I. A. P. Mathematics Lecture Series 1999
Notes for 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

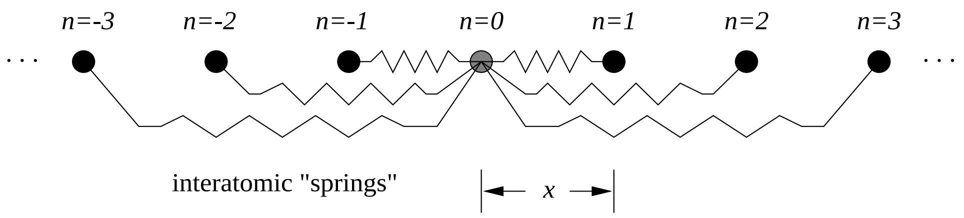

Figure 1: The linear-chain crystal lattice $\mathcal{Z}$.

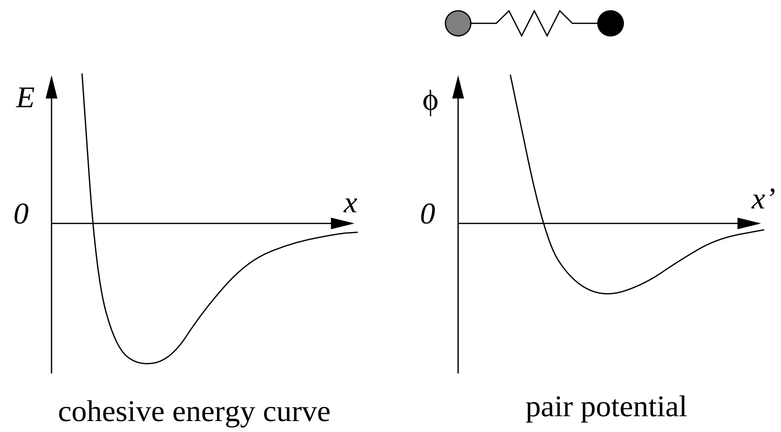

Figure 2: A typical curve of cohesive energy E versus first neighbor spacing x and the associated pair potential ("spring energy") ϕ versus distance x'.

1 Introduction to Two-Body Lattice Inversion

Example 1 *The linear chain $\mathcal{Z}$.* (N.-X. Chen 1990, P. L. Chebychev, 1851)

$$E(x) = \sum_{n=1}^{\infty} \phi(nx)$$

The total energy per atom $E(x)$ is assumed to be a sum of (unknown) "spring energies" $\phi(|nx|)$, evaluated at the crystal lattice points nx, $n = \pm1, \pm2, \pm3, \ldots$. Solve for $\phi(x)$.

Example 2 *A "charged" linear chain.*

$$E(x) = \sum_{n=1}^{\infty} a(n)\phi(nx)$$

Idea: (A. F. Möbius, 1832) Assume

$$\phi(x) = \sum_{n=1}^{\infty} b(n)E(nx)$$

and find $b(n)$.

$$\begin{aligned}
E(x) &= a(1)\phi(x) + a(2)\phi(2x) + a(3)\phi(3x) + \dots \\
E(2x) &= a(1)\phi(2x) + a(2)\phi(4x) + a(3)\phi(6x) + \dots \\
E(3x) &= a(1)\phi(3x) + a(2)\phi(6x) + a(3)\phi(9x) + \dots \\
&\vdots
\end{aligned}$$

$$\begin{aligned}
\phi(x) &= b(1)E(x) + b(x)E(2x) + b(3)E(3x) + \dots \\
&= a(1)b(1)\phi(x) \left.\begin{array}{l} +a(2)b(1) \\ +a(1)b(2) \end{array}\right| \cdot\phi(2x) \left.\begin{array}{l} +a(3)b(1) \\ +a(1)b(3) \end{array}\right| \cdot\phi(3x) \left.\begin{array}{l} +a(4)b(1) \\ +a(2)b(2) \\ +a(1)b(4) \end{array}\right| \cdot\phi(4x) \\
&\quad \left.\begin{array}{l} +a(5)b(1) \\ +a(1)b(5) \end{array}\right| \cdot\phi(5x) \left.\begin{array}{l} +a(6)b(1) \\ +a(3)b(2) \\ +a(2)b(3) \\ +a(1)b(6) \end{array}\right| \cdot\phi(6x) + \dots
\end{aligned}$$

