2D periodic charge sheets: electrostatics

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1 Motivation

These notes deal with the electrostatics of periodic 2D charge distributions as well as vertically stacked 2D distributions which have the same in-plane periodicity but which may have different charge distributions inside their unit cells. The main mathematical enabler is that the Poisson equation can be solved analytically in the mixed representation of Fourier space for in-plane behavior (g_{xy}) and real space (z) in the normal direction.

The key physical result is is Eq. (3) that gives the electrostatic potential from a single 2D periodic sheet at $z = 0$ evaluated any position x, y, z as a Fourier series over in-plane modes. The contribution of finite wavelength in-plane fluctuations ($g_{xy} \neq 0$) as a function of z going away from the sheet are exponentially suppressed: i.e., the "corrugation" of the charge distribution away from its uniform average only shows up in the near-field close to the sheet. Far away from the sheet, the potential is that of a sheet with uniform charge distribution. Far and near in z are with respect to the in-plane lattice constant setting the length scale.

These results are useful in doing analytical models of electrostatic systems (arrays of charges, dipoles, etc.), modeling interfaces of ionic materials, etc. An example is provided by the $LaAlO_3/SrTiO_3$ (LAO/STO) interface where we have polar/nonpolar materials and one wishes to understand the electrostatics and effects of the surfaces on the interfaces, etc.

2 Mathematical results

2.1 Single 2D periodic sheet

We tart with a single 2D sheet in the xy plane at $z = 0$ which has a periodic charge distribution $\sigma(x, y)$. We separate out the average charge density in a unit cell to be $\bar{\sigma}$ and the remainder (fluctuations or nonhomogeneity) will be written in a Fourier series over the

2D reciprocal lattice vectors $g_{xy} = (g_x, g_y)$:

$$\sigma(x,y) = \bar{\sigma} + \sum_{g_{xy}\neq 0} \hat{\sigma}(g_{xy}) e^{i g_{xy}\cdot r_{xy}} \,. \tag{1}$$

Here $r_{xy} = (x, y)$ is a 2D position in the xy plane. The Fourier components are

$$\hat{\sigma}(g_{xy}) = \frac{1}{A}\int_{u.c.} dx\, dy\, \sigma(x,y) e^{-i g_{xy}\cdot r_{xy}} \tag{2}$$

where A is the unit cell area in the xy plane and the integral is over one unit cell ($u.c.$) in the xy plane. Note that $\bar{\sigma} = \hat{\sigma}(0)$ but we separate out $\bar{\sigma}$ with a different symbol since the $g_{xy} \neq 0$ components behave quite differently.

The corresponding three dimensional charge density is

$$\rho(x,y,z) = \sigma(x,y)\delta(z)\,.$$

We would like to solve the Poisson equation

$$\nabla^2 \phi = -4\pi\rho\,.$$

One can plug the above form into this equation and find for the Fourier transform of ϕ, called $\hat{\phi}$, at wave vector $g = (g_x, g_y, g_z)$

$$\hat{\phi}(g) = \frac{4\pi\hat{\sigma}(g_{xy})}{g_z^2 + g_{xy}^2}\,.$$

The Fourier integral over g_z back to z can be done analytically and one gets the mixed transform

$$\hat{\phi}(g_{xy}, z) = \frac{2\pi\hat{\sigma}(g_{xy}) e^{-|z||g_{xy}|}}{|g_{xy}|}\,.$$

Obviously, there is some problem with $g_{xy} = 0$ which has to be handled separately. For one thing, $\hat{\sigma}(0) = 0$ is absolutely essential which is true sine we separated out the average by hand. The contribution of $\bar{\sigma}$ to the potential is handled here by hand since we know the answer: we have just included the solution of the Poisson equation for a uniform sheet of charge $\bar{\sigma}$ which we know gives a linear potential $-2\pi\bar{\sigma}|z|$. So the complete solution to this problem is

$$\phi(x,y,z) = \phi_0 - 2\pi\bar{\sigma}|z| + \sum_{g_{xy}\neq 0} \frac{2\pi\hat{\sigma}(g_{xy})}{|g_{xy}|} e^{i g_{xy}\cdot r_{xy}} e^{-|z||g_{xy}|} \tag{3}$$

where ϕ_0 is an arbitrary overall constant that reflects the long-range of the Coulomb interaction and ambiguity in determining the overall potential. A main observation is that the part coming from the nonhomogeneity decays exponentially away from the sheet — corrugations die off quickly. The length scale is that of the periodic lattice a (since the smallest $|g_{xy}|$ is $\sim 2\pi/a$).

