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Algebraic rings of integers and some 2D lattice problems in physics

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Abstract. This paper develops the Möbius inversion formula for the Gaussian integers and Eisenstein's integers, and gives two applications. The first application is to the two-dimensional arithmetic Fourier transform (AFT), which is suitable for parallel processing. The second application is to two-dimensional inverse lattice problems, and is illustrated with the recovery of interatomic potentials from the cohesive energy for monolayer graphite. The paper demonstrates the potential application in the physical science of integral domains other than the standard integers.

1. Introduction

Recently, a number of authors have applied the one-dimensional Möbius inversion formula [1] to a variety of inverse problems, leading to concise analytic expressions, and to rapidly convergent series for practical calculation. The applications have included the inverse blackbody radiation problem, recovery of the temperature distribution of the shell of a black hole and interstellar dust, the inverse heat capacity problem for phonon density of states, the inverse carrier density problem for electron density of states, the inverse cohesion problem, and so on [2–7]. Each of these applications can be regarded as examples of the Möbius inversion formula, with equal and unequal weights [2, 6–8].

The present work extends the Möbius function and the Möbius inversion formula to integral domains other than the standard integers. Applications are given to the two-dimensional (2D) arithmetic Fourier transform (AFT), and the *ab initio* calculation of the C–C pair interaction in monolayer graphite. All the contents are introduced in an elementary way for the physicist's convenience. It shows the potential applications of the theory of integral domains to physical sciences.

2. Inverse cohesion problem for a 2D lattice

Suppose that the vertices of an infinite two-dimensional square lattice are all occupied with interacting atoms, so that any one of them experiences a potential as

$$E(x) = \tfrac{1}{2} \sum_{(m,n)\neq(0,0)} \Phi\left(\sqrt{m^2+n^2}x\right) = 2\sum_{m=0}^{\infty}\sum_{n=1}^{\infty} \Phi\left(\sqrt{m^2+n^2}x\right). \qquad (1)$$

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The inverse cohesion problem for a two-dimensional lattice is to determine $\Phi(x)$ from $E(x)$ based on the above relation. For solving the equation, Chen and Ren proposed an iterative method based on the classical one-dimensional Möbius inversion formula with the concept of most close-packed direction instead of the nearest neighbour distance [8], which has been directly applied to various kinds of 3D crystal lattice structures. Ninham *et al* inverted double series such as (1) by writing [6]

$$\Phi(x) = \sum_{k=1}^{\infty} \omega(k) E(\sqrt{k}x) \tag{2}$$

where the coefficients $\omega(k)$ can be found recursively, and this recursive calculation can be simplified as the Dirichlet inverse from number theory. Their use of number theory is not applicable to three-dimensional crystal structure problems, for which we need to use a specially generalized Dirichlet product [9].

Originally the Möbius function $\mu(n)$ was introduced to describe the unique factorization of any natural number [1, 10], i.e.

$$n = p_1^{r_1(n)} p_2^{r_2(n)} \cdots p_k^{r_k(n)} \tag{3}$$

with $p_i \neq p_j$, when $i \neq j$, where p_i is a prime number, and $r_i \geqslant 1$. For any algebraic structure which possesses analogous factorization properties, an analogue of the Möbius function and Möbius inversion formula may be anticipated. The most general algebraic structure of this type is a *ring*, but in practice a few additional restrictions seem necessary, and these direct us to those structures known as *integral domains*. We consider one such example in the present section. A second example will be found in section 4.

The *Gaussian integers* are defined to be the set $G = \{z = m + n\mathrm{i} \backslash m, n \in \boldsymbol{Z}\}$ with the standard definition of addition and multiplication of complex numbers used to define addition and multiplication of Gaussian integers. The roles of zero and unity are played by $0 + 0\mathrm{i}$ and $1 + \mathrm{i}$, abbreviated as 0 and 1 as usual. Divisors of a Gaussian integer are defined in the obvious manner, and any divisor of unity is called a *unit*. There are clearly four of these: 1, -1, i, $-\mathrm{i}$. The set of units is denoted by U. If $u \in U$, then one says that uz is *associated* with the Gaussian integer z. One calls a Gaussian integer *prime* if it is neither zero nor a unit. It can be proved that any Gaussian integer can be factored into a product of primes, in a manner such as

