The general method to solve the inverse lattice problems in physics

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Abstract

By a system of linear equations on a multiplicative semigroup, we present a general mathematical method to determine the interatomic potential of various lattice structures in order to compute the performances of materials, and show the relation between the method and the Möbius inversion. © 2003 Elsevier Science (USA). All rights reserved.

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1. Introduction

The mathematical model of inverse lattice problem is to determine the pair potential \( \Phi(x) \) between atoms from the summation

\[
E(x) = \frac{1}{2} \sum_{n=1}^{\infty} r(b_n) \Phi(b_n x).
\]

Here \( x \) is the lattice constant, \( E(x) \) is the cohesive energy for each atom in a crystal lattice, \( b_n \) is the distance from a lattice point to the origin, \( r(b_n) \) is the number of lattice points whose distance to the origin is equal to \( b_n \), and \( \{b_n\} \) and \( \{r(b_n)\} \) are determined by the structure of the actual crystal. This model was proposed by Carlsson et al. [1]. Chen et

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al. have solved the one-dimensional and two-dimensional inverse lattice problems by the Möbius inversion [2–4]. Much work has been done for some three-dimensional inverse lattice problems [5–7], but the methods used are very complex and cannot be used in all the lattice structures. Further, the results for some three-dimensional lattice structures are wrong because the three-dimensional lattices do not satisfy the semigroup condition, and we have to deal with the inversion problems of summations with unequally weighted terms.

In this paper, the general method, based on constructing a system of linear equations on a multiplicative semigroup, is presented to solve all the inverse lattice problems, and show the relation between the method and the Möbius inversion formula.

2. The system of linear equations on multiplicative semigroup

Let \( f(x) \), \( g(x) \) be the functions defined on \( x > 0 \) and satisfy the equation

\[
g(x) = \sum_{n=1}^{\infty} \lambda(\alpha_n) f(\alpha_n x),
\]

where the function \( g(x) \) and the sequences \( \{\lambda(\alpha_n)\}, \{\alpha_n\} \) are known. (2) is a summation with unequally weighted terms, and we shall solve the function \( f(x) \) from (2).

If the sequence \( P = \{\alpha_n\} \) satisfies the following conditions:

(i) For any \( \alpha_n, \alpha_m \in P \), the product \( \alpha_n \alpha_m \in P \);

(ii) \( \{\alpha_n\} \) is a monotonic increasing sequence with \( \alpha_1 = 1 \), i.e., \( 1 = \alpha_1 < \alpha_2 < \cdots < \alpha_n < \alpha_{n+1} < \cdots \),

then \( P \) is called a semigroup sequence because \( P \) is a multiplicative semigroup by (i).

We conclude that if \( P = \{\alpha_n\} \) in (2) is a semigroup sequence and \( \lambda(\alpha_1) \neq 0 \), then Eq. (2) has a unique solution \( f(x) \).

The proof is based on constructing a system of linear equations.

From (2), for any \( \alpha_m \in P \), we have

\[
g(\alpha_mx) = \sum_{n=1}^{\infty} \lambda(\alpha_n) f(\alpha_n \alpha_mx).
\]

Since \( P \) is a multiplicative semigroup, then \( \alpha_n \alpha_m \in P \). We define

\[
\lambda\left(\frac{\alpha_k}{\alpha_m}\right) = \lambda_{mk} = \begin{cases} \lambda(\alpha_n) & \text{when } \alpha_k/\alpha_m = \alpha_n \in P, \\ 0 & \text{when } \alpha_k/\alpha_m \notin P. \end{cases}
\]

So (3) can be expressed as

\[
g(\alpha_mx) = \sum_{k=1}^{\infty} \lambda\left(\frac{\alpha_k}{\alpha_m}\right) f(\alpha_k x),
\]

i.e.,

\[
g(\alpha_mx) = \sum_{n=1}^{\infty} \lambda\left(\frac{\alpha_n}{\alpha_m}\right) f(\alpha_n x) = \sum_{n=1}^{\infty} \lambda_{mn} f(\alpha_n x).
\]
We write $g(\alpha mx), f(\alpha nx)$ simply as $g_m, f_n$, respectively, and write (5) as
\[ g_m = \sum_{n=1}^{\infty} \lambda_{mn} f_n \quad (m = 1, 2, 3, \ldots), \] (6)
which is a system of linear equations with infinite equations. This system of linear equations can be expressed as the form of infinite matrix
\[
\begin{pmatrix}
g_1 \\
g_2 \\
g_3 \\
\vdots \\
g_m \\
\vdots
\end{pmatrix} =
\begin{pmatrix}
\lambda_{11} & \lambda_{12} & \lambda_{13} & \ldots & \lambda_{1n} & \ldots \\
\lambda_{21} & \lambda_{22} & \lambda_{23} & \ldots & \lambda_{2n} & \ldots \\
\lambda_{31} & \lambda_{32} & \lambda_{33} & \ldots & \lambda_{3n} & \ldots \\
\vdots & \vdots & \vdots & \ddots & \vdots & \ddots \\
\lambda_{m1} & \lambda_{m2} & \lambda_{m3} & \ldots & \lambda_{mn} & \ldots \\
\vdots & \vdots & \vdots & \ddots & \vdots & \ddots
\end{pmatrix}
\begin{pmatrix}
f_1 \\
f_2 \\
f_3 \\
\vdots \\
f_n \\
\vdots
\end{pmatrix}.
\] (7)