2.2 A stack of periodic sheets

Now consider a set of parallel sheets indexed by j at positions z_j with periodic charge distributions σ_j sharing the same in-plane periodic lattice. Hence,

$$\rho(x,y,z) = \sum_j \sigma_j(x,y)\delta(z-z_j)\,.$$

Generalizing the above result is straightforward and gives

$$\phi(x,y,z) = \phi_0 - 2\pi\sum_j \bar{\sigma}_j|z-z_j| + \sum_{g_{xy}\neq 0}\frac{2\pi e^{ig_{xy}\cdot r_{xy}}}{|g_{xy}|}\sum_j e^{-|z-z_j||g_{xy}|}\hat{\sigma}_j(g_{xy})\,. \tag{4}$$

2.3 Electrostatic energy of a stack of sheets

The electrostatic energy per unit cell (*u.c.* below) can be written in two equivalent ways:

$$E_H = \int_{u.c.} dx\,dy\int dz\,\frac{|\vec{E}|^2}{8\pi} = \frac{1}{2}\int_{u.c.} dx\,dy\int dz\,\rho\,\phi\,. \tag{5}$$

The second form is easiest to do here since we have expressions for both ρ and ϕ. Doing the algebra gives

$$\begin{aligned} E_H &= \frac{A}{2}\cdot\Bigg[\phi_0\sum_j\bar{\sigma}_j - 2\pi\sum_{j,k}\bar{\sigma}_j\bar{\sigma}_k|z_j-z_k| \\ &\qquad + \sum_{g_{xy}\neq 0}\frac{2\pi}{|g_{xy}|}\sum_{j,k}\hat{\sigma}_j(g_{xy})^*\hat{\sigma}_k(g_{xy})\exp\left(-|g_{xy}||z_j-z_k|\right)\Bigg]\,. \end{aligned} \tag{6}$$

This splits into the overall constant part, the interactions between the average sheet charges only, and self-energy and interactions among the fluctuating parts of the sheet charges. The self-energy is the contributions of $j = k$ in the third term: this is the (positive) energy to assemble the (fluctuating) charge of the sheet — it is not an interaction energy but is intrinsic to that sheet charge itself.

2.4 Net neutral stack of sheets

This simply means that $\sum_j \bar{\sigma}_j = 0$ and thus the arbitrary ϕ_0 contribution to the energy E_H drops out, as it should. We can simplify the above energy expression and also explicitly

separate out the self-energies from the interactions:

$$E_H = \frac{A}{2}\Bigg[-4\pi\sum_{j<k}\bar{\sigma}_j\bar{\sigma}_k|z_j-z_k| + \sum_{g_{xy}\neq 0}\frac{4\pi}{|g_{xy}|}\sum_{j<k}\hat{\sigma}_j(g_{xy})^*\hat{\sigma}_k(g_{xy})\exp\left(-|g_{xy}||z_j-z_k|\right) + \sum_{g_{xy}\neq 0}\frac{2\pi}{|g_{xy}|}\sum_j|\hat{\sigma}_j(g_{xy})|^2\Bigg] . \quad (7)$$

The first two terms are the interaction terms between sheets and the third term is the total self-energy to assemble each sheet separately. The first interaction term is the long-range part (linear part) due to the average sheet densities (same charge pairs repel, opposite charge sheets attract), and the second interaction term is short ranged (exponential damping) interaction between the fluctuations in charge density around their averages. The self-energy is entirely due to the fluctuations since on average (i.e. at long range) a sheet of charge doesn't repel or attract itself.