$$z = \epsilon P_1^{k_1} P_2^{k_2} \cdots P_i^{k_i} \cdots P_t^{k_t} \tag{4}$$

similar to (3) which is unique apart from the order of the factors, the presence of units, and the ambiguity between primes associated with each other. For the purpose of physical applications, elements of the set G simply correspond to all 2D lattice points, and the set G^* of non-zero Gaussian integers becomes a multiplicative semigroup. The Möbius function of a non-zero Gaussian integer z can now be defined as

$$\mu(z) = \begin{cases} 1 & \text{if } z \in U, \\ (-1)^t & \text{if } z \text{ factors as the product of } t \text{ distinct primes,} \\ & \textit{with no two factors being associated,} \\ 0 & \text{otherwise.} \end{cases} \tag{5}$$

Obviously, the Möbius function takes the same value for any two associated Gaussian integers, and a sum rule of $\mu(z)$ is given as

$$\sum_{d|z} \mu(d) = \begin{cases} 0 & \text{if } z \notin U, \\ 4 & \text{if } z \in U. \end{cases} \tag{6}$$

This is similar to the sum rule

$$\sum_{d|n} \mu(d) = \delta_{n1} \tag{7}$$

for the Möbius function $\mu(n)$ on the natural numbers $\boldsymbol{N}$. To see whether the Gaussian integer $m + \mathrm{i}n$ has a prime, it is equivalent to whether $m + \mathrm{i}n$ has non-trivial factors. The first case is that neither m nor n is zero, for $m + \mathrm{i}n$ being factorized, $m^2 + n^2$ must factorize as an ordinary natural number. The second case is that one of m and n is zero, then $m + \mathrm{i}n$ is prime in G^* if and only if $m^2 + n^2$ is prime in $\boldsymbol{N}$. These results can be expressed as

$$\begin{cases} m^2 + n^2 \text{ is prime in } \boldsymbol{N} & \text{if } mn \neq 0, \\ |z| \neq p^2 + q^2 \text{ is a prime in } \boldsymbol{N} & \text{if } mn = 0. \end{cases} \tag{8}$$

Using these observations, which can be proved rigorously, the function Möbius function for the set G^* of non-zero Gaussian integers is easily evaluated (table 1).

Table 1. Gaussian Möbius functions.

m	$n \rightarrow$	0	1	2	3	4	5	6	7	8
1		1	−1	−1	1	−1	1	−1	0	1
2		0	−1	0	−1	0	−1	0	−1	0
3		−1	1	−1	1	0	1	1	1	−1
4		0	−1	0	0	0	−1	0	1	0
5		1	1	−1	1	−1	−1	−1	1	−1
6		0	−1	0	1	0	−1	0	1	0
7		−1	0	−1	1	1	1	1	1	−1
8		0	1	0	−1	0	−1	0	−1	0

Note that the Möbius function or the inversion coefficient only takes the value of 1, −1 and 0 as usual; it is an obvious advantage over the Ninham's result.

For solving equation (1)

$$E(x) = \tfrac{1}{2} \sum_{(m,n)\neq(0,0)} \Phi\left(\sqrt{m^2 + n^2}x\right)$$

we can apply the Möbius inversion formula on the algebraic ring of integers, which leads to

$$\begin{aligned} \Phi(x) &= \tfrac{1}{8} \sum_{(m,n)\neq(0,0)} \mu(m + n\mathrm{i}) E\left(\sqrt{m^2 + n^2}x\right) \\ &= \tfrac{1}{2} \sum_{m=1}^{\infty} \sum_{n=0}^{\infty} \mu(m + n\mathrm{i}) E\left(\sqrt{m^2 + n^2}x\right). \end{aligned} \tag{9}$$

In fact,

$$\begin{aligned} &\tfrac{1}{8} \sum_{(m,n)\neq(0,0)} \mu(m + n\mathrm{i}) E\left(\sqrt{m^2 + n^2}x\right) \\ &\quad = \tfrac{1}{8} \sum_{(m,n)\neq(0,0)} \mu(m + n\mathrm{i}) \left[\tfrac{1}{2} \sum_{(p,q)\neq(0,0)} \Phi\left(\sqrt{(m^2 + n^2)(p^2 + q^2)}x\right) \right] \\ &\quad = \tfrac{1}{16} \sum_{z_1} \mu(z_1) \sum_{z_2} \Phi(|z_1 z_2|x) = \tfrac{1}{16} \sum_{z} \left[\sum_{z_1|z} \mu(z_1) \right] \Phi(|z|x) \\ &\quad = \tfrac{1}{4} \sum_{z\in U} \Phi(|z|x) = \Phi(x). \end{aligned}$$

This solution (9) from the proper Möbius method is significantly simpler than all the previous formulae for analysis and easier for calculation. This method is also suitable for binary systems.