We denote
\[ G = (g_m) = \begin{pmatrix} g_1 \\ g_2 \\ g_3 \\ \vdots \\ g_m \\ \vdots \end{pmatrix}, \quad F = (f_n) = \begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ \vdots \\ f_n \\ \vdots \end{pmatrix}. \] (8)

\[ R = (\lambda_{mn}) = \begin{pmatrix} \lambda_{11} & \lambda_{12} & \lambda_{13} & \ldots & \lambda_{1n} & \ldots \\ \lambda_{21} & \lambda_{22} & \lambda_{23} & \ldots & \lambda_{2n} & \ldots \\ \lambda_{31} & \lambda_{32} & \lambda_{33} & \ldots & \lambda_{3n} & \ldots \\ \vdots & \vdots & \vdots & \ddots & \vdots & \ddots \\ \lambda_{m1} & \lambda_{m2} & \lambda_{m3} & \ldots & \lambda_{mn} & \ldots \\ \vdots & \vdots & \vdots & \ddots & \vdots & \ddots \end{pmatrix}. \] (9)

So
\[ G = RF. \] (10)

According to condition (ii) and (4), we have $\lambda_{mn} = 0$ when $m > n$. Then $R$ is a upper-triangular matrix with $\lambda_{mm} = \lambda(\alpha_1) \neq 0$, 
\[ R = \begin{pmatrix} \lambda_{11} & \lambda_{12} & \lambda_{13} & \ldots & \lambda_{1n} & \ldots \\ 0 & \lambda_{22} & \lambda_{23} & \ldots & \lambda_{2n} & \ldots \\ 0 & 0 & \lambda_{33} & \ldots & \lambda_{3n} & \ldots \\ \vdots & \vdots & \vdots & \ddots & \vdots & \ddots \\ 0 & 0 & 0 & \ldots & \lambda_{mm} & \ldots \end{pmatrix}. \] (11)
which implies that $R$ is an invertible matrix. If there is a matrix

$$R^{-1} = (\mu_{mn}) = \begin{pmatrix}
\mu_{11} & \mu_{12} & \mu_{13} & \cdots & \mu_{1n} & \cdots \\
\mu_{21} & \mu_{22} & \mu_{23} & \cdots & \mu_{2n} & \cdots \\
\mu_{31} & \mu_{32} & \mu_{33} & \cdots & \mu_{3n} & \cdots \\
\vdots & \vdots & \vdots & \ddots & \vdots & \ddots \\
\mu_{m1} & \mu_{m2} & \mu_{m3} & \cdots & \mu_{mn} & \cdots \\
\vdots & \vdots & \vdots & \ddots & \vdots & \ddots
\end{pmatrix}$$

(12)

such that the product $R^{-1}R = I$ is a unit matrix, then

$$F = (R^{-1}R)F = R^{-1}(RF) = R^{-1}G,$$

(13)
i.e.,

$$\begin{pmatrix}
f_1 \\
f_2 \\
f_3 \\
\vdots \\
f_m \\
\vdots
\end{pmatrix} = \begin{pmatrix}
\mu_{11} & \mu_{12} & \mu_{13} & \cdots & \mu_{1n} & \cdots \\
\mu_{21} & \mu_{22} & \mu_{23} & \cdots & \mu_{2n} & \cdots \\
\mu_{31} & \mu_{32} & \mu_{33} & \cdots & \mu_{3n} & \cdots \\
\vdots & \vdots & \vdots & \ddots & \vdots & \ddots \\
\mu_{m1} & \mu_{m2} & \mu_{m3} & \cdots & \mu_{mn} & \cdots \\
\vdots & \vdots & \vdots & \ddots & \vdots & \ddots
\end{pmatrix} \begin{pmatrix}
g_1 \\
g_2 \\
g_3 \\
\vdots \\
g_n \\
\vdots
\end{pmatrix}.$$  

(14)

So

$$f_m = \sum_{n=1}^{\infty} \mu_{mn}g_n \quad (m = 1, 2, 3, \ldots).$$  

(15)

Taking $m = 1$, we have $f_1 = \sum_{n=1}^{\infty} \mu_{1n}g_n$, i.e.,

$$f(\alpha_1x) = f(x) = \sum_{n=1}^{\infty} \mu_{1n}g(\alpha_nx).$$  

(16)

We may determine $\mu_{mn}$ as follows. Let the unit matrix

$$I = (\delta_{mn}), \quad \delta_{mn} = \begin{cases} 1 & \text{when } m = n, \\ 0 & \text{when } m \neq n. \end{cases}$$

By the multiplication of matrix $R^{-1}R = I$, we have

$$\delta_{mn} = \sum_{j=1}^{\infty} \mu_{mj}\lambda_{jn}.$$  

(17)

Since $\lambda_{jn} = 0$ when $j > n$, then

$$\delta_{mn} = \sum_{j=1}^{n} \mu_{mj}\lambda_{jn}.  $$

(17)

By $\lambda_{nn} = \lambda(\alpha_1) \neq 0$, we have, for any $m$,

$$\mu_{mn}\lambda_{mn} = \begin{cases} \delta_{m1} & \text{when } n = 1, \\ \delta_{mn} - \sum_{j=1}^{n-1} \mu_{mj}\lambda_{jn} & \text{when } n > 1, \end{cases}$$
\[ \mu_{mn} = \begin{cases} \delta_{mn} & \text{when } n = 1, \\ \lambda_{nn} \sum_{j=1}^{n-1} \mu_{mj} \lambda_{jn} & \text{when } n > 1, \end{cases} \quad (18) \]

which is a recursion formula for \( n = 1, 2, \ldots \).