Equate coefficients of $\phi(nx)$:

$$\begin{aligned}
a(1)b(1) &= 1 \\
a(2)b(1) + a(1)b(2) &= 0 \\
a(3)b(1) + a(1)b(3) &= 0 \\
a(4)b(1) + a(2)b(2) + a(1)b(4) &= 0 \\
&\vdots
\end{aligned}$$

$$\sum_{d|n} a(d)b(n/d) = I(n) = \begin{cases} 1 & \text{if } n = 1 \\ 0 & \text{if } n > 1 \end{cases}$$

Solve recursively for $b(n)$, if $a(1) \neq 0$:

$$\begin{aligned}
b(1) &= \frac{1}{a(1)} \\
b(2) &= -\frac{1}{a(1)}\,[a(2)b(1)] \\
b(3) &= -\frac{1}{a(1)}\,[a(3)b(1)]
\end{aligned}$$

$$
\begin{aligned}
b(4) &= -\frac{1}{a(1)}\left[a(4)b(1)+a(2)b(2)\right] \\
&\vdots \\
b(n) &= -\frac{1}{a(1)}\sum_{d|n,d<n} a(n/d)b(d)
\end{aligned}
$$

Back to Example 1:
$a(n) = 1 \equiv u(n)$ = "unit function"
$b(n) \equiv \mu(n)$ = "Möbius function"

n	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	...
$\mu(n)$	1	-1	-1	0	-1	1	-1	0	0	1	-1	0	-1	1	1	...

What is the pattern?

2 Background from Number Theory

Definition 1 *An* **arithmetical function** $a(n)$ *is a mapping from the positive integers to the real or complex numbers.*

Definition 2 *The* **Dirichlet product** *of two arithmetical functions is given by*

$$(a * b)(n) = \sum_{d|n} a(n/d)b(d).$$

One can show $a * (b * c) = (a * b) * c$, $a * b = b * a$ and $I * a = a$ (so $I(n)$ = "identity"). The set of arithmetical functions with $*$ forms a "group".

Definition 3 *If* $a(1) \neq 0$, *then the* **Dirichlet inverse** *of* $a(n)$ *denoted* $a^{-1}(n)$ *is defined by* $a * a^{-1} = I$.

Existence and uniqueness of $a^{-1}(n)$ is established by the recursion for $b(n)$ above, if $a(1) \neq 0$.

Theorem 1 (Möbius Inversion Formula) *If* $a(1) \neq 0$,

$$\sum_{d|n} a(n/d)f(d) = F(n) \quad \Rightarrow \quad f(n) = \sum_{d|n} a^{-1}(n/d)F(d)$$

PROOF: $a^{-1} * F = a^{-1} * (a * f) = (a^{-1} * a) * f = I * f = f$. $\square$

Definition 4 *If* $a(mn) = a(m)a(n)$ *for relatively prime integers* m *and* n *(with greatest common factor* 1*), the* $a(n)$ *is said to be* **multiplicative**.

Theorem 2 *An explicit formula for the* **Möbius function** $\mu \equiv u^{-1}$ *is:*

$$\mu(n) = \begin{cases} 1 & \textit{if } n = 1 \\ (-1)^k & \textit{if } n \textit{ is a product of } k \textit{ distinct primes} \\ 0 & \textit{if } n \textit{ is divisible by a square} \end{cases}$$

PROOF: (Laguerre,1874) We must show $(\mu * u)(n) = I(n)$ with this formula for $\mu(n)$. The case $n = 1$ is trivial, $\sum_{d|1} \mu(d) = \mu(1) = 1$. For $n > 1$, let the prime decomposition of n be $p_1^{\alpha_1} \cdots p_k^{\alpha_k}$. Observe that the sum of the divisors of n can be written as the following product, $\sum_{d|n} d = \prod_{i=1}^{k} (1 + p_i + p_i^2 + \ldots + p_i^{\alpha_i})$. From the definition, $\mu(n)$ is multiplicative, $\Rightarrow \sum_{d|n} \mu(d) = \prod_{i=1}^{k} [\mu(1) + \mu(p_i) + \mu(p_i^2) + \ldots + \mu(p_i^{\alpha_i})] = \prod_{i=1}^{k} (1 - 1 + 0 \ldots + 0) = 0.$ □

Solution to Example 1:

$$\phi(x) = \sum_{n=1}^{\infty} \mu(n) E(nx)$$

Solution to Example 2:

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

Definition 5 *If* $a(mn) = a(m)a(n)$ *for all* $m, n \geq 1$*, then* $a(n)$ *is said to be* **completely multiplicative**.