An example of using such a result is the following. Let us say we are studying LAO/STO (00) and are concerned with the electrostatics of the polar LAO segment. Each consecutive LaO and AlO_2 layer can be modeled as a periodic 2D array of point charges (La^{3+}, Al^{3+}, and O^{2-}). For a polar stoichiometric LAO film, we have net neutrality. Looking at Eq. (7), we see that for a fixed configuration, the interaction of layers separated by more than a few a is given to high accuracy by just the interaction of averaged sheet charges: e.g., the electrostatic effect of the topmost LAO surface layer on the interface is quantitatively given by assuming it is a uniform sheet of charge (instead of at atomic lattice of points) once the film is thicker than a few in-plane a lattice constants.

Next, we might consider doing some ionic exchanges or intermixtures: e.g. swapping some Ti from interface with Al on LAO surface. This can lower the total energy since it will reduce the polar field in the LAO. But we might ask what arrangement of Ti on the surface is best electrostatic ally? And the formula tells us to focus on the self-energy part: the energy to assemble the surface sheet itself is the critical thing to consider to leading order: the best ones minimize opposite charge distances and maximize same charge distances. For example, a square checkerboard pattern of + and - charges is better than lining up all + in a a row and - in the next row (close nearest neighbor same charges). And one can quantitatively compute and compare.

3 Simple examples

3.1 A square lattice of point charges

Consider a square lattice in the xy plane with lattice constant a. Inside each unit cell there is a unit positive point charge. For convenience we put it at the origin and center the square on this point (so the primitive cell spans $-a/2 < x, y < a/2$). As noted above, this unit cell is not charge neutral and thus the Coulombic integrals are ill defined: the value of the Hartree energy E_H can be anything we like since ϕ_0 is completely arbitrary in Eq. (6). Mathematically, this is because the sum over $1/|r_{xy}|$ over a 2D lattice is (infrared or long-ranged) divergent. The remedy is to make the cell neutral so we add a uniform background negative charge of $-1/a^2 = -1/A$. So

$$\sigma(x, y) = \delta(x)\delta(y) - 1/A$$

and we have the simple Fourier transforms

$$\bar{\sigma} = 0 \qquad , \qquad \hat{\sigma}(g_{xy}) = 1/A\,.$$

The Hartree self-energy of this assembly is as per Eq. (7)

$$E_H = \frac{A}{2} \sum_{g_{xy} \neq 0} \frac{2\pi}{A^2 |g_{xy}|} = \frac{\pi}{A} \sum_{g_{xy} \neq 0} \frac{1}{|g_{xy}|}\,.$$

This is also divergent but in the ultraviolet/short range sense: the parts coming from short wavelengths $g_{xy} \to \infty$ are giving a non-converging sum. Being an ultraviolet problem, this is not due to some long range interaction but due to some very small length scale issues. The problem is simple: we've assumed a mathematical point charge and the $|\vec{E}|^2/8\pi$ electrostatic self-energy integral for a point charge is divergent. This is what we see here: the electrostatic repulsive energy to assemble a unit of charge into an infinitely small volume is divergent.

The solution is to make a finite-sized charge instead of a point charge. Since we are in 2D, we will smooth out the point charge into a finite-sized 2D object like a disk. Analytically, a normalized Gaussian is a good choice as integrals with Gaussians are generally easy. So we do the replacement in real space

$$\delta(x)\delta(y) \to \frac{\exp\left[-\frac{(x^2+y^2)}{2\rho^2}\right]}{2\pi\rho^2}$$

which means a Gaussian unit disk of extent ρ. In Fourier space we have

$$\hat{\sigma}(g_{xy}) = \frac{\exp(-|g_{xy}|^2\rho^2/2)}{a^2}\,.$$

The Hartree energy is now

$$E_H = \frac{\pi}{A} \sum_{g_{xy} \neq 0} \frac{\exp(-|g_{xy}|^2\rho^2)}{|g_{xy}|}$$

which is absolutely convergent. This is the total Hartree energy and actually contains a part that is the self-energy of the Gaussian distribution which is not of physical interest and we will deal with it further below.