3. Application to the 2D arithmetic Fourier transform

The discrete Fourier transform (DFT) is an essential part of numerous physical and technical problems such as band structure, signal processing, pattern recovery, etc. The popularity of the fast Fourier transform (FFT) [11] is primarily due to its reduction of the number of multiplicative operations from $O(N^2)$ to $O(N \log N)$ for computing $2N + 1$ Fourier coefficients. The arithmetic Fourier transform (AFT) [12] is based on the Möbius inversion formula of classical number theory [1], in which the number of multiplications is further reduced significantly down to $O(N)$ since the Möbius functions only take the value in $\{-1, 0, 1\}$. At the same time, the remaining addition operations can be performed much more quickly by a parallel processor.

A 2D AFT algorithm has been proposed by Tufts *et al* [13]. Also, a row-column algorithm has been developed by Kelly and co-workers [14]. All of those methods require that the row, column, and the global means of the function must be removed before transforming. In the present work, a new 2D AFT technique based on the Möbius inversion formula on the ring of Gaussian integers [1, 10] is introduced in a concise manner.

Suppose that a function $f(x, y)$ is defined on R^2 with a period of 2π for both the x and y, and with the zero 'direct component', that is,

$$f(x, y) = \sum_{m,n=-\infty}^{\infty} c_{m,n} e^{i(mx+ny)} \tag{10}$$

with

$$\int_D f(x, y)\, dx\, dy \equiv \int_0^{2\pi} \int_0^{2\pi} f(x, y)\, dx\, dy = 0 \tag{11}$$

where $D = [0, 2\pi] \times [0, 2\pi]$, and

$$c_{m,n} = \frac{1}{4\pi^2} \int_D f(x, y) e^{-i(mx+ny)}\, dx\, dy. \tag{12}$$

Now let us use the notation $\alpha = m + ni$, and write $c_{m,n} = c_\alpha$. The sum in (10) is equivalent to a sum over α, with α taking all values in the set G^* of non-zero Gaussian integers. As discussed in section 2, for the Gaussian integers we have a unique factorization property and a Möbius inversion formula, which will be used below.

Writing $\beta = a + bi \in G^*$, we have

$$\begin{aligned} S_\alpha \equiv \sum_{\beta \in G^*} c_{\alpha\beta} &= \frac{1}{4\pi^2} \int_D \left[\sum_{\beta \in G^*} e^{-i[(am-bn)x+(bm+an)y]} \right] f(x, y)\, dx\, dy \\ &= \frac{1}{4\pi^2} \int_D \left[\sum_{\beta \in G^*} e^{-ia(mx+ny)} e^{-ib(-nx+my)} \right] f(x, y)\, dx\, dy. \end{aligned} \tag{13}$$

Noting that

$$\sum_{n=-\infty}^{\infty} e^{inx} = 2\pi \sum_{q=-\infty}^{\infty} \delta(x - 2q\pi) \tag{14}$$

and considering $\beta = a + b\mathrm{i}$, it is given that

$$S_\alpha = \frac{1}{4\pi^2}\int_D \left[-1 + 4\pi^2 \sum_{p,q=-\infty}^{\infty} \delta(mx + ny - 2p\pi)\delta(-nx + my - 2q\pi)\right] f(x, y)\,\mathrm{d}x\,\mathrm{d}y$$
$$= \sum_{p,q=-\infty}^{\infty} \int_D \delta(mx + ny - 2p\pi)\delta(-nx + my - 2q\pi) f(x, y)\,\mathrm{d}x\,\mathrm{d}y.$$

Since D is a bounded region, when $|p|$, $|q|$ are large enough, the corresponding terms vanish, thus only finitely many terms make a contribution to the above summation.

