{2\ell + 1}{4\pi}} \sum_{k=0}^{\ell} \tilde{\alpha}_k(\ell,0)(-1)^k \times$$

$$\frac{1}{2} \left( \int_{-D}^{z'-s_j} dz'' - \int_{z'-s_j}^{+D} dz'' \right) z''(t-2k)e^{-z''^2p^2} \times$$

$$\int_0^{+\infty} dq \, q^{2k+1} e^{-q^2} q^2.$$

Here the hypergeometric function is written again by a finite sum with coefficients $\tilde{\alpha}_k(\ell)$. After some algebraic manipulations with finite $\ell$ summation $E$ is expressed as

$$E(z') = \sum_{j=1}^{d} \sum_{\lambda=0}^{\ell_{\max}} \sum_{k=0}^{\ell_{\max}-\lambda} q_{2\lambda+1,j} C(j,2\lambda+1+2k,k) +$$

$$\sum_{j=1}^{d} \sum_{\lambda=0}^{\ell_{\max}-\lambda} q_{2\lambda,j} C(j,2\lambda+1+2k,k) +$$

$$\sum_{j=1}^{d} \sum_{\lambda=0}^{\ell_{\max}-\lambda} q_{2\lambda+1,j} C(j,2\lambda+1+2k,k) +$$

$$q_{t,j} = \frac{1}{2} \left( \int_{-D}^{z'-s_j} dz - \int_{z'-s_j}^{+D} dz \right) q^3(zp)'e^{-z^2p^2},$$

$$C(j,\ell,k) = \frac{2A_j(\ell,0)p^\ell}{p^2U \sqrt{2\ell+1}} \left[ (\ell) \Gamma(k + \frac{1}{2}) \right] \Gamma(k + \frac{1}{2}).$$

Here, the explicit form of the hypergeometric coefficients $\tilde{\alpha}$ is applied and $C(j,\ell,k)$ is defined as a dimensionless quantity. The one dimensional integral has the dimension of a surface charge $[q_{t,j}] = 1/m^2$. In the expression above the $[\cdots]$ bracketing is used again to denote the floor function.

If $t$ is odd ($t = 2\lambda + 1$)

$$q_{2\lambda+1,j} = \frac{-e^{-(z'-s_j)^2p^2}p^2}{2} \sum_{n=0}^{\ell_{\max}} \lambda!(z'-s_j)p^{2n}$$

(see Gradshteyn, 3.351/2.). For $z' = s_j$ only the $n = 0$ term is non-zero. For even $t$ ($t = 2\lambda$) the result

$$q_{2\lambda,j} = \begin{cases} \lambda = 0 & q_{0,j} = \frac{\pi^{3/2}}{2} \text{Erf}\left((z'-s_j)p\right) \\ \lambda > 0 & q_{2\lambda,j} = f(\lambda)q_{0,j} - \frac{\pi}{2} e^{-(z'-s_j)^2p^2} \times \\ & \sum_{n=1}^{\lambda} \left(f(\lambda)/f(n)\right) ((z'-s_j)p)^{2n-1} \end{cases}$$

is proven in Appendix [18] and expressed with the help of the error function Erf$(\cdots)$ and a gamma function

$$f(\lambda) = \frac{1}{\sqrt{\pi}} \Gamma\left(\lambda + \frac{1}{2}\right) = \left\{ \begin{array}{ll} 1 & \lambda = 0 \\ (2\lambda - 1)!!/2\lambda & \lambda > 0 \end{array} \right.$$

which shows also the identity

$$\sum_{n=0}^{\lambda} f(n) \frac{\lambda^n}{n!} = 2f(\lambda + 1) \quad (51)$$

proven by induction to $\lambda$. This identity is used below in the calculations of the boundary properties of E. Eq.(19) is also valid in the case of $z' = s_j$. Further algebraic manipulations on $E$ leads to the expression

$$E(z') = \sum_{j=1}^{d} \frac{\sqrt{\pi}p^2}{2} \text{Erf}\left((z'-s_j)p\right)P_0(j,p,0) - \sum_{j=1}^{d} \frac{e^{-(z'-s_j)^2p^2}p^2}{2} \sum_{n=0}^{\ell_{\max}} P_n(j,p,n)((z'-s_j)p)^{2n-1},$$