Just to do some sanity checks, let's consider the limit of $a \to \infty$: the lattice gets very large and the point charges get very separated. In this limit, the mutual interactions between the point charges and backgrounds should go to zero since each unit cell is neutral overall and so the main remaining energy should just be the self-energy to assemble the Gaussian distribution. To see this, let's write things out explicitly with $g_{xy} = 2\pi(m,n)/a$ for integers n and m which we can turn into an integral since $1/a \to 0$:

$$\begin{aligned}
E_H &= \frac{\pi}{A} \sum_{g_{xy}\neq 0} \frac{\exp(-|g_{xy}|^2\rho^2)}{|g_{xy}|} \\
&= \frac{\pi}{A} \sum_{(m,n)\neq(0,0)} \frac{\exp(-(2\pi\rho/a)^2(m^2+n^2))}{(2\pi/a)\sqrt{m^2+n^2}} \\
&= \frac{1}{2a} \sum_{(m,n)\neq(0,0)} \frac{\exp(-(2\pi\rho/a)^2(m^2+n^2))}{\sqrt{m^2+n^2}} \\
&\approx \frac{1}{2a} \int_{-\infty}^{\infty} dm \int_{-\infty}^{\infty} dn \; \frac{\exp(-(2\pi\rho/a)^2(m^2+n^2))}{\sqrt{m^2+n^2}} \\
&\approx \frac{1}{2a} \int_0^{\infty} u\, du \int_0^{2\pi} d\theta \; \frac{\exp(-(2\pi\rho/a)^2 u^2)}{u} \\
&\approx \frac{\pi}{a} \int_0^{\infty} du \; \exp(-(2\pi\rho/a)^2 u^2) = \frac{\sqrt{\pi}}{4\rho}\,.
\end{aligned}$$

As expected, the energy per unit cell for $a \to \infty$ is some constant independent of the size of the cell: this is just the self energy to assemble the Gaussian disk. Also, it scales like $1/\rho$ as expected since the Gaussian charge is of extent ρ and Coulomb's law says the potential is $\sim 1/\rho$ inside the Guassian distribution and there is a unit of charge.

The actual interaction energy we care about for the periodic system with finite a is thus the difference between the integral and the sum:

$$E_H^{int} = E_H(a) - E_H(a\to\infty) = \frac{1}{2a} \sum_{(m,n)\neq(0,0)} \frac{\exp(-(2\pi\rho/a)^2(m^2+n^2))}{\sqrt{m^2+n^2}} - \frac{\sqrt{\pi}}{4\rho}\,.$$

Loosely, we can estimate that this will be $\sim -1/a$ since we expect the main physical interaction is that of a point charge with the uniform background: both are one unit of charge, of opposite sign, and about $1/a$ apart on average. And the background charge in one unit cell screens the point charge so we expect very weak interaction between unit cells. The point of the above formula is that one can calculate it as accurately as needed and take the $\rho \to 0$ limit with no problems.

3.2 Highly anisotropic rectangular array of point charges

Instead of a 1×1 square lattice of point charges (and compensating background), consider the $1 \times M$ unit cell, or more precisely $a \times Ma$, where M is an integer that will become large to give high anisotropy. The limit of huge M is that of a line point charges equally spaced by a along x and the next periodic line is Ma away along y. Thus $A = Ma^2$. What is the Hartree energy for this assembly? Does it converge and under what conditions?

The initial phase of the calculations are identical to the square lattice above. Putting in the actual rectangular unit cell, the Hartree energy is

$$\begin{aligned} E_H &= \frac{\pi}{A} \sum_{g_{xy} \neq 0} \frac{\exp(-|g_{xy}|^2 \rho^2)}{|g_{xy}|} \\ &= \frac{\pi}{Ma^2} \sum_{(m,n) \neq (0,0)} \frac{\exp(-(2\pi\rho/a)^2 (m^2 + n^2/M^2))}{(2\pi/a)\sqrt{m^2 + n^2/M^2}} \\ &= \frac{1}{2Ma} \sum_{(m,n) \neq (0,0)} \frac{\exp(-(2\pi\rho/a)^2 (m^2 + n^2/M^2))}{\sqrt{m^2 + n^2/M^2}} \,. \end{aligned}$$

