I. A. P. Mathematics Lecture Series 1999

Solutions to the Homework Problems due Friday, January 15, 1999

Lecture 5: *Lattice Inversion Problems with Applications in Solid State Physics*

Martin Bazant, E-mail: bazant@math.mit.edu, Office: 2-339, Phone: 3-1715

1. **Césaro Semigroups.**

$$\varepsilon_m(\varepsilon_n(x)) = a(m)\,(a(n)x) = a(mn)x = \varepsilon_{mn}(x)$$

$$x^{a(mn)} = \left(x^{a(m)}\right)^{a(n)}$$

$$\frac{\left(\frac{x}{1-x\log a(n)}\right)}{1-\left(\frac{x}{1-x\log a(n)}\right)\log a(m)} = \frac{x}{1-x\log a(n)-x\log a(m)} = \frac{x}{1-x\log a(m)a(n)} = \frac{x}{1-x\log a(mn)}$$

$$\begin{aligned}\frac{[xa(n)/\left(1-x(a(n)-1)\right)]a(m)}{1-[xa(n)/\left(1-x(a(n)-1)\right)]\left(a(m)-1\right)} &= \frac{xa(m)a(n)}{1-x\left(a(n)-1\right)-xa(n)\left(a(m)-1\right)}\\ &= \frac{xa(m)a(n)}{1-x\left(a(m)a(n)-1\right)} = \frac{xa(mn)}{1-x\left(a(mn)-1\right)}\end{aligned}$$

Extra Credit: Here's another one:

$$\varepsilon_n(x) = x + \log a(n)$$

Check:

$$(x+\log a(m)) + \log a(n) = x + \log a(m)a(n) = x + \log a(mn)$$

Did you think of a different one?

2. **Two-body inversion on the linear chain $\mathcal{Z}$**

Rewrite the problem

$$\sum_{k=0}^{\infty}(-1)^k f\left((2k+1)x\right) = \frac{1}{x^2}$$

in the Césaro form:

$$\sum_{n=1}^{\infty} a(n)f(nx) = F(x)$$

where $F(x) = 1/x^2$ and

$$a(n) = \begin{cases} (-1)^k & \text{if } n = 2k+1, k = 0,1,2,\ldots \\ 0 & \text{otherwise}\end{cases}$$

Invert:

$$f(x) = \sum_{n=1}^{\infty} a^{-1}(n) F(nx)$$

where $a^{-1}(n)$ is the Dirichlet inverse of $a(n)$.

Claim: $a(n)$ is completely multiplicative.

Proof: $a(mn) = 0 = 0 \cdot a(n) = a(m)a(n)$ if is m is even. If both m and n are odd, $m = 2k+1$ and $n = 2k' + 1$, then

$$a(mn) = a((2k+1)(2k'+1)) = a(2(2kk'+k+k')+1) = (-1)^{2kk'+k+k'} = (-1)^k(-1)^{k'} = a(m)a(n)$$

Therefore, $a^{-1}(n) = a(n)\mu(n)$ by Theorem 3, and the solution is:

$$f(x) = \sum_{n=1}^{\infty} a(n)\mu(n)F(nx) = \sum_{k=0}^{\infty}(-1)^k \mu(2k+1)F((2k+1)x) = \frac{A}{x^2}$$

where

$$A = \sum_{k=0}^{\infty} \frac{(-1)^k \mu(2k+1)}{(2k+1)^2}$$

Now we prove this is really the solution. First we show that the sum actually converges:

$$|A| \leq \sum_{n=1}^{\infty} \left| \frac{a(n)\mu(n)}{n^2} \right| \leq \sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6} < \infty$$

where we note that $|a(n)| \leq 1$ and $|\mu(n)| \leq 1$. Then we show that the absolute convergence condition of Césaro's theorem holds:

$$\sum_{n=1}^{\infty} \sum_{n'=1}^{\infty} |a(n)a^{-1}(n')f(nn'x)| \leq \sum_{n=1}^{\infty} \sum_{n'=1}^{\infty} |f(nn'x)| = \frac{|A|}{x^2} \left(\sum_{n=1}^{\infty} \frac{1}{n^2} \right)^2 \leq \left(\frac{\pi^2}{6} \right)^3 \frac{1}{x^2} < \infty$$

3. **Two-body inversion on the simple cubic lattice $\mathcal{Z}^3$**

(a) To count the number of neighbors $a(n)$ at a distance $\sqrt{n}$ from the origin in $\mathcal{Z}^3$, consider cubes of increasing size centered on the origin. On the cube of side $2 \cdot 1$, there is one point per face at a distance 1, one per edge at $\sqrt{2}$ and one per corner at a distance $\sqrt{3}$. On the cube of side $2 \cdot 2$, there is one point per face (in the center) at 2, four per face (around the center) at $\sqrt{5}$ and also four per face at $\sqrt{6}$. There are no points at $\sqrt{7}$. On the same cube, there is one point per edge at distance $\sqrt{8}$, two per edge at distance $\sqrt{9}$. Be careful: on the next bigger cube of side $2 \cdot 3$, there are more points, one per face (at the center) at distance $\sqrt{9}$. That's it for $n \leq 9$. Since a cube has 6 faces, 12 edges and 8 corners, we have:

n	1	2	3	4	5	6	7	8	9	...
a(n)	6	12	8	6	24	24	0	12	30	...