Obviously, \( \{\mu_{mn}\} \) are well determined by \( \{\lambda_{mn}\} \) and \( R^{-1} \) is determined uniquely by \( R \).

Since the inverse matrix \( R^{-1} \) is unique, then the solution of Eq. (16) is unique.

From (16), we only require the results for \( m = 1 \). By \( \lambda_{nn} = \lambda(\alpha_1) \neq 0 \), it follows that

\[ \delta_{1n} = \sum_{j=1}^{n} \mu_{1j} \lambda_{jn}. \quad (19) \]

\[ \mu_{1n} = \begin{cases} \frac{1}{\lambda(\alpha_1)} & \text{when } n = 1, \\ \frac{-1}{\lambda(\alpha_1)} \sum_{j=1}^{n-1} \mu_{1j} \lambda_{jn} & \text{when } n > 1. \end{cases} \quad (20) \]

Since \( \mu_{1n} \) is determined by \( n \), we write \( \mu_{1n} \) as \( \mu(\alpha_n) \). Thus, (19) becomes

\[ \delta_{1n} = \sum_{j=1}^{n} \mu(\alpha_j) \lambda_{jn} = \sum_{j=1}^{n} \mu(\alpha_j) \lambda \left( \frac{\alpha_n}{\alpha_j} \right) = \sum_{\alpha_j \alpha_k = \alpha_n} \mu(\alpha_j) \lambda(\alpha_k) = \begin{cases} 1, & n = 1, \\ 0, & n > 1. \end{cases} \quad (20) \]

(20) becomes

\[ \mu(\alpha_n) = \begin{cases} \frac{1}{\lambda(\alpha_1)} & \text{when } n = 1, \\ \frac{-1}{\lambda(\alpha_1)} \sum_{j=1}^{n-1} \mu(\alpha_j) \lambda \left( \frac{\alpha_n}{\alpha_j} \right) & \text{when } n > 1. \end{cases} \quad (21) \]

i.e.,

\[ \mu(\alpha_n) = \begin{cases} \frac{1}{\lambda(\alpha_1)} & \text{when } n = 1, \\ \frac{-1}{\lambda(\alpha_1)} \sum_{\alpha_j \alpha_k = \alpha_n, \alpha_j \neq \alpha_n} \mu(\alpha_j) \lambda(\alpha_k) & \text{when } n > 1, \end{cases} \quad (22) \]

and Eq. (16) becomes

\[ f(x) = \sum_{n=1}^{\infty} \mu(\alpha_n) g(\alpha_n x). \quad (23) \]

We call (23) the inversion formula of (2).

In addition, we must assume that the series \( \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \mu(\alpha_n) \lambda(\alpha_m) f(\alpha_n \alpha_m x) \) converges absolutely because the multiplication of matrix in (13) must satisfy associative law, which is usually satisfied in applications.

The semigroup condition (i) is necessary, if not, we cannot construct the system of linear equations (6). Some results of inverse lattice problems were wrong in the past, because the semigroup condition (i) was omitted. However, in most cases of applications, the sequence \( \{\alpha_n\} \) in (2) does not satisfy condition (i) or (ii). Since \( \{\alpha_n\} \) is unbounded in the inverse lattice problems, it may be treated as follows.

**Case 1.** The sequence \( \{\alpha_n\} \) in (2), with \( 1 = \alpha_1 < \alpha_2 < \cdots < \alpha_n < \alpha_{n+1} < \cdots \), does not satisfy the semigroup condition (i).
We may choose the multiplicative semigroup \( \{ \alpha'_n \} \) generated by \( \{ \alpha_n \} \), with \( \alpha'_1 < \alpha'_2 < \cdots < \alpha'_{n+1} < \cdots \), as the semigroup sequence \( P \). Since \( P = \{ \alpha'_n \} \supseteq \{ \alpha_n \} \), (2) can be changed to

\[
g(x) = \sum_{n=1}^{\infty} \hat{\lambda}(\alpha'_n) f(\alpha'_n x),
\]
where

\[
\hat{\lambda}(\alpha'_n) = \begin{cases} 
\lambda(\alpha_m) & \text{when } \alpha'_n = \alpha_m \in \{ \alpha_n \}, \\
0 & \text{when } \alpha'_n \notin \{ \alpha_n \}.
\end{cases}
\]

Since \( \alpha'_1 = \alpha_1 \), \( f(x) \) can be solved by (23) when \( \lambda(\alpha_1) \neq 0 \).

Case 2. The sequence \( \{ \alpha_n \} \) in (2), with \( 0 < \alpha_1 < \alpha_2 < \cdots < \alpha_n < \alpha_{n+1} < \cdots \), does not satisfy conditions (i) and \( \alpha_1 \neq 1 \).

From (2), we may let

\[
G(x) = g\left(\frac{1}{\alpha_1 x}\right) = \sum_{n=1}^{\infty} \lambda(\alpha_n) f\left(\frac{\alpha_n}{\alpha_1 x}\right).
\]

Denote \( \beta_n = \alpha_n/\alpha_1 \) and \( \lambda^*(\beta_n) = \lambda(\alpha_1 \beta_n) = \lambda(\alpha_n) \) \((n = 1, 2, \ldots)\), then

\[
G(x) = \sum_{n=1}^{\infty} \lambda^*(\beta_n) f(\beta_n x),
\]
and \( 1 = \beta_1 < \beta_2 < \cdots < \beta_n < \cdots \), which is Case 1.