The difference from the square lattice is the asymmetric treatment of the two axes. For finite M, this is an absolutely convergent sum. To get a better feeling for its behavior for large M, we separate out the $m = 0$ term (long range term along x) from the others:

$$\begin{aligned} E_H &= \frac{1}{2Ma} \left[\sum_{n \neq 0} \frac{\exp(-(2\pi\rho/a)^2 (n/M)^2)}{|n|/M} + \sum_{m \neq 0, n} \frac{\exp(-(2\pi\rho/a)^2 (m^2 + n^2/M^2))}{\sqrt{m^2 + n^2/M^2}} \right] . \\ &= \frac{1}{a} \sum_{n>0} \frac{\exp[-(2\pi\rho/(aM))^2 n^2]}{n} + \frac{1}{Ma} \sum_{m>0, n} \frac{\exp(-(2\pi\rho/a)^2 (m^2 + n^2/M^2))}{\sqrt{m^2 + n^2/M^2}} \,. \end{aligned}$$

What can we say for large M? In the second term, we can turn the sum over n into an integral over n for $M \gg 1$ since the variation of the sum with respect to n is then very small. Calling $u = n/M$, we end with

$$E_H \approx \frac{1}{a} \sum_{n>0} \frac{\exp[-(2\pi\rho/(aM))^2 n^2]}{n} + \frac{1}{a} \sum_{m>0} \int_{-\infty}^{\infty} du \, \frac{\exp(-(2\pi\rho/a)^2 (m^2 + u^2))}{\sqrt{m^2 + u^2}} \,.$$

The second term, the sum over $m > 0$, converges very nicely since the integrand is always bounded from above by $\exp(-(2\pi\rho/a)^2 m^2)/m$ which itself decays very quickly. This is just saying that the short wavelength part of the sum having to do with the energy to assemble the Gaussian disks plus whatever short-range interactions they have along x (the m-direction) converges to a finite answer that doesn't depend on M once M is large enough. Basically, for $m \neq 0$ we are talking about rapid charge fluctuations in the x direction and its interactions with periodic copies Ma away along y are completely suppressed for large M. It is the first term that describes the long range interactions along the x direction expressed as a sum over n which requires more thought.

We can estimate this sum easily: for $M \gg 1$, the exponent term is very close to unity for small n and then we are just summing $1/n$. The exponent starts cutting off the sum once $n \geq aM/(2\pi\rho)$. We are basically summing $1/n$ from one to this number. The sum over $1/n$ from 1 to K is roughly $\ln K$ when we approximate by an integral which is good for large K. So we expect

$$E_H \approx \frac{1}{a} \ln\left(\frac{aM}{2\pi\rho}\right) + \text{constant (something finite in } \rho \text{ and } a)\,.$$

This is logarithmically divergent for $M \to \infty$ which may seem strange at first since we worked so hard to get of all the divergences.

However, there is a physical reason for this having to do with the strange and/or problematic way we've laid out the charges. Each unit cell has a unit point charge at the origin but the compensating negative unit charge is spread uniformly over a very tall and skinny rectangle of dimensions $a \times Ma$; the negative charge density has small areal density $-1/(Ma^2)$. It is only when we are at least Ma far away from the positive point charge that the negative background charge can actually compensate/screen the positive charge and make the sum of the potential from both become small (and thus make our sums convergent). So for distances from the positive charge much smaller that Ma, we expect to just see the potential from the positive charge alone with a very weak contribution from the negative background. Since the Hartree energy of Eq. (5) is the integral over one unit cell of the potential felt from all charges on the charges in that unit cell, we see that the potential in the reference cell (say the origin) is mainly dominated by those within Ma along the x axis in each direction, and these contributions are just basically from unit charges. So we'd expect something like

$$E_H \approx \frac{1}{2}\left[\sum_{j=-M}^{-1} + \sum_{j=1}^{M}\right]\left(\frac{1}{|j|a}\right) \approx \frac{\ln M}{a}\,.$$

The remaining differences with the previous expressions are constants and the fact that we don't have point charges but Gaussian disks, etc. If the compensating negative background charge were more localized about the positive charge, say within a large but fixed distance, then this divergence would go away and we'd again get a finite answer.