(b) Use the recursion to get $b(n) = a^{-1}(n)$:

$$\begin{aligned}
b(1) &= \frac{1}{a(1)} = \frac{1}{6} \\
b(2) &= -\frac{a(2)b(1)}{a(1)} = -\frac{1}{3} \\
&\vdots \\
b(8) &= -\frac{a(8)b(1) + a(4)b(2) + a(2)b(4)}{a(1)} = -1 \\
b(9) &= -\frac{a(9)b(1) + a(3)b(3)}{a(1)} = -\frac{29}{54} \\
&\vdots
\end{aligned}$$

n	1	2	3	4	5	6	7	8	9	...
$a^{-1}(n)$	$\frac{1}{6}$	$-\frac{1}{3}$	$-\frac{2}{9}$	$\frac{1}{2}$	$-\frac{2}{3}$	$\frac{2}{9}$	0	-1	$-\frac{29}{54}$	...

(c) The first 8 nonzero terms in the Möbius expansion of $\phi(x)$ (valid for $x > 0$):

$$\phi(x) = \sum_{n=1}^{\infty} a^{-1}(n)e^{-nx^2} = \frac{1}{6}e^{-x^2} - \frac{1}{3}e^{-2x^2} - \frac{2}{9}e^{-3x^2} + \frac{1}{2}e^{-4x^2} - \frac{2}{3}e^{-5x^2} + \frac{2}{9}e^{-6x^2} - e^{-8x^2} - \frac{29}{54}e^{-9x^2} + \ldots$$

Proving this result would be tricky since we don't yet know how to bound $a(n)$ and $a^{-1}(n)$ as $n \to \infty$. If these sequences were known to be bounded, then a rigorous proof using Césaro's theorem) could follow from the observation, $e^{-x} < 1/x$ for all $x > 0$.

4. **Three-body inversion on the square lattice $\mathcal{Z}^2$.** (Extra Credit)

The inversion problem is to find $g(r)$:

$$\sum_{\alpha,\beta \in \mathcal{Z}^2} h(\theta_{\alpha,\beta})g(d_\alpha x)g(d_\beta x) = F(x)$$

where

$$h(\theta) = (1 + \cos\theta)$$

$$F(x) = \begin{cases} (x-1)^4 & \text{if } 0 < x < 1 \\ 0 & \text{if } x \geq 1 \end{cases}$$

- $x \geq 1$. In this region, $F(x) = 0$. Since $d_\alpha \geq 1$ for all $\alpha \in \mathcal{Z}^2$, $d_\alpha x > 1$ when $x \geq 1$. Therefore we must have:

  $$g(x) = 0, \quad \text{for} \quad x \geq 1$$

  i.e. $g(x)$ will have a "finite cutoff". As the lattice spacing x is reduced, neighbors will enter the cutoff and successively make new contributions to the sum...

- $1/\sqrt{2} \leq x < 1$. In this region, the (four) first neighbors of the origin, at a distance $r(1)x = x$ are close enough to the origin to interact with a nonzero contribution to the sum. However, second neighbors at a distance $r(2)x = \sqrt{2}x \geq 1$ are not. So, for these values of x the sum reduces to this:

  $$a(1,1)g(x)^2 = (x-1)^4, \quad 1/\sqrt{2} \leq x < 1$$

  where

  $$a(1,1) = \sum h(\theta_{\alpha,\beta}) = 4h(\pi/2) + 2h(\pi) = 8$$

  since there are 4 90° and 2 180° angles subtended by bonds with the four atoms in the first shell. Therefore,

  $$g(x) = (x-1)^2/\sqrt{8}, \quad 1/\sqrt{2} \leq x < 1$$

  Note that no iteration is necessary.

- $1/2 \leq x < 1/\sqrt{2}$. Now the (four) second neighbors are also within the cutoff since $r(2)x = \sqrt{2}x \geq \sqrt{2}/2 > 1/2$, but not the (four) third neighbors $r(3) = 2x$. So, in this case we have (following the rearrangement of the sum given in the lecture notes):

  $$a(1,1)g(x)^2 + a(1,2)g(x)g(\sqrt{2}x) + a(2,2)g(\sqrt{2}x)^2 = (x-1)^4$$

  where

  $$a(1,2) = 8h(\pi/4) + 8h(3\pi/4) = 16$$
  $$a(2,2) = a(1,1) = 8.$$

  Plugging in these values

  $$8(g(x) + g(\sqrt{2}x))^2 = (x-1)^4$$

  we get the recursion for $g(x)$:

  $$g(x) = (x-1)^2/\sqrt{8} - g(\sqrt{2}x)$$

  We iterate once, and the recursion terminates because $2x > 1$,

  $$\begin{aligned} g(x) &= (x-1)^2/\sqrt{8} - (\sqrt{2}x-1)^2/\sqrt{8} + g(2x) \\ &= (x-1)^2/\sqrt{8} - (\sqrt{2}x-1)^2/\sqrt{8}, \quad 1/2 \leq x < 1/\sqrt{2} \end{aligned}$$

Note that $g(x)$ is a continuously differentiable sum of parabolae with discontinuous second derivatives (where new parabolic terms for successive shells enter as x is decreased) at the set of points $\{1/\sqrt{n}, n \in \mathcal{N} | a(n) \neq 0\}$.