It is based on these techniques that we can solve all the lattice problems by the inversion formula (23).

3. The Möbius inversion formula on multiplicative semigroup

Chen has used the Möbius inversion formula in number theory to solve one-dimensional inverse lattice problem in 1989 [2]. Maddox said: "A more demanding question is whether it will be feasible to extend the trick to problems that are not simply one-dimensional," and indicated that it would be a challenge [8]. Chen et al. solved the two-dimensional inverse lattice problem by extending the Möbius inversion formula to the unique factorization multiplicative semigroups of the Gaussian ring and the Eisenstein’s ring [3,4]. Because the three-dimensional lattices do not satisfy the semigroup condition (i), and we have to deal with the summations of unequally weighted terms such as (2), they are more difficult to solve by the classical Möbius inversion.

On the other hand, the Möbius inversion formula has been extended to a partially ordered set by Rota in 1964 [9]. But it cannot be used here directly because we have to deal with the summations of finite and equally weighted terms. However, we may extend Rota’s Möbius inversion formula by his idea of associative algebra on a partially ordered set. In this section, we deduce the same inversion formula (23) by the extended Möbius inversion formula.

A partially ordered set \( P \) is a nonempty set with a binary relation "\( \leq \)" satisfying the following conditions:
(a) Reflexive: $\alpha \preceq \alpha$ for all $\alpha \in P$;
(b) Transitive: if $\alpha \preceq \beta$ and $\beta \preceq \gamma$, then $\alpha \preceq \gamma$;
(c) Anti-symmetric: if $\alpha \preceq \beta$ and $\beta \preceq \alpha$, then $\alpha = \beta$.

$\alpha \prec \beta$ means $\alpha \preceq \beta$ and $\alpha \neq \beta$.
$\alpha \not\preceq \beta$ means that $\alpha \preceq \beta$ is not true. A partially ordered set $P$ is locally finite if the set $\{\gamma \in P: \alpha \preceq \gamma \preceq \beta\}$ is finite for all $\alpha, \beta \in P$. If there exist $\varepsilon \in P$, for any $\alpha \in P$ the relation $\varepsilon \preceq \alpha$ holds, then $\varepsilon$ is called the minimal element in $P$. It is clear that the minimal element $\varepsilon$ is unique when it exists.

Let $P$ be a locally finite partially ordered set with the minimal element, and let $A(P)$ be the set of all real-valued functions of two variables which are defined on $P \times P$, and satisfy $\lambda(\alpha, \beta) = 0$ when $\alpha \not\preceq \beta$. For any $\lambda, \eta \in A(P)$, define the convolution $h = \lambda * \eta$ by

$$h(\alpha, \beta) = \sum_{\alpha \preceq \gamma \preceq \beta} \lambda(\alpha, \gamma)\eta(\gamma, \beta).$$

(24)

It can be verified that $h \in A(P)$ and $A(P)$ is an associative algebra over the real field [9]. The identity in $A(P)$ is

$$\delta(\alpha, \beta) = \begin{cases} 1, & \alpha = \beta, \\ 0, & \text{otherwise}. \end{cases}$$

(25)

An element $\lambda \in A(P)$ is called a unit if there exists $\mu \in A(P)$ such that

$$\delta = \mu * \lambda = \lambda * \mu.$$  

(26)

Such $\mu$ in (26) is unique when it exists [10]. We call $\mu$ the inverse element of $\lambda$. It can be proved that $\lambda$ is an unit in $A(P)$ if and only if $\lambda(\alpha, \alpha) \neq 0$ for all $\alpha \in P$, and its inverse element $\mu$ can be determined by the recursion formula [10],

$$\delta(\alpha, \beta) = \sum_{\alpha \preceq \gamma \preceq \beta} \mu(\alpha, \gamma)\lambda(\gamma, \beta).$$

(27)

i.e.,

$$\mu(\alpha, \beta) = \begin{cases} \frac{1}{\lambda(\alpha, \alpha)}, & \alpha = \beta, \\ -\frac{1}{\lambda(\beta, \beta)} \sum_{\alpha \preceq \gamma < \beta} h(\alpha, \gamma)\lambda(\gamma, \beta), & \alpha < \beta, \\ 0, & \text{otherwise}. \end{cases}$$

(28)

We extend the Möbius inversion formula as follows.

Let $P$ be a locally finite partially ordered set with the minimal element. Suppose $P$ is a countable set, and $f, g$ are the real-valued functions defined on $P$ satisfying the relation

$$g(\alpha) = \sum_{\alpha \preceq \beta} \lambda(\alpha, \beta) f(\beta)$$

(29)

for all $\alpha \in P$. If $\lambda$ is a unit in $A(P)$, then the Möbius inversion formula follows

$$f(\alpha) = \sum_{\alpha \preceq \beta} \mu(\alpha, \beta) g(\beta),$$

(30)

where $\mu$ is the inverse element of $\lambda$. In fact
\[
\sum_{\alpha \preceq \beta} \mu(\alpha, \beta)g(\beta) = \sum_{\alpha \preceq \beta} \mu(\alpha, \beta) \sum_{\beta \preceq \gamma} \lambda(\beta, \gamma) f(\gamma) = \sum_{\alpha \preceq \beta} \sum_{\beta \preceq \gamma} \mu(\alpha, \beta)\lambda(\beta, \gamma) f(\gamma)
\]
\[
= \sum_{\alpha \preceq \gamma} \left[ \sum_{\alpha \preceq \beta} \mu(\alpha, \beta)\lambda(\beta, \gamma) \right] f(\gamma) = \sum_{\alpha \preceq \gamma} \delta(\alpha, \gamma) f(\gamma) = f(\alpha).
\]

Of course, we must assume that the series
\[
\sum_{\alpha \preceq \beta} \sum_{\beta \preceq \gamma} \mu(\alpha, \beta)\lambda(\beta, \gamma) f(\gamma)
\]
converges absolutely. It is clear that (29) may be a summation with unequally weighted terms. We may call \( \mu \) in (30) the Möbius function on \( P \), which is determined by \( \lambda \) in (29).