$$- \sum_{j=1}^{d} \frac{e^{-(z'-s_j)^2p^2}p^2}{2} \sum_{n=1}^{\ell_{\max}} P_n(j,p,n)((z'-s_j)p)^{2n-1}. \quad (52)$$
where

\[
P_e(j, p, n) = \frac{2}{n!} \sum_{k=n}^{\left\lceil \frac{\text{max} - 1}{d} \right\rceil} \frac{2A_j(2k+1)(p/2)^{2k+1}}{p^2 U} \frac{\sqrt{\pi}}{\sqrt{4k+3}} \Gamma(2k+2) \left( \sum_{\lambda=n}^{k} \frac{(-1)^{k-\lambda}}{k!} \binom{k}{\lambda} \right) \; ;
\]

\[
P_o(j, p, n) = \frac{1}{f(n)} \sum_{k=n}^{\left\lceil \frac{\text{max}}{d} \right\rceil} \frac{2A_j(2k)(p/2)^{2k}}{p^2 U} \frac{\sqrt{\pi}}{\sqrt{4k+1}} \Gamma(2k+1) \left( \sum_{\lambda=n}^{k} \frac{(-1)^{k-\lambda}}{k!} \binom{k}{\lambda} \right) ;
\]

\[
P_o(j, p, 0) = C(j, 0, 0) = \frac{2A_j(0, 0)}{p^2 U} .
\]

The \(k\) sums above are numerically feasible representations. Summing up \(P_o(j, p, 0)\) from Eq.(53) to all sites \(j\) results zero by the Ewald neutrality Eq.(37). This identity is used to check the boundary properties of \(E\). A detailed justification of the vanishing site sum of \(P_o(j, p, 0)\) starting from Eq.(47) can be found in Appendix C. The whole space integral of \(E\) connects the boundary values of \(\phi_{\text{Ewald}}(0, z)\),

\[
C_2 = \int_{-\infty}^{+\infty} \! dz' E(z') = \lim_{D \to +\infty} \sum_{j=1}^{d} \frac{\sqrt{\pi} p^2}{2} P_o(j, p, 0) \int_{-D}^{+D} \! \text{Erf}(z' - s_jz)p dz' - \\
\frac{p\sqrt{\pi}}{2} \sum_{j=1}^{d} \left[ \sum_{\lambda=0}^{\left\lceil \frac{\text{max} - 1}{d} \right\rceil} \sum_{n=0}^{\lambda} \binom{\lambda}{n} f(n) \right] C(j, 2t + 1, t - \lambda) = -\sqrt{4\pi} \sum_{j=1}^{d} s_jz A_j(0, 0) - \frac{p\sqrt{\pi}}{2} \sum_{j=1}^{d} C(j, 1, 0) = \\
-\frac{\sqrt{4\pi}}{U} \sum_{j=1}^{d} s_jz A_j(0, 0) - \frac{1}{U} \sqrt{\frac{4\pi}{3}} \sum_{j=1}^{d} A_j(1, 0).
\]

and results the value of \(C_2\). For the third sum in the second line one can apply the identity from Eq.(51) and the equation Eq.(C6) from Appendix C.

The equation

\[
\sum_{j=1}^{d} \int \mathbb{R}^3 d^3 r \; z \rho_j(\mathbf{r} - \mathbf{s}_j) = \int_{\mathbb{R}} d z \int_{\mathcal{U}} dx dy \; z \rho(\mathbf{r})
\]

derived by the fact that the Bravais vectors have zero \(z\) components can be used in the \(z\) component dipole compensation. The resulted relation

\[
\int_{\mathbb{R}} d z \int_{\mathcal{U}} dx dy \; z \rho(\mathbf{r}) = -\sqrt{\frac{4\pi}{3}} \sum_{j=1}^{d} A_j(1, 0) + \sum_{j=1}^{d} s_jz Z_j \\
\sqrt{\frac{4\pi}{3}} \sum_{j=1}^{d} s_jz A_j(0, 0) = C_2 U + \sum_{j=1}^{d} s_jz Z_j
\]