It is usually very difficult to derive explicit formulae for $a^{-1}(n)$, except ...

Theorem 3 *If* $a(n)$ *is completely multiplicative, then* $a^{-1}(n) = a(n)\mu(n)$.

PROOF: $\sum_{d|n} a(n/d)a(d)\mu(d) = a(n)\sum_{d|n} \mu(d) = a(n)\sum_{d|n} u(n/d)\mu(d) = a(n)(u * \mu)(n) = a(n)I(n) = I(n)$, where in the last step we note that $a(1) = 1$. □

Example 3 *Solve for* $f(x)$*:*

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

Solution: Because $(mn)^s = m^s n^s$:

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

What conditions are needed to *prove* such a formula?
How can the Möbius/Chebychev trick be generalized?

Definition 6 *The set of functions* $\{\varepsilon_n(x)\}$ *is called a* **Césaro semigroup** *if it is closed under composition, i.e.* $\varepsilon_{mn}(x) = \varepsilon_m(\varepsilon_n(x))$ *for all* $m, n \in \mathcal{N}$ *and* $x \in \Re$*. Note that* $\varepsilon_1(x) = x$*.*

Theorem 4 (Césaro, 1885) *Let $\{\varepsilon_n(x)\}$ be a Césaro semigroup. If*

$$\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}|a(m)a^{-1}(n)f(\varepsilon_{mn}(x))| < \infty, \quad x \in \Re$$

and $a(1) \neq 0$, then

$$\sum_{n=1}^{\infty} a(n)f(\varepsilon_n(x)) = F(x), \quad \Rightarrow \quad f(x) = \sum_{n=1}^{\infty} a^{-1}(n)F(\varepsilon_n(x)).$$

PROOF:

$$\begin{aligned}
\sum_{n=1}^{\infty} a^{-1}(n)F(\varepsilon_n(x)) &= \sum_{n=1}^{\infty} a^{-1}(n)\sum_{n'=1}^{\infty} a(n')f(\varepsilon_{n'}(\varepsilon_n(x))) \\
&= \sum_{n=1}^{\infty}\sum_{n'=1}^{\infty} a^{-1}(n)a(n')f(\varepsilon_{nn'}(x)) \\
&= \sum_{m=1}^{\infty}\left(\sum_{n|m} a^{-1}(n)a(m/n)\right) f(\varepsilon_m(x)) \qquad (m = nn') \\
&= \sum_{m=1}^{\infty} I(m)f(\varepsilon_m(x)) \\
&= f(\varepsilon_1(x)) = f(x)
\end{aligned}$$

where the absolute convergence condition justifies rearranging the summation. □

Example 4 *(Möbius, 1832) Solve for $f(x)$:*

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

Solution: Since $(x^m)^n = x^{mn}$,

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

A Proof of Example 1: If there exist $M > 0, s > 1$ such that $|\phi(x)| < M/x^s$, then

$$\sum_{n=1}^{\infty}\sum_{n'=1}^{\infty}|u(n)\mu(n')\phi(nn'x)| \leq \sum_{n=1}^{\infty}\sum_{n'=1}^{\infty}|\phi(nn'x)| < \frac{M}{x^2}\left(\sum_{n=1}^{\infty}\frac{1}{n^s}\right)^2 < \infty$$

3 Two-Body Inversion in Higher Dimensions

For a general crystal lattice $\mathcal{L}$:

$$E(x) = \sum_{\alpha\in\mathcal{L}} \phi(d_\alpha x)$$

where the sum excludes the origin and d_α is the distance from the origin to α. To simplify, group $\{d_\alpha x\}$ into "**shells**" of radius $r(n)$ containing $a(n)$ neighbors, $n \in \mathcal{N}$, with $r(1) = 1$:

$$E(x) = \sum_{n=1}^{\infty} a(n)\phi(r(n)x)$$

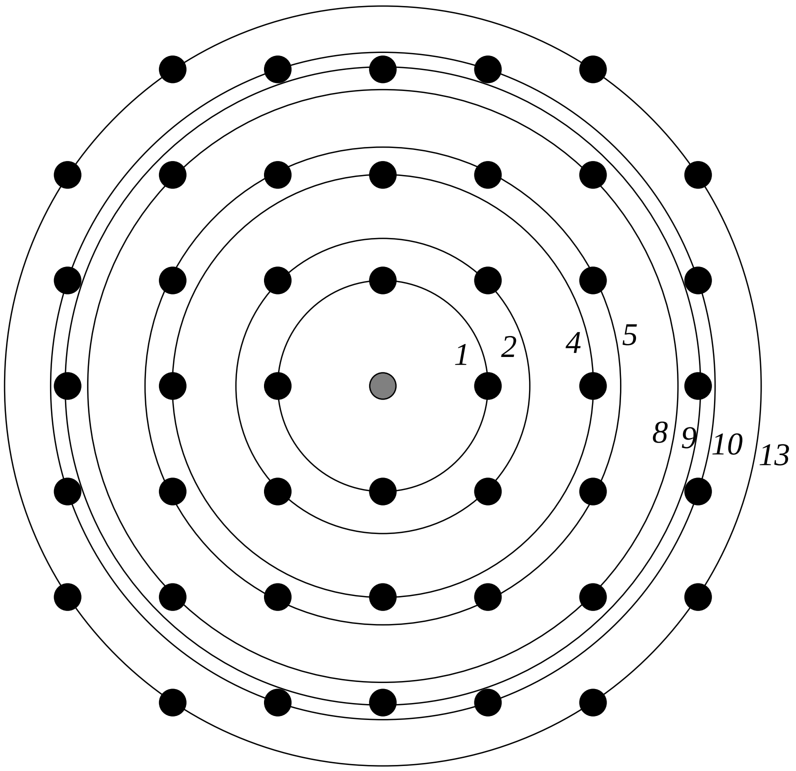

Figure 3: Neighbors of the origin in $\mathcal{Z}^2$ grouped into shells of radius $\sqrt{n}$ for $n = 1, 2, 4, 5, 8, 9, 10, 13, \ldots$.

Example 5 *Solve for $\phi(x)$ with $E(x) = 1/x^6$ on the square lattice $\mathcal{Z}^2$.*

Solution: Since $d_{(i,j)} = \sqrt{i^2 + j^2}$,

$$\begin{aligned} E(x) &= 4\sum_{i=0}^{\infty}\sum_{j=1}^{\infty} \phi(\sqrt{i^2 + j^2}x) \\ &= 4\sum_{n=1}^{\infty} a(n) f(\sqrt{n}x) \end{aligned}$$

where

n	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	...
$a(n)$	1	1	0	1	2	0	0	1	1	2	0	0	2	0	0	...

Since $r(n) = \sqrt{n}$ is completely multiplicative, use Césaro's theorem:

$$\phi(x) = \frac{1}{4}\sum_{n=1}^{\infty} a^{-1}(n) E(\sqrt{n}x)$$

Compute the Dirichlet inverse $a^{-1}(n) = 1, -1, 0, 0, -2, 0, 0, 0, -1, 2, \ldots$ to obtain the solution:

$$\phi(x) = \frac{1}{4}\sum_{n=1}^{\infty} \frac{a^{-1}(n)}{n^3 x^6} = \frac{1}{4x^6}\left(1 - \frac{1}{2^3} - \frac{2}{5^3} - \frac{1}{9^3} + \frac{2}{10^3} + \ldots\right)$$

Problem: If $r(n)$ is not completely multiplicative, then Césaro's theorem does not apply! However, an inversion formula still exists (Carlsson, Gelatt, Ehrenreich, 1980, Bazant, 1995).

Theorem 5 *Under certain technical conditions, if $a(1) \neq 0$, then the pair potential problem can be solved for any crystal lattice by the recursion:*

$$\phi(x) = \frac{1}{a(1)}\left[E(x) - \sum_{n=2}^{\infty} a(n)\phi(r(n)x)\right]$$

or the explicit formula:

$$\phi(x) = \frac{E(x)}{a(1)} - \sum_{n=2}^{\infty}\frac{a(n)E(r(n)x)}{a(1)^2} + \sum_{n=2}^{\infty}\sum_{n'=2}^{\infty}\frac{a(n)a(n')E(r(n)r(n')x)}{a(1)^3} - \ldots$$