The inversion formula (23) can be obtained from the extended Möbius inversion formula (30).

Suppose \( P = \{\alpha_n\} \) is a semigroup sequence. Denote \( \alpha_m \preceq \alpha_n \) if \( \alpha_n/\alpha_m = \alpha_k \in P \). We can verify that \( P \) is a locally finite partially ordered set with the minimal element \( \alpha_1 = 1 \). From (2), we have

\[
g(\alpha_m x) = \sum_{n=1}^{\infty} \lambda(\alpha_n f(\alpha_n \alpha_m x) \quad (m = 1, 2, \ldots),
\]

where \( \lambda(\alpha_1) \neq 0 \). Let

\[
\tilde{\lambda}(\alpha_m, \alpha_n) = \begin{cases} \lambda(\alpha_k), & \frac{\alpha_m}{\alpha_n} = \alpha_k \in P, \\ 0, & \text{otherwise}. \end{cases}
\]

Obviously, \( \tilde{\lambda}(\alpha_m, \alpha_n) = 0 \) when \( \alpha_m \npreceq \alpha_n \), hence \( \tilde{\lambda} \in A(P) \). Since \( \tilde{\lambda}(\alpha_m, \alpha_n) = \lambda(\alpha_m/\alpha_n) = \lambda(\alpha_1) \neq 0 \), then \( \tilde{\lambda} \) is a unit in \( A(P) \). By the semigroup condition (i), (31) can be written as

\[
g(\alpha_m x) = \sum_{n=1}^{\infty} \tilde{\lambda}(\alpha_m, \alpha_n) f(\alpha_n \alpha_m x) = \sum_{\alpha_n \preceq \alpha_j} \tilde{\lambda}(\alpha_m, \alpha_j) f(\alpha_j x),
\]

where \( \alpha_j = \alpha_n \alpha_m \), i.e.,

\[
g(\alpha_m x) = \sum_{\alpha_n \preceq \alpha_j} \tilde{\lambda}(\alpha_m, \alpha_n) f(\alpha_n x).
\]

We write (33) simply as

\[
g(\alpha_m) = \sum_{\alpha_n \preceq \alpha_m} \tilde{\lambda}(\alpha_m, \alpha_n) f(\alpha_n).
\]

In fact, this is Eq. (29). By the Möbius inversion formula (30), we have

\[
f(\alpha_m) = \sum_{\alpha_n \preceq \alpha_m} \tilde{\mu}(\alpha_m, \alpha_n) g(\alpha_n),
\]

where \( \tilde{\mu} \) is the inverse element of \( \tilde{\lambda} \) in \( A(P) \). Taking \( \alpha_m = \alpha_1 \), we have

\[
f(\alpha_1) = \sum_{\alpha_n \preceq \alpha_1} \tilde{\mu}(\alpha_1, \alpha_n) g(\alpha_n).
\]
Since $\alpha_1$ is the minimal element, by the recursion formula (28), we obtain

\[
\tilde{\mu}(\alpha_1, \alpha_n) = \begin{cases} 
1, & \alpha_n = \alpha_1, \\
-1 \frac{1}{\lambda(\alpha_j, \alpha_1)} \sum_{\alpha_1 \leq \alpha_j < \alpha_n} \tilde{\mu}(\alpha_1, \alpha_j) \tilde{\lambda}(\alpha_j, \alpha_n), & \alpha_n \neq \alpha_1.
\end{cases}
\]

(37)

We write $\mu(\alpha_j) = \tilde{\mu}(\alpha_1, \alpha_j)$, and notice that

\[
\tilde{\lambda}(\alpha_1, \alpha_j) = \lambda(\alpha_j/\alpha_1) = \lambda(\alpha_k)
\]

when $\alpha_j \alpha_k = \alpha_n$. So that

\[
\tilde{\mu}(\alpha_1, \alpha_n) = \mu(\alpha_n) = \begin{cases} 
1, & \alpha_n = \alpha_1, \\
-1 \frac{1}{\lambda(\alpha_j, \alpha_1)} \sum_{\alpha_j \alpha_k = \alpha_n, \ j \neq n} \mu(\alpha_j) \lambda(\alpha_k), & \alpha_n \neq \alpha_1.
\end{cases}
\]

(38)

which is Eq. (22). Since $\alpha_1$ is the minimal element, (36) becomes

\[
f(\alpha_1) = \sum_{n=1}^{\infty} \mu(\alpha_n) g(\alpha_n),
\]

(39)

i.e.,

\[
f(\alpha_1 x) = f(x) = \sum_{n=1}^{\infty} \mu(\alpha_n) g(\alpha_n x),
\]

which is the inversion formula (23). So we may call $\mu(\alpha_n)$ in (21) or (22) the Möbius function on $P$, which is determined by $\lambda(\alpha_n)$, and call (23) the Möbius inversion formula.