expresses the finite voltage \(C_2\) as the \(z\) component slab dipole (surface, area) density and gives the expected macroscopic electrostatics of the system.
The method is based on the pseudo-charge method for Poisson equation for two dimensional periodic systems. It uses a localized site density scheme, which expresses the local electronic site charge densities $\rho$ bounded domains $\Omega$ of the Ewald technique. The proper boundary condition for the slab geometry is written as a locally finite sum. The finite voltage at the infinite boundaries in the yield the multipole freedoms and unambiguously define the Ewald densities of every site. Solutions of the multipole compensation equations compensate the site monopoles but also all higher multipoles by the additional generalized Ewald site densities beyond the Ewald technique, the approach not only results in the correct macroscopic electrostatics, but also allows for self-consistent calculations of the finite voltage. The proper boundary condition for the slab geometry, i.e. the finite voltage at the infinite boundaries in the $z$-direction, results in the correct macroscopic electrostatics. The finite potential difference at the boundaries is expressed by the total dipole (surface, area) density. To our knowledge, the explicit treatment of the general slab boundary conditions presents the most simple and direct way for self-consistent calculations of the finite voltage. The expressions presented here, may easily be applied to the electrostatics of lattices with point-like multipoles for molecular dynamical simulations.

In Appendix B we shortly sketch how our ideas apply to the 1D periodic problem, which differs in methodology from the treatments presented elsewhere, however resulting in the same expressions.

Turning to the calculation of the potential by Eq. (43) one arrives to the final expression

$$
\phi^\text{Ewald}(0, z) = \frac{d}{2} \sum_{j=1}^{d} P_o(j, p, 0) \sqrt{\pi}((z - s_{jz})p) \text{Erf}((z - s_{jz})p) + \frac{d}{2} \sum_{j=1}^{d} P_o(j, p, 0)e^{-(z-s_{jz})^2 p^2}$$

$$- \sum_{j=1}^{d} \sum_{n=0}^{\lfloor \frac{2n+1}{2} \rfloor} \left( f(n)P_e(j, p, n) \right) \frac{P}{4} \sqrt{\pi} \text{Erf}((z - s_{jz})p)$$

$$+ \sum_{j=1}^{d} \sum_{n=1}^{\lfloor \frac{2n+1}{2} \rfloor} \left( f(n)P_e(j, p, n) \right) \frac{P}{4} e^{-(z-s_{jz})^2 p^2} \sum_{t=1}^{n} ((z - s_{jz})p)^{2t-1} f(t)$$

$$+ \sum_{j=1}^{d} \sum_{n=1}^{\lfloor \frac{2n+1}{2} \rfloor} (n-1)!P_o(j, p, n) \frac{P}{4} e^{-(z-s_{jz})^2 p^2} \sum_{t=0}^{n-1} ((z - s_{jz})p)^{2t} \frac{1}{t!} + C_2$$

(A57)

A straightforward calculation leads to the observation that only the first term and the third one in the second line have contribution at the boundaries. The calculation of the boundary values yields the same results what is already calculated in Eq. (43).

V. SUMMARY

The paper proposes a general approach to solve the Poisson equation for two dimensional periodic systems. The method is based on the pseudo-charge method and uses a localized site density scheme, where the total charge density is written as a locally finite sum. The bounded domains $\Omega'_n$ coincide with the compact support of the local electronic site charge densities $\rho_n(r - s_j)$. Going beyond the Ewald technique, the approach not only compensates the site monopoles but also all higher multipoles by the additional generalized Ewald site densities. Solutions of the multipole compensation equations yield the multipole freedoms and unambiguously define the Ewald densities of every site.

The proper boundary condition for the slab geometry, i.e. the finite voltage at the infinite boundaries in the $z$-direction, results in the correct macroscopic electrostatics. The finite potential difference at the boundaries is expressed by the total dipole (surface, area) density. To our knowledge, the explicit treatment of the general slab boundary conditions presents the most simple and direct way for self-consistent calculations of the finite voltage. The expressions presented here, may easily be applied to the electrostatics of lattices with point-like multipoles for molecular dynamical simulations.