4 Three-Body Inversion

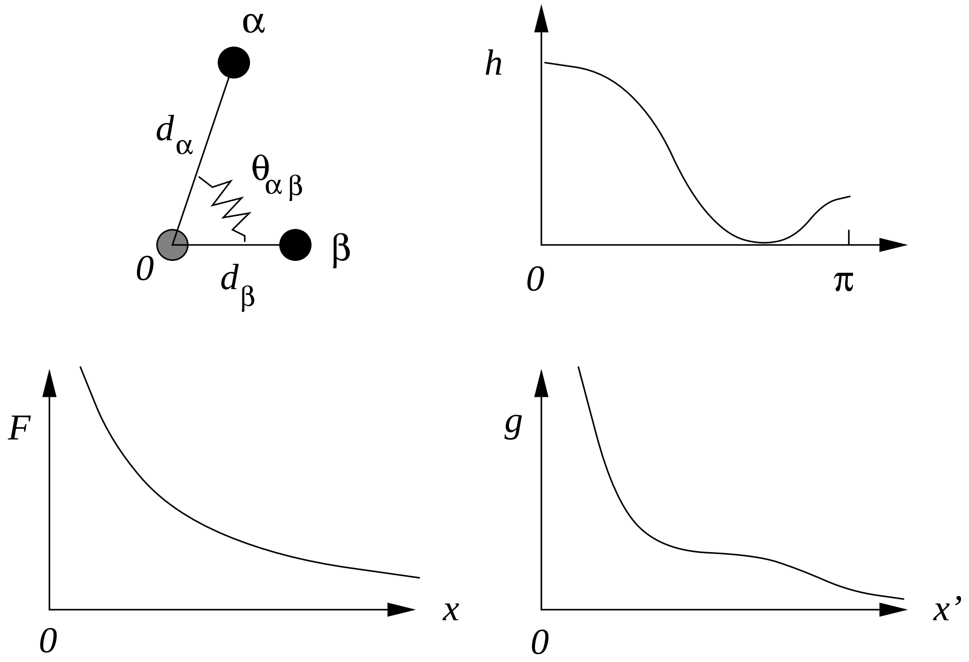

Figure 4: Two neighbors of the origin α and β coupled by an "angular spring" and typical plots of the angular function $h(\theta)$, the many-body energy $F(x)$ and the (unknown) radial function $g(x')$.

A real material possesses *many-body* interactions, i.e. "springs" involving three or more atoms at a time. For example, "covalent bonds" are often modeled by a three-body potential:

$$\sum_{\alpha,\beta} h(\theta_{\alpha,\beta})g(d_\alpha x)g(d_\beta x) = F(x)$$

where $\theta_{\alpha,\beta}$ is the angle between α and β subtended at the origin, $h(\theta)$ is the "angular function" (spring favoring certain angles), $g(x)$ is the "three-body radial function" (controling the strength of angular spring), and $F(x)$ is the "three-body energy". For example, the angle θ_o is favored with the choice,

$$h(\theta) = (\cos\theta - \cos\theta_o)^2$$

To simplify, group lattice points into shells as before:

$$F(x) = \sum_{m=1}^{\infty}\sum_{n=m}^{\infty} a(m,n)g(r(m)x)g(r(n)x)$$

where

$$\begin{aligned} a(m,n) &= \sum_{d_\alpha=r(m),d_\beta=r(n)} h(\theta_{\alpha,\beta}) \text{ if } m<n \\ &= \sum_{d_\alpha=d_\beta=r(n),\alpha<\beta} h(\theta_{\alpha,\beta}) \text{ if } m=n \end{aligned}$$

Problem: The inversion problem for $g(x)$ is **nonlinear**, and hence Césaro can't help! However, recursion still works (Bazant, 1995).

$$F(x) = a(1,1)g(x)^2 + A[g](x)g(x) + B[g](x)$$

where

$$\begin{aligned} A[g](x) &= \sum_{n=2}^{\infty} a(1,n)g(r(n)x) \qquad (m=1, n>1) \\ B[g](x) &= \sum_{m=2}^{\infty}\sum_{n=m}^{\infty} a(m,n)g(r(m)x)g(r(n)x) \qquad (m>1, n\geq m) \end{aligned}$$

Theorem 6 *If a (positive) solution exists to the three-body potential inversion problem, it is given by the recursion:*

$$g(x) = \frac{1}{2a(1,1)}\left(-A[g](x) + \sqrt{A[g](x)^2 - 4a(1,1)B[g](x)}\right)$$

This formula is difficult to evaluate by hand, but it's no problem for a computer!

Hint: On the homework (problem 4), the recursion terminates after only a few iterations since $F(x)$ has a "**finite cutoff**": $F(x) = 0$ for $x > 1$.