For example, let

\[
g(x) = \sum_{n=1}^{\infty} f(nx).\]

Here $P = \{1, 2, \ldots \}$ is a semigroup sequence and $\lambda(n) = 1$ ($n = 1, 2, \ldots$). By (38) or (22)

\[
\mu(1) = \lambda^{-1}(1) = 1,
\]

\[
\mu(2) = -\lambda^{-1}(1) [\mu(1) \lambda(2)] = -1,
\]

\[
\mu(3) = -\lambda^{-1}(1) [\mu(1) \lambda(3)] = -1,
\]

\[
\mu(4) = -\lambda^{-1}(1) [\mu(1) \lambda(4) + \mu(2) \lambda(2)] = 0,
\]

\[
\mu(5) = -\lambda^{-1}(1) [\mu(1) \lambda(5)] = -1,
\]

\[
\mu(6) = -\lambda^{-1}(1) [\mu(1) \lambda(6) + \mu(2) \lambda(3) + \mu(3) \lambda(2)] = 1,
\]

\[\vdots\]

It can be proved that $\mu(n)$ is just the Möbius function in number theory [10]

\[
\mu(n) = \begin{cases} 
1, & n = 1, \\
(-1)^r, & if \ n \ is \ the \ product \ of \ r \ distinct \ prime \ factors, \\
0, & otherwise.
\end{cases}
\]

So

\[
f(x) = \sum_{n=1}^{\infty} \mu(n) g(nx) = g(x) - g(2x) - g(3x) - g(5x) + g(6x) - g(7x) + \cdots,
\]
which accords with Chen’s result [2] and [11]. However, this example is a special case because it deals with the summation having equally weighted terms.

4. Examples

4.1. Fibonacci structure

Let \( F = \{b_n\} \) be the Fibonacci sequence, i.e., \( b_0 = b_1 = 1, \ b_{n+1} = b_n + b_{n-1} \ (n = 1, 2, \ldots) \). Let us solve \( \Phi(x) \) from the summation

\[
E(x) = \frac{1}{2} \sum_{n=0}^{\infty} \Phi(b_n x).
\]

(40)

Obviously,

\[
2E(x) = 2\Phi(x) + \sum_{n=2}^{\infty} \Phi(b_n x)
\]

\[
= 2\Phi(x) + \Phi(2x) + \Phi(3x) + \Phi(5x) + \Phi(8x) + \cdots + \Phi(b_n x) + \cdots
\]

(41)

and \( F = \{1, 2, 3, 5, 8, 13, 21, \ldots, b_n, \ldots\} \) is not a semigroup sequence by (i), which is Case 1. We choose the multiplicative semigroup generated by \( F \) as the semigroup sequence \( P \),

\[
P = \{1, 2, 3, 4, 5, 6, 8, 9, 10, 12, 13, 15, 16, 18, 20, 21, \ldots, \alpha_n, \ldots\}.
\]

(42)

So \( P \supseteq F \) and (41) is equivalent to

\[
2E(x) = \sum_{n=1}^{\infty} \lambda(\alpha_n) \Phi(\alpha_n x),
\]

(43)

where

\[
\lambda(y) = \begin{cases} 
2 & \text{if } y = 1, \\
1 & \text{if } y \in F \text{ and } y \neq 1, \\
0 & \text{otherwise}.
\end{cases}
\]

(44)

The Möbius function \( \mu(\alpha_n) \) can be computed by (21):

\[
\mu(\alpha_1) = \mu(1) = \lambda^{-1}(1) = \frac{1}{2},
\]

\[
\mu(\alpha_2) = \mu(2) = -\frac{1}{2} \mu(1) \lambda(2) = -\frac{1}{4},
\]

\[
\mu(\alpha_3) = \mu(3) = -\frac{1}{2} \left[ \mu(1) \lambda(3) + \mu(2) \lambda \left( \frac{3}{2} \right) \right] = -\frac{1}{2} \left[ \frac{1}{2} + 0 \right] = -\frac{1}{4},
\]

\[
\mu(\alpha_4) = \mu(4) = -\frac{1}{2} \left[ \mu(1) \lambda(4) + \mu(2) \lambda(2) + \mu(3) \lambda \left( \frac{4}{3} \right) \right]
\]

\[
= -\frac{1}{2} \left[ 0 - \frac{1}{4} + 0 \right] = \frac{1}{8}.
\]
\[
\mu(\alpha_5) = \mu(5) = -\frac{1}{2} \left[ \mu(1)\lambda(5) + \mu(2)\lambda\left(\frac{5}{2}\right) + \mu(3)\lambda\left(\frac{5}{3}\right) + \mu(4)\lambda\left(\frac{5}{4}\right) \right]
\]
\[= -\frac{1}{2} \left[ \frac{1}{2} + 0 + 0 + 0 \right] = -\frac{1}{4}, \]
\[
\mu(\alpha_6) = \mu(6) = -\frac{1}{2} \left[ \mu(1)\lambda(6) + \mu(2)\lambda(3) + \mu(3)\lambda(2) + \mu(4)\lambda\left(\frac{6}{4}\right) + \mu(5)\lambda\left(\frac{6}{5}\right) \right]
\]
\[= -\frac{1}{2} \left[ 0 - \frac{1}{4} - 0 + 0 + 0 \right] = -\frac{1}{4}, \]
\[
\mu(\alpha_7) = \mu(8) = -\frac{1}{2} \left[ \mu(1)\lambda(8) + \mu(2)\lambda(4) + \mu(3)\lambda\left(\frac{8}{3}\right) + \mu(4)\lambda(2) + \mu(5)\lambda\left(\frac{8}{5}\right) + \mu(6)\lambda\left(\frac{8}{6}\right) \right]
\]
\[= -\frac{1}{2} \left[ \frac{1}{2} + 0 + 0 + \frac{1}{8} + 0 + 0 \right] = -\frac{5}{16}, \]

(see Table 1). So

\[\Phi(x) = 2 \left[ \frac{1}{2} E(x) - \frac{1}{4} E(2x) - \frac{1}{4} E(3x) + \frac{1}{8} E(4x) - \frac{1}{4} E(5x) + \cdots \right]. \tag{45}\]

This result may be applied to the inversion of the interatomic potential for a one-dimensional quasi-crystal.

