Additional problem  
for homework #3  

Numerically determine the Madelung constant, to 5 significant figures, for an infinite PLANE of ions of alternating sign, if the plane consists of a 2-d square lattice with a nearest-neighbor distance R.

Some thoughts....

In the text and in class, the Madelung constant, $\alpha$, for an infinite LINE of ions of alternating sign with a nearest-neighbor distance R was determined analytically. A method for calculating it numerically was also present in class.

If the ion of interest is at the origin, the contribution to $\alpha$ from the ions along the x and y axes are identical to the one dimensional problem. The contribution from the remainder of the ions in the four quadrants must now be determined. Adding the contribution from such terms is naturally written as a DOUBLE sum over ... say $i$ and $j$. This series “converges” more slowly than that for one dimension. If you are not careful in how you perform the summation, the double series will appear to diverge (even though it does not!)

Rewrite the double sum as a single sum whose terms alternate in sign. Each of the terms in the single sum must, therefore, represent the contribution from several like charged ions in the two dimensional lattice. The resulting one dimensional series will have alternating terms, and will converge slowly. The convergence of this one dimensional series can be accelerated by using the Padé method.

Note, if one uses multiple Padé sequences, the contribution to $\alpha$ from off-axis ions in one quadrant can be found to 5 significant figures by considering only 28 off-axis ions. If you brute force the double sum, you will have to use so many terms (10’s of thousands of ions or more) in the series, that round-off errors will render your result questionable.