We introduce the transformation of variables

$$u = mx + ny$$
$$v = -nx + my.$$

Notice that the Jacobian can be expressed as

$$\Delta \equiv \begin{vmatrix} m & n \\ -n & m \end{vmatrix} = m^2 + n^2 = |\alpha|^2 \neq 0$$

and

$$x = (mu - nv)/\Delta$$
$$y = (nu + mv)/\Delta.$$

Therefore, equation (13) can be expressed as

$$S_\alpha = \frac{1}{\Delta}\sum_{p,q=-\infty}^{\infty}\int_{D'} \delta(u - 2p\pi)\delta(v - 2q\pi) f\left(\frac{mu - nv}{\Delta}, \frac{nu + mv}{\Delta}\right)\mathrm{d}u\,\mathrm{d}v$$
$$= \frac{1}{\Delta}\sum_{(u,v)\in D'(\alpha)} f\left(\frac{mu - nv}{\Delta}, \frac{nu + mv}{\Delta}\right) = \frac{1}{\Delta}\sum_{(x,y)\in D(\alpha)} f(x, y)$$
$$= \frac{1}{|\alpha|^2}\sum_{(x,y)\in D(\alpha)} f(x, y) \tag{15}$$

where $D(\alpha)$ is determined uniquely by $\alpha = m + \mathrm{i}n$. In other words, for certain (m, n), only a finite number of points $\{2\pi(mp - nq)/(m^2 + n^2),\ 2\pi(np + mq)/(m^2 + n^2)\}$ would be inside the field $[0, 2\pi] \times [0, 2\pi]$, and p, q are integers. This finite point set is also called the interpolation point set.

For the equation

$$S_\alpha = \sum_{\beta\in G^*} c_{\alpha\beta} \tag{16}$$

we have the corresponding Möbius inversion formula as

$$\sum_{z\in U} c_{z\alpha} = \tfrac{1}{4}\sum_{\beta\in G^*}\mu(\beta)S_{\alpha\beta} \tag{17}$$

since the right-hand side of (17) is equal to

$$\tfrac{1}{4}\sum_{\beta\in G^*}\mu(\beta)S_{\alpha\beta} = \tfrac{1}{4}\sum_{\beta\in G^*}\mu(\beta)\sum_{\gamma} c_{\alpha\beta\gamma}$$
$$\stackrel{\beta'=\beta\gamma}{=} \tfrac{1}{4}\sum_{\beta'\in G^*} c_{\alpha\beta'}\sum_{\beta|\beta'}\mu(\beta) = 4[\tfrac{1}{4}]\sum_{\beta'\in U} c_{\beta'\alpha}$$
$$= c_\alpha + c_{\mathrm{i}\alpha} + c_{-\alpha} + c_{-\mathrm{i}\alpha}.$$

Thus

$$W_1 \equiv c_\alpha + c_{\mathrm{i}\alpha} + c_{-\alpha} + c_{-\mathrm{i}\alpha} = \tfrac{1}{4}\sum_{\beta\in G^*}\frac{\mu(\beta)}{|\alpha\beta|^2}\sum_{(x,y)\in D(\alpha\beta)} f(x,y). \tag{18}$$

Now, let us consider

$$F(x,y) \equiv f(x+s\pi, y+t\pi) = \sum_{m,n=-\infty}^{\infty} c_{m,n}\mathrm{e}^{\mathrm{i}[m(x+s\pi)+n(y+t\pi)]}$$
$$= \sum_{m,n=-\infty}^{\infty} c_{m,n}\mathrm{e}^{\mathrm{i}(ms+nt)\pi}\mathrm{e}^{\mathrm{i}(mx+ny)}.$$

From the periodicity of $f(x,y)$ and $c_{0,0}=0$, it is also given that

$$\int_0^{2\pi}\int_0^{2\pi} F(x,y)\,\mathrm{d}x\,\mathrm{d}y = 0.$$

Again writing that $\alpha = m+n\mathrm{i}$, from equation (18) we have

$$c_\alpha \mathrm{e}^{\mathrm{i}(ms+nt)\pi} + c_{\alpha\mathrm{i}}\mathrm{e}^{\mathrm{i}(-ns+mt)\pi} + c_{-\alpha}\mathrm{e}^{\mathrm{i}(-ms-nt)\pi} + c_{-\alpha\mathrm{i}}\mathrm{e}^{\mathrm{i}(ns-mt)\pi}$$
$$= \tfrac{1}{4}\sum_{\beta\in G^*}\frac{\mu(\beta)}{|\alpha\beta|^2}\sum_{(x,y)\in D(\alpha\beta)} f(x+s\pi, y+t\pi). \tag{19}$$