4.2. Square lattice structure

This inversion problem is to solve \(\Phi(x)\) from \(E(x)\), based on the summation

\[E(x) = \frac{1}{2} \sum_{(m,n)\neq (0,0)} \Phi(\sqrt{m^2 + n^2}x). \tag{46}\]

It is equivalent to the summation

\[2E(x) = \sum_{\alpha_n \in S} \lambda(\alpha_n)\Phi(\alpha_n x), \tag{47}\]

where \(x\) is the lattice constant; the set

\[S = \{ \sqrt{m^2 + n^2}; \ m, n \in \mathbb{Z}, \ m^2 + n^2 \neq 0 \}\]
\[= \{1, \sqrt{2}, \sqrt{4}, \sqrt{5}, \sqrt{8}, \sqrt{10}, \sqrt{13}, \ldots, \alpha_n, \ldots \}\]
Table 1
The values of Möbius function for Fibonacci structure

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<th>λ(αn)</th>
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is just a semigroup sequence, and λ(α_n) is the number of solutions of the equation
\[ x^2 + y^2 = \alpha_n^2 \] in integers. By the Möbius inversion formula (23), we have

\[ \Phi(x) = 2 \sum_{\alpha_n \in S} \mu(\alpha_n) E(\alpha_n x), \]

(48)
i.e.,

\[ \Phi(x) = 2 \left[ \frac{1}{4} E(x) - \frac{1}{4} E(\sqrt{2}x) - \frac{1}{12} E(\sqrt{5}x) - \frac{1}{4} E(3x) + \cdots \right], \]

(49)

(see Table 2), where µ(α_n) is determined by (21).

It should be noted that this problem has a more concise solution based on the Möbius inversion formula on the Gaussian ring [3].

4.3. Bcc lattice structure

This inversion problem is to solve \( \Phi(x) \) from \( E(x) \) based on the summation

\[ E(x) = \frac{1}{2} \sum_{(l,m,n) \neq (0,0,0)} \Phi(|l \vec{a} + m \vec{b} + n \vec{c}| x), \]

(50)

where

\[ \vec{a} = \left\{ \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right\}, \quad \vec{b} = \left\{ -\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right\}, \quad \vec{c} = \left\{ -\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right\} \]

(51)
Table 2
The values of Möbius function for square structure

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are the basis vectors, $x$ is the lattice constant. (50) is equivalent to the summation

$$E(x) = \frac{1}{2} \sum_{b_n \in S} r(b_n) \Phi(b_n x),$$

(52)

where the set

$$S = \{ |l\vec{a} + m\vec{b} + n\vec{c}| : l, m, n \in \mathbb{Z}, l^2 + m^2 + n^2 \neq 0 \}$$

is not a semigroup sequence, which is Case 2, and $r(b_n)$ is the number of solutions of the equation $|x\vec{a} + y\vec{b} + z\vec{c}| = b_n$ in integers. By (52)

$$2E\left(\sqrt[3]{\frac{4}{3}}\right) = \sum_{n=1}^{\infty} r(b_n) \Phi\left(\sqrt[3]{\frac{4}{3}} b_n x\right).$$

(53)

Let

$$B = \left\{ b_n \sqrt[3]{\frac{4}{3}} : b_n \in S \right\} = \left\{ 1, \sqrt[3]{\frac{4}{3}}, \sqrt[3]{\frac{16}{9}}, \sqrt[3]{\frac{64}{27}}, \sqrt[3]{\frac{8}{3}}, \ldots, \alpha_n, \ldots \right\},$$

and let $P$ be the multiplicative semigroup generated by $B$. So

$$P = \left\{ 1, \sqrt[3]{\frac{4}{3}}, \sqrt[3]{\frac{16}{9}}, \sqrt[3]{\frac{64}{27}}, \sqrt[3]{\frac{8}{3}}, \ldots, \alpha_n, \ldots \right\}.$$
is a semigroup sequence. Let

$$E^*(x) = 2E\left(\frac{4}{\sqrt{3}x}\right) = \sum_{n=1}^{\infty} \lambda(\alpha_n)\Phi(\alpha_n x),$$

(54)

where

$$\lambda(y) = \begin{cases} 
    r(b_k) & \text{if } \sqrt{\frac{4}{\sqrt{3}}}y = b_k \in S, \\
    0 & \text{otherwise}. 
\end{cases}$$

(55)

By the Möbius inversion formula (23)

$$\Phi(x) = \sum_{n=1}^{\infty} \mu(\alpha_n)E^*(\alpha_n x) = 2\sum_{n=1}^{\infty} \mu(\alpha_n)E\left(\frac{4}{\sqrt{3}x}\right),$$

(56)

i.e.,

$$\Phi(x) = 2\left[\frac{1}{8}E\left(\sqrt{\frac{4}{3}x}\right) - \frac{3}{32}E\left(\sqrt{\frac{16}{9}x}\right) + \frac{9}{128}E\left(\sqrt{\frac{64}{27}x}\right) + \cdots\right],$$

(57)

(see Table 3), where $\mu(\alpha_n)$ is determined by (21).