APPENDIX A: CALCULATION OF THE $I_3$, $I_4$ INTEGRALS

By the Fourier transformations

$$\frac{1}{\sqrt{2\pi}} \int_R dx \frac{1}{1 + x^2} e^{ix} = \frac{1}{2} \frac{\pi}{e^{i|\tau|}}$$

$$\frac{1}{\sqrt{2\pi}} \int_R dx e^{-\left(\frac{K_{||}}{x^2}\right)^2 x^2} e^{i(\delta - \tau)\bar{x}} = \frac{1}{\sqrt{2}} e^{-i\frac{\xi\tau^2}{K_{||}}}$$

$$\frac{1}{\sqrt{2\pi}} \int_R dx e^{-\left(\frac{K_{||}}{x^2}\right)^2 x^2} e^{i(\delta - \tau)\bar{x}} = \frac{1}{\sqrt{2}} e^{-i\frac{\xi\tau^2}{K_{||}}}$$

(A1)

(see Gradshteyn 3.354/5., 3.323/2., 3.462/2.) where $\delta_j = K_{||} (z - s_{jz})$ and by the convolution theorem one can calculate the required integrals

$$I_3 = \frac{1}{\sqrt{2\pi}} \int_R d\tau \mathcal{F}[f](\tau) \mathcal{F}[g](\delta_j - \tau) = \mathcal{F}[fg](\delta_j) = \frac{\pi}{2} e^{K_{||}^2 / (4\pi^2)} (D(\delta_j) + D(-\delta_j))$$

$$I_4 = i\frac{\pi}{2} e^{K_{||}^2 / (4\pi^2)} (D(\delta_j) - D(\delta_j))$$

(A2)

where

$$D(\delta) = e^{\delta} \text{Erfc}\left(\frac{K_{||}}{2p} + \frac{p\delta}{K_{||}}\right).$$

(A3)

APPENDIX B: CALCULATION OF THE $q_{2\lambda}$ INTEGRAL

Easy to find out the recursive relation

$$q_{2\lambda,j} = -\frac{(z' - s_{jz})^{2\lambda-1}}{2p^2} e^{-(z'-s_{jz})^2 p^2} + \frac{2\lambda - 1}{2p^2} q_{2\lambda-2,j}$$

(B1)
for the needed integral. Using this relation one can forbe the final result presented in Eq.(49) and prove it easily by induction to $\lambda$.

**APPENDIX C: SPECIAL SUMS FOR THE BOUNDARY BEHAVIOR**

The $P_o(j, p, 0)$ quantity is the coefficient of the error function resulted from the integral $\varphi_{2, j, 0}$, see Eq.(47). By this observation one can do the calculation on the following way:

$$
\sum_{j=1}^{d} P_o(j, p, 0) = \sum_{j=1}^{d} \sum_{\lambda=0}^{\lfloor \frac{j}{2} \rfloor} \sum_{k=0}^{\lfloor \frac{j}{2} \rfloor} C(j, 2\lambda + 2k, k) f(\lambda) = \\
\sum_{j=1}^{d} C(j, 0, 0) + \sum_{j=1}^{d} \sum_{\lambda=0}^{\lfloor \frac{j}{2} \rfloor} C(j, 2t\tau - \lambda) \frac{2(2\lambda - 1)!!}{2^\lambda} \\
= \sum_{j=1}^{d} \frac{2A_{j(00)}}{p^2U} + \\
\sum_{j=1}^{d} \sum_{i=1}^{\left( \begin{array}{c} j \\ 2 \end{array} \right) - 1} (-1)^i p^{-3} A_{j(2i0)} \frac{2\pi}{p^2U} \frac{N_{2t}}{\pi^2} \frac{1+t}{4\pi} S(t, \lambda) \\
(C1)
$$

where

$$
S(t, \lambda) = f(\lambda) \tilde{a}_{t-\lambda}(2t)(t-\lambda)!(-1)^\lambda, \\
\tilde{a}_{t-\lambda}(2t) = \prod_{i=0}^{t-\lambda}(t+1+i)(t+\lambda-i) \\
(t+1)(t+\frac{1}{2})(t-\lambda)!(t-\lambda)!
(C2)
$$