(i) Let $s=\frac{n}{\Delta}$, $t=\frac{-m}{\Delta}$. Then

$$W_2 \equiv c_\alpha \mathrm{e}^{\mathrm{i}0\pi} + c_{\alpha\mathrm{i}}\mathrm{e}^{-\mathrm{i}\pi} + c_{-\alpha}\mathrm{e}^{\mathrm{i}0\pi} + c_{-\alpha\mathrm{i}}\mathrm{e}^{\mathrm{i}\pi}$$
$$= c_\alpha - c_{\alpha\mathrm{i}} + c_{-\alpha} - c_{-\alpha\mathrm{i}}$$
$$= \frac{1}{4}\sum_{\beta\in G^*}\frac{\mu(\beta)}{|\alpha\beta|^2}\sum_{(x,y)\in D(\alpha\beta)} f\left(x+\frac{n}{m^2+n^2}\pi, y+\frac{-m}{m^2+n^2}\pi\right). \tag{20}$$

(ii) Let $s=\frac{m+n}{2\Delta}$, $t=\frac{-m+n}{2\Delta}$. Then

$$W_3 \equiv \mathrm{i}[c_\alpha - c_{\alpha\mathrm{i}} - c_{-\alpha} + c_{-\alpha\mathrm{i}}]$$
$$= \frac{1}{4}\sum_{\beta\in G^*}\frac{\mu(\beta)}{|\alpha\beta|^2}\sum_{(x,y)\in D(\alpha\beta)} f\left(x+\frac{m+n}{2(m^2+n^2)}\pi, y+\frac{-m+n}{2(m^2+n^2)}\pi\right). \tag{21}$$

(iii) Let $s=\frac{m-n}{2\Delta}$, $t=\frac{m+n}{2\Delta}$. Then

$$W_4 \equiv \mathrm{i}[c_\alpha + c_{\alpha\mathrm{i}} - c_{-\alpha} - c_{-\alpha\mathrm{i}}]$$
$$= \frac{1}{4}\sum_{\beta\in G^*}\frac{\mu(\beta)}{|\alpha\beta|^2}\sum_{(x,y)\in D(\alpha\beta)} f\left(x+\frac{m-n}{2(m^2+n^2)}\pi, y+\frac{m+n}{2(m^2+n^2)}\pi\right). \tag{22}$$

From the above, we have

$$c_{\alpha\mathrm{i}} - c_{-\alpha\mathrm{i}} = \frac{\mathrm{i}}{2}(W_2 - W_3). \tag{23}$$

Finally, it is given that

$$c_\alpha = \tfrac{1}{4}[(W_1+W_2) - \mathrm{i}(W_3+W_4)] \tag{24}$$
$$c_{-\alpha} = \tfrac{1}{4}[(W_1+W_2) + \mathrm{i}(W_3+W_4)] \tag{25}$$
$$c_{\alpha\mathrm{i}} = \tfrac{1}{4}[(W_1-W_2) + \mathrm{i}(W_3-W_4)] \tag{26}$$
$$c_{-\alpha\mathrm{i}} = \tfrac{1}{4}[(W_1-W_2) - \mathrm{i}(W_3-W_4)]. \tag{27}$$

In many cases, $f(x,y)$ is real, and all the W_1, W_2, W_3 and W_4 are real, hence $\bar{c_\alpha} = c_{-\alpha}$. From the above, we see that the multiplicative operations in this AFT are much less than that in FFT, which is quite suitable for a parallel processing design. However, the sampling distribution needs further improvement for practical application.