3.3 Lattice of point charges above a compensating uniform sheet

We slightly generalize the square lattice result by explicitly consider one sheet of positive point charges in a square lattice at $z_1 = 0$ and a negatively charged uniform sheet which compensates it at $z_2 = d$. So $\bar{\sigma}_1 = -\bar{\sigma}_2 = 1/A = 1/a^2$, $\hat{\sigma}_1(g_{xy}) = 1/A$, and $\hat{\sigma}_2(g_{xy}) = 0$. This could represent a uniform electron gas separated from the electron donors on a surface by some insulating and non polar film.

The Hartree energy of this system is a minor variation of the simple square lattice from above

$$E_H \;=\; \frac{2\pi d}{A} + \frac{\pi}{A}\sum_{g_{xy}\neq 0}\frac{\exp(-|g_{xy}|^2\rho^2)}{|g_{xy}|}\,.$$

Thus, compared to the coplanar square lattice, we just have an extra energy cost of separating two uniform charged sheets of opposite sign by distance d which is linear in d (linear potential or linear volume over which $E^2/8\pi$ is integrated).

3.4 Two parallel lattices of opposite sign (dipole array)

Consider a final system of two sheets of charge that are separated by a distance d. On the top sheet we put Gaussian "point" charges of unit positive charge on a lattice, and on the bottom sheet we put unit negative charges at the same positions — perfect alignment. We can view this as a vertical array of dipoles of magnitude d that are placed on a lattice. So if top sheet has density $\sigma_2(x,y)$, then the bottom sheet has density $\sigma_1(x,y) = -\sigma_2(x,y)$ and

$$-\bar{\sigma}_1 = \bar{\sigma}_2 = 1/A \qquad , \qquad -\hat{\sigma}_1(g_{xy}) = \hat{\sigma}_2(g_{xy}) = \exp(-|g_{xy}|^2\rho^2/2)/A\,.$$

The Hartree energy of Eq. (7), after some minor algebra, becomes

$$E_H = \frac{2\pi d}{A}\cdot\left[1 + \sum_{g_{xy}\neq 0}\frac{(1-e^{-|g_{xy}|d})e^{-|g_{xy}|^2\rho^2}}{d|g_{xy}|}\,.\right]$$

This is very well behaved as the long-range behavior of the summand close to $g_{xy}\to 0$ is finite (instead of diverging like $1/|g_{xy}|$ in the previous examples). This is because our long-range interaction is between dipoles and not point charges and dipole-dipole interactions at long length scales (small $|g_{xy}|$) fall off quite rapidly. For example, the logarithmic divergence in the second example is removed completely since we have a new fixed cutoff distance d (instead of the increasing Ma) to render things well behaved. Extensions to cases where the distributions of charges on the two sheets are Gaussians of different extents is also possible. Also notice that the summand is smooth and well behaved around $g=0$ so we can formally write the sum as

$$E_H = \frac{2\pi d}{A}\cdot\sum_{g_{xy}}\frac{(1-e^{-|g_{xy}|d})e^{-|g_{xy}|^2\rho^2}}{d|g_{xy}|}\,.$$

Let's start with a square lattice of point charges for simplicity so g_{xy} also lies on a square lattice. We will always be taking $\rho \ll a, d$ as a reasonable condition on ρ as we seek the limit of point charges. The two limits that can be treated analytically are (i) $d \ll a$ where the dipoles are quite close compared to the in-plane lattice constant, and (ii) $d \gg a$ where the sheets are well separated compared to the in-plane lattice constant. For the first case

of short dipoles $d \ll a$, the summand is very smooth so we can replace it by an integral remembering that the density of g_{xy} vectors is one per $(2\pi/a)^2 = 4\pi^2/A$ area:

$$E_H = \frac{2\pi d}{A} \cdot \frac{A}{(2\pi)^2} \int_0^\infty 2\pi g \, dg \, \frac{(1-\exp(-gd))\exp(-\rho^2 g^2)}{gd} = \int_0^\infty dg (1-\exp(-gd))\exp(-\rho^2 g^2)\,.$$