The first term in Eq.(C1) vanishes by the charge neutrality conditions stated in Eq.(37). Using the above expression for $\tilde{a}_{t-\lambda}(2t)$ one gets

$$
S(t, 0) = \frac{(2t-1)!!}{2^t}, \quad \lambda = 0 \\
S(t, \lambda) = \frac{(2t-1)!!}{4^t(2t-\lambda)!!}(-1)^\lambda, \quad \lambda > 0
(C3)
$$

and then one can easily establish that

$$
t \text{ is odd: } S(t, \lambda) = -S(t, t-\lambda) \quad \lambda = 0, \ldots, \frac{t-1}{2} \\
t \text{ is even: } S(t, \lambda) = S(t, t-\lambda) \quad \lambda = 0, \ldots, \frac{t}{2} - 1.
(C4)
$$

By this property for odd $t$ it is trivial that the last summation in Eq.(C1) gives zero. For even $t$ ($t = 2\delta$)

$$
\sum_{\lambda=0}^{t} S(2\delta, \lambda) = \frac{(2\delta-1)!!}{4^\delta} + \sum_{\lambda=1}^{2\delta} \frac{(2\delta-1)!!}{4^\delta} \frac{1}{\lambda!} \frac{1}{4^\delta} (-1)^\lambda = \\
\frac{(2\delta-1)!!}{4^\delta} \sum_{\lambda=0}^{2\delta} \left( \frac{2\delta}{\lambda} \right) (-1)^\lambda = 0.
(C5)
$$

Checking the boundary behavior of the Ewald potential in Eq.(51) one needs the equation

$$
\sum_{t=0}^{\lfloor \frac{t \max}{2} \rfloor} \sum_{\lambda=0}^{t} f(\lambda + 1)C(j, 2t + 1, t - \lambda) = C(j, 1, 0)f(1),
(C6)
$$

which can be proven on a similar way given above using the

$$
\tilde{a}_{t-\lambda}(2t + 1) = \prod_{i=0}^{t-\lambda}(t+3/2+i)(t+1+i) \\
(t+1)(t+1/2)(t-\lambda)!(t-\lambda)!
(C7)
$$

expression for the expansion coefficients of the hypergeometric function in Eq.(51).

**APPENDIX D: THE ONE DIMENSIONAL PERIODIC CASE**

This appendix shortly sketches how the method inherited from the above presented treatment apply to the one dimensional periodic case. The general solution, characterized by the multipole moments of the unitcell and based on the Poisson summation formula, is already presented in the literature see Refs.10,11. The Ewald method for point-like Coulomb and dipole-dipole interactions was worked out first by Porto12.

Fourier expansions in the Poisson equation yields the 2D modified Helmholtz equation

$$
\left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} - K^2 \right) \varphi_{\text{Ewald}}(x, y, K) = \rho_{\text{Ewald}}(x, y, K). \\
(D1)
$$

The equation requires different treatments for $K \neq 0$ and for the case of $K = 0$. The $K \neq 0$ case is solved with the help of the Green function

$$
G(K, \rho - \rho') = -\frac{1}{2\pi} K_0(K |\rho - \rho'|), \\
(D2)
$$

where $K_0$ is the modified Bessel function of the second kind ($K_n$) for $n = 0$. Unlike in the 2D periodic case now one can use the Laplace transform of the Green function

$$
\tilde{\varphi}_{\text{Ewald}}(x, y, K) = \left( \frac{1}{2\pi} \right) \times \\
\int_{R^2} dx' dy' \left[ \int_0^{\infty} dt \frac{e^{-K^2 t^2}/4t}{2t} e^{-t(x-x')^2-t(y-y')^2} \right] \\
\sum_{j=1}^{d} \int_{R} dz' \tilde{\rho}_j(x', s_j) e^{-iKz'} \\
(D3)
$$

and then apply the Fourier transforms ($t > 0$ by the Laplace transform)

$$
e^{-t(\tau-\tau')} = \frac{1}{\sqrt{2\pi}} \int_{R} d\omega \frac{e^{-\omega^2t}/(4t)}{\sqrt{2t}} e^{i\omega(\tau-\tau')} \\
(D4)
for the two exponential terms in the bracket. Of course, the \( dt \) integration behind the \( \omega_x \) and \( \omega_y \) integrals can also be executed and results the two dimensional version of Eq. (13), but its calculation turns to difficulties after applying the already introduced multipole shaped Ewald densities. Executing the integrations in a different order