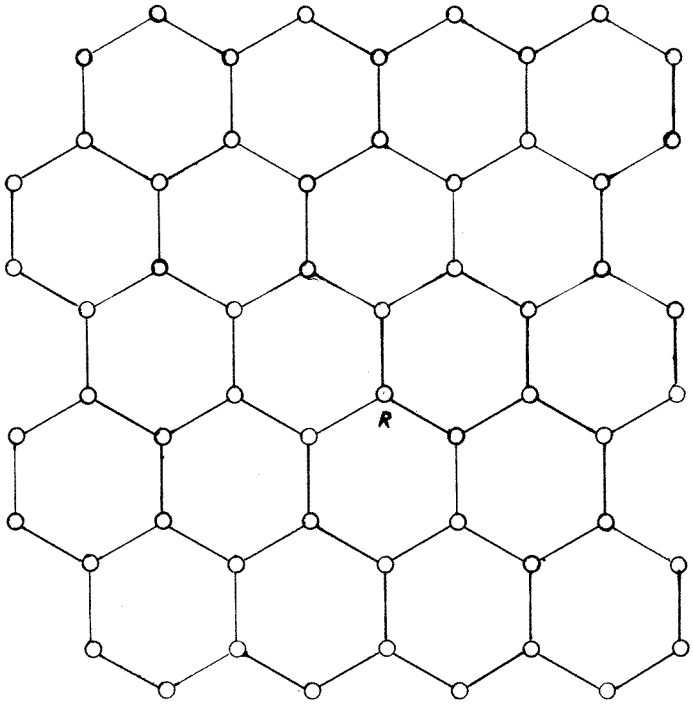

Figure 1. A 2D hexagonal lattice. Here R is the point about which rotation occurs.

4. 2D hexagonal lattice problem and ring of Eisenstein's integers

4.1. Möbius inverse formula on Eisenstein's ring

The 2D hexagonal lattice such as a monolayer graphite is essentially a complex lattice as shown in figure 1. Rotate it through 180° around a reference point R, then superimpose the new pattern on the original one. Obviously, the final result is equivalent to a superposition of two face-centred hexagonal lattices with lattice constants x and $\sqrt{3}x$ respectively (figure 2), and each of them can be represented as a ring of Eisenstein's integers [1, 10], i.e.

$$\boldsymbol{E} = \{a + b\omega \mid a, b \in \boldsymbol{Z}\} \tag{28}$$

where a, b are integers, and

$$\omega = \frac{1 + \sqrt{3}\mathrm{i}}{2} = \mathrm{e}^{\mathrm{i}\pi/3}. \tag{29}$$

Since $\omega^2 = \omega - 1$, the product of two Eisenstein's integers is itself an Eisenstein's integer. The idea of factorization, of units, and of association of elements go through as for the Gaussian integers, except that the units are

$$\boldsymbol{U} = \{\pm 1, \pm\omega, \pm\omega^2\} \tag{30}$$

which represents all the roots of $z^6 = 1$. Any non-zero Eisenstein's integer is therefore associated with five other distinct Eisenstein's integers.

This also includes a multiplicative semigroup with unique factorization considering the associative relations.

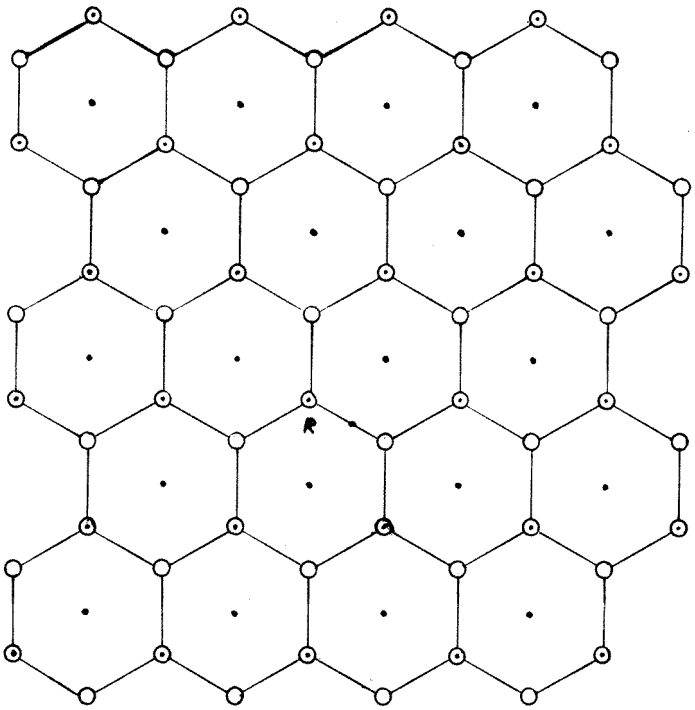

Figure 2. Put the two pictures before and after rotation together. The final result is a superposition of two face-centred hexagons.