4.4. Hcp lattice structure

This inversion problem is to solve $\Phi(x)$ from $E(x)$ based on the summation

$$E(x) = \frac{1}{2}\left[ \sum_{(l,m,n) \neq (0,0,0)} \Phi(\sqrt{\frac{4}{3}x}l\vec{a} + m\vec{b} + n\vec{c})x) + \sum_{(l,m,n)} \Phi(\sqrt{\frac{4}{3}x}l\vec{a} + m\vec{b} + n\vec{c} + \vec{d})x) \right],$$

(58)

where $\vec{d} = [1/2, \sqrt{3}/6, \sqrt{6}/3], \vec{a} = [1, 0, 0], \vec{b} = [-1/2, \sqrt{3}/2, 0], \vec{c} = [0, 0, 2\sqrt{6}/3]$ are basis vectors, and $x$ is the lattice constant. Define the set $S$ by

$$S = \{l\vec{a} + m\vec{b} + n\vec{c}: l, m, n \in \mathbb{Z}, l^2 + m^2 + n^2 \neq 0\}$$

$$\cup \{l\vec{a} + m\vec{b} + n\vec{c} + \vec{d}: l, m, n \in \mathbb{Z}\}$$

$$= \left\{1, \sqrt{2}, \sqrt{3}, \sqrt{\frac{8}{3}}, \sqrt{\frac{11}{3}}, 2, \sqrt{\frac{17}{3}}, \ldots, b_n, \ldots\right\}.$$

Let

$$r(b_n) = r_1(b_n) + r_2(b_n),$$

where $r_1(b_n)$ is the number of solutions of equation $|x\vec{a} + y\vec{b} + z\vec{c}| = b_n$ in integers, and $r_2(b_n)$ is the number of solutions of equation $|x\vec{a} + y\vec{b} + z\vec{c} + \vec{d}| = b_n$ in integers. So (58) is equivalent to
Table 3
The values of Mobius function for bcc structure

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<th>$\mu(a_n)$</th>
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$$E(x) = \frac{1}{2} \sum_{b_n \in S} r(b_n) \Phi(b_n x)$$

$$= \frac{1}{2} \left[ 12 \Phi(x) + 6 \Phi(\sqrt{2} x) + 2 \Phi \left( \sqrt{\frac{8}{3}} x \right) + 18 \Phi(\sqrt{3} x) + 12 \Phi \left( \sqrt{\frac{11}{3}} x \right) + 6 \Phi(2x) + 12 \Phi(\sqrt{5} x) + 12 \Phi \left( \sqrt{\frac{17}{3}} x \right) + \ldots \right].$$

(59)

Since $S$ is obviously not a semigroup sequence, which is Case 1, let $P$ be the multiplicative semigroup generated by $S$, so that

$$P = \left\{ 1, \sqrt{2}, \sqrt{\frac{8}{3}}, \sqrt{3}, \sqrt{\frac{11}{3}}, 2, \sqrt{5}, \sqrt{\frac{16}{3}}, \sqrt{\frac{17}{3}}, \ldots, a_n, \ldots \right\}$$
where $E(x) = \sum_{n=1}^{\infty} \lambda(\alpha_n) \Phi(\alpha_n x)$.

By the Möbius inversion formula (23)

$$
\Phi(x) = \sum_{n=1}^{\infty} \mu(\alpha_n) E^*(\alpha_n x) = 2 \sum_{n=1}^{\infty} \mu(\alpha_n) E(\alpha_n x)
$$

is a semigroup sequence. By (59), we have

$$
E^*(x) = 2E(x) = \sum_{n=1}^{\infty} \lambda(\alpha_n) \Phi(\alpha_n x),
$$

where

$$
\lambda(y) = \begin{cases} 
  r(b_m) & \text{if } y = b_m \in S, \\
  0 & \text{otherwise}.
\end{cases}
$$

By the Möbius inversion formula (23)

$$
\Phi(x) = 2 \sum_{n=1}^{\infty} \mu(\alpha_n) E(\alpha_n x) = 2 \sum_{n=1}^{\infty} \mu(\alpha_n) E(\alpha_n x)
$$

$$
= 2 \left[ \frac{1}{12} E(x) - \frac{1}{24} E(\sqrt{2} x) - \frac{1}{72} E\left(\sqrt{\frac{8}{3}} x\right) - \frac{1}{8} E(\sqrt{3} x) - \frac{1}{12} E\left(\sqrt{\frac{11}{3}} x\right) \right]
$$

$$
- \frac{1}{48} E(2x) - \frac{1}{12} E(\sqrt{5} x) + \frac{1}{72} E\left(\sqrt{\frac{16}{3}} x\right) - \frac{1}{12} E\left(\sqrt{\frac{17}{3}} x\right) + \cdots
$$

(see Table 4), where $\mu(\alpha_n)$ is determined by (21).

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5. Conclusion and discussion

From the above discussion, all the inverse lattice problems can be solved successfully based on the Möbius inversion formula (23). The Möbius function $\mu(\alpha_n)$ can be easily obtained by a small program, since it is determined by the recursion formula (21). By the method presented in this paper, we are building a database to determine the interatomic potential of various lattice structure in order to compute the performances of materials. Of more importance, the work shows that a potential application of the algebra to the physical sciences.

Acknowledgment

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References