\[
\int_0^\infty dt \int_\mathbb{R} d\omega_x \int_\mathbb{R} d\omega_y \int_\mathbb{R}^3 d^3p' \quad \text{(D5)}
\]

allows one to introduce the Fourier vector \( \mathbf{K}^T(\omega_x, \omega_y) = (\omega_x, \omega_y, K) \) similar to that is used above in Eq. (10). The cylindrical arrangement of the system suggests the application of Eq. (45) to represent the spherical harmonics in cylindrical coordinate system and the solution, according to the assumption of the finite number of non-zero electrostatic multipole moments, is looked for in the form of

\[
\phi_\text{Ewald}(x,y,0) = \sum_{j=1}^d \sum_{\ell,m} A_{j\ell} f_j(\vartheta_j) \zeta_{m0} e^{i\varphi_j}, \quad \text{(D12)}
\]

where \( \zeta_{m0} \) is already introduced by Eq. (14) and \( \vartheta_j = \sqrt{(x-s_{jx})^2 + (y-s_{jy})^2} \). Applying again the appropriate (Eq. (10)) representation of the \( Y_\ell \) functions, the original equation yields a second order linear inhomogeneous ordinary differential equation for \( f_j \),

\[
f_j'' + \frac{1}{\vartheta_j^2} f_j' - \frac{m^2}{\vartheta_j^4} f_j = \frac{N_j}{L} \sqrt{\frac{2\ell + 1}{4\pi} \left( \frac{\ell + |m|!}{(\ell - |m|)! 2|m|} \right)^2} \times \sum_{k=0}^{2\lambda} \tilde{\alpha}_k(\ell, m)(-1)^k e^{-\vartheta_j^2 p^2} q^{2k+|m|} \frac{\Gamma(2k+1)}{p^{2k+1}}, \quad \text{(D13)}
\]

where \( 2\lambda = \ell - 2k - |m| \). Only the mod(\( \ell - |m|, 2 \)) = 0 case has nonzero contribution. The general solutions of the homogeneous equation are

\[
f_{t,0}(\vartheta) = A_0 \log(\vartheta) + B_0, \quad m = 0 \quad \text{and} \quad f_{t,|m|}(\vartheta) = A_m(\vartheta)^{-|m|} + B_m(\vartheta)^{|m|}, \quad |m| > 0 \quad \text{(D14)}
\]

The solutions of the inhomogeneous equation for both \( \ell = 0 \) and \( |m| > 0 \) can be obtained by the constant variation method. For example, for \( m = 0 \)

\[
A_0(\vartheta) = -\frac{1}{L \sqrt{\pi}} e^{-\vartheta^2},
\]

\[
B_0(\vartheta) = \frac{1}{L \sqrt{\pi}} \left( -\frac{\text{Ei}(-\vartheta^2)}{2} + e^{-\vartheta^2} \log(\vartheta) \right) \quad \text{(D15)}
\]

which results

\[
\phi_\text{Ewald}(x,y,K) = \sum_{j=1}^d \frac{q_j}{4\pi L} \left( \Gamma(0, p^2 q_j^2) - \frac{A_0}{4\pi} \log(p^2 q_j^2) \right) \quad \text{(D16)}
\]

by the charge neutrality. Because of the identity (see Gradsteyn & Ryzhik, 8.312/1.)

\[
\Gamma(0, x) - \frac{A_0}{4\pi} \log(x) = -\log(x) \left( 1 + \frac{A_0}{4\pi} \right) - \gamma - \int_0^x dt \frac{e^{-t} - 1}{t}, \quad x > 0, \quad \text{(D17)}
\]

the choice of \( A_0 = -\sqrt{4\pi} \) together with the charge neutrality ensures the required vanishing potential at the infinity (open boundary).
As it is shown above in the simple example the obtained results are the same what are already presented by Langridge and co-workers\textsuperscript{10} or by Porto\textsuperscript{12} but of course, the followed path is methodologically different.

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