Therefore, the cohesive energy of the hexagonal lattice is equal to

$$E(x) = \tfrac{1}{2} \sum_{\alpha \in \boldsymbol{E}^*} \tfrac{1}{2}[\Phi(|\alpha|x) + \Phi(\sqrt{3}|\alpha|x)] \tag{31}$$

where $\alpha = a + b\omega$ represents an Eisenstein's integer, and $\boldsymbol{E}^*$ is the set of non-zero Eisenstein's integers. Based on the Möbius theorem on the Eisenstein's ring, the solution of (31) can be given immediately as

$$[\Phi(x) + \Phi(\sqrt{3}x)] = \frac{4}{6^2} \sum_{\alpha \in \boldsymbol{E}^*} \mu(\alpha) E(|\alpha|x).$$

Therefore, as the previous section, it leads to

$$\Phi(x) = \tfrac{1}{9} \sum_{n=0}^{\infty} (-1)^n \sum_{\alpha \in \boldsymbol{E}^*} \mu(\alpha) E(|\alpha| 3^{\frac{n}{2}} x). \tag{32}$$

This result is quite concise and easy for practical calculation. The Möbius function on the ring of Eisenstein's integers is shown in table 2. Note that the rotation of the lattice is equivalent to constructing a principal ideal in the theory of rings, which is similar to a normalized subgroup in the group theory.

The pair potentials between distinct atoms can be obtained by solving the inverse problems for a binary structure.

Table 2. Eisenstein's Möbius functions.

m	$n \rightarrow$	0	1	2	3	4	5	6	7	8
1		1	−1	−1	−1	1	−1	−1	1	−1
2		−1	−1	1	−1	1	1	1	−1	−1
3		0	−1	−1	0	−1	0	0	−1	−1
4		0	1	1	−1	0	−1	1	1	0
5		−1	−1	1	0	−1	−1	1	−1	1
6		0	−1	1	0	1	1	0	−1	1
7		1	1	−1	−1	1	−1	−1	−1	0
8		0	−1	−1	−1	0	1	1	0	0

4.2. Application to graphite monolayer

It is well known that graphite has a layer structure with very strong interactions in planes and very weak interactions between planes. Now let us calculate the in-plane elastic constants of monolayer graphite by using the Möbius inverse formula on the Eisenstein ring.

4.2.1. Calculation of pair potential The *ab initio* calculated total energy for a monolayer graphite sheet using the FLAPW method has been completed [15]. Here, the Rose function is taken to fit the total energy curve as

$$E(x) = -a(1 + \alpha(x - x_0))\mathrm{e}^{-\alpha(x-x_0)} \tag{33}$$

where x is the lattice constant and x_0 is the lattice constant at equilibrium state. The parameters in (33) are listed in table 3.

Table 3. Parameters for fitting total energy of graphite monolayer.

		a (eV/atom)	$\alpha(\mathrm{A}^{-1})$	x_0 (A)
1	*ab initio* limited basis [15]	7.41	3.038	1.429
2	*ab initio* converged basis [15]	8.69	2.842	1.415
3	Experiment	7.39 [16]	3.029 [17]	1.421 [16]

The calculated C–C pair potential can be obtained using (32). If it is also fit in Rose form as

$$\phi(r) = -a(1 + \alpha(r - r_0))\mathrm{e}^{-\alpha(r-r_0)} \tag{34}$$

then the fitting parameters are as shown in table 4.

Table 4. The calculated C–C pair potential based on the Rose equation.

	a (eV)	$\alpha(\mathrm{A}^{-1})$	r_0 (A)
1	3.456	3.095	1.594
2	3.795	2.900	1.622
3	3.422	3.083	1.589

Note that table 4 corresponds to table 3 associated with three sources of total energy curves respectively.

4.2.2. Calculated results of elastic constants. For convenience, we define

$$e_{ij} = \frac{c}{2} C_{ij} \tag{35}$$

where c is lattice constant of bulk hcp crystal in c-axes direction, e_{ij} and C_{ij} are the ijth elastic constants and the ij-component of elastic modulus tensor respectively. Then e_{ij} can be expressed as

$$e_{ij} = \frac{1}{s_0} \frac{\partial^2 \mathcal{E}}{\partial \epsilon_i \partial \epsilon_j}\bigg|_{\epsilon_i=0,\epsilon_j=0} \tag{36}$$

where s_0 is the equilibrium atom area in plane,

$$s_0 = \frac{3\sqrt{3}}{4} x_0^2 \tag{37}$$

and $\mathcal{E}$ is the deformation energy per atom in the monolayer.