The integrand can be split in two: $\exp(-\rho^2 g^2)$ which is a self energy and can be integrated simply as a Gaussian integral and $\exp(-gd - \rho^2 g^2)$ which can be well approximated by $\exp(-dg)$ since $\rho \ll d$, and then that integral is also doable. So

$$\text{When } d \ll a \quad \rightarrow \quad E_H = 2 \cdot \frac{\sqrt{\pi}}{4\rho} - \frac{1}{d}$$

which is two self energies for each sheet separately (per charge) and then the attractive interaction of two point charges of opposite sign a distance d apart. For the second limit of $d \gg a$, we must separate out the $g_{xy} = 0$ term from the sum, and the notice that $\exp(-d|g_{xy}|)$ will be very small for $g_{xy} \neq 0$. So to exponential accuracy we will get

$$\text{When } d \gg a \quad \rightarrow \quad E_H = \frac{2\pi d}{A} + 2 \cdot \frac{\pi}{A} \sum_{g_{xy} \neq 0} \frac{\exp(-\rho^2 |g_{xy}|^2)}{|g_{xy}|}$$

where we have the self-energy of the two separate point charge arrays as the second term and the first is the interaction of two uniform and oppositely charged sheets a distance d apart: for $d \gg a$, the actual layout of the charges on each sheet is not important for their interaction but just their average density (again due to exponential suppression of fluctuations about uniformity).

A second case of interest is the highly anisotropic $1 \times M$ layout from above. As before, we can separate out the $m = 0$ long-range part from $m \neq 0$ to get

$$\begin{aligned} E_H &= \frac{1}{a} \sum_n \frac{(1-\exp\left[-(2\pi d/(aM))|n|\right])\exp[-(2\pi\rho/a)^2 n^2/M^2]}{|n|} \\ &\quad + \frac{2}{Ma} \sum_{m>0,n} \frac{\left(1-\exp\left[-(2\pi d/a)\sqrt{m^2+n^2/M^2}\right]\right)\exp[-(2\pi\rho/a)^2(m^2+n^2/M^2)]}{\sqrt{m^2+n^2/M^2}}\,. \end{aligned}$$

Turning the second sum into an integral with $u = n/M$ for $M \gg 1$ as before then ends with

$$\begin{aligned} E_H &\approx \frac{1}{a} \sum_n \frac{(1-\exp\left[-(2\pi d/(aM))|n|\right])\exp[-(2\pi\rho/(aM))^2 n^2]}{|n|} \\ &\quad + \frac{2}{a} \sum_{m>0} \int_{-\infty}^{\infty} du \, \frac{\left(1-\exp\left[-(2\pi d/a)\sqrt{m^2+u^2}\right]\right)\exp[-(2\pi\rho/a)^2(m^2+u^2)]}{\sqrt{m^2+u^2}}\,. \end{aligned}$$

The second sum is quite well behaved for $m > 0$: it looks like the isolated sheet case when $d \gg a$, and, at any rate, is some constant term with no real strong M dependence. The first term is the long-range part. As usual we assume that $\rho \ll d$. Then the summand has three

different behaviors: (i) for $|n| < aM/(2\pi d)$ it is basically a constant and equal to $2\pi d/(aM)$; (ii) for $aM/(2\pi d) < |n| < aM/(2\pi\rho)$ it is basically $1/|n|$; and (iii) for $|n| > aM/(2\pi\rho)$ it is quite small due to the Gaussian damping. Thus the sum can be approximately done for (i) by just multiplying the value by the number of n contributing and for (ii) by integrating $1/|n|$ over the range of the sum. We end with

$$E_H \approx \frac{2}{a} + \frac{2}{a}\ln(d/\rho) + \text{constant depending on } d/a \text{ and } \rho/a.$$

While the factors of 2 should not be taken completely seriously, the point is that this is well converged and largely independent of M. The logarithmic behavior is no longer of M/ρ but of d/ρ. This reflects the fact that after a distance d from a dipole, the field gets very weak so it is well-behaved at long ranges. In other words, there is a well-defined $M \to \infty$ limit so the system of two lines of parallel dipoles is well-defined.