The strains are given by the following transformations:

$$x' = x(1+\epsilon)\ \ y' = y \qquad \text{for } e_{11}$$
$$x' = x(1+\epsilon_1)\ \ y' = y(1+\epsilon_2) \qquad \text{for } e_{12}$$

and

$$x' = \frac{x}{\sqrt{1+\epsilon^2}}\ \ y' = y + \frac{x\epsilon}{\sqrt{1+\epsilon^2}} \qquad \text{for } e_{66}.$$

According to a similar method to that discussed before, the deformation energy $\mathcal{E}(\epsilon_i, \epsilon_j)$ can be expressed as the sums of pair potential and then the elastic constants can be expressed as

$$e_{11} = \frac{1}{24\sqrt{3}x_0} \sum_{\alpha\in E} \{|\alpha|\phi'(|\alpha|x_0) + \sqrt{3}|\alpha|\phi'(\sqrt{3}|\alpha|x_0)\}$$
$$+ \frac{1}{8\sqrt{3}} \sum_{\alpha\in E} \{|\alpha|^2\phi''(|\alpha|x_0) + 3|\alpha|^2\phi''(\sqrt{3}|\alpha|x_0)\} \tag{38}$$

and

$$e_{12} = e_{66} = -\frac{1}{24\sqrt{3}x_0} \sum_{\alpha\in E} \{|\alpha|\phi'(|\alpha|x_0) + \sqrt{3}|\alpha|\phi'(\sqrt{3}|\alpha|x_0)\}$$
$$+ \frac{1}{24\sqrt{3}} \sum_{\alpha\in E} \{|\alpha|^2\phi''(|\alpha|x_0) + 3|\alpha|^2\phi''(\sqrt{3}|\alpha|x_0)\} \tag{39}$$

where ϕ' and ϕ'' are the first and the second derivative of ϕ respectively. Thus, we have

$$e_{11} = \frac{1}{6\sqrt{3}} \mathcal{E}'(x_0) + \frac{1}{2\sqrt{3}} \mathcal{E}''(x_0) \tag{40}$$

and

$$e_{12} = e_{66} = -\frac{1}{6\sqrt{3}} \mathcal{E}'(x_0) + \frac{1}{6\sqrt{3}} \mathcal{E}''(x_0). \tag{41}$$

The equilibrium condition of a lattice is

$$E'(x_0) = 0$$

therefore

$$e_{11} = 3e_{12} = 3e_{66} = \frac{1}{2\sqrt{3}} \mathcal{E}''(x_0). \tag{42}$$

Table 5. The comparison of calculated and experimental elastic constants with unit of N/m.

		e_{11}	e_{12}	e_{66}
Calculated	1	315.9	105.3	105.3
	2	324.2	108.1	108.1
	3	313.2	104.5	104.5
Experiment [17]		378.6	94.5	—
Experiment [18]		355.1	60.3	147.4

The experimental values of e_{ij} are calculated from the relation $e_{ij} = \frac{c}{2}C_{ij}$, in which $c = 6.7$A [16]. The calculated results are listed in table 5.

The calculated results are quite acceptable although many-body interactions have been ignored [18].

5. Conclusion and discussion

From the above discussion, the inverse 2D lattice problem can be solved successfully based on different kinds of Möbius inversion theorems in the theory of rings. The solutions presented in this work are not only concise for theoretical analysis, but also rapidly convergent for practical calculations in physics. This provides a convenient bridge between the electronic structure calculation and mechanical, thermal or chemical properties. Also, we would like to mention some other interesting works on the applications of Möbius inversion formulae to physical problems, such as the Möbius method based on partially ordered sets for the cluster variation method in statistical physics [19], and the Möbius inversion formula for supersymmetry in quantum field theory [20].

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Appendix. Some notes on AFT

This appendix illustrates an improved practical implementation of the one-dimensional AFT, which can also be generalized to the two-dimensional AFT. Suppose that a function $f(x)$ is defined on $(-\infty, \infty)$ with period 2π and zero direct component, that is

$$f(x) = \sum_{n=-\infty}^{\infty} c_n \mathrm{e}^{\mathrm{i}nx} \tag{A1}$$

where

$$c_n = \frac{1}{2\pi}\int_0^{2\pi} \mathrm{e}^{-\mathrm{i}nx} f(x)\,\mathrm{d}x \qquad \text{with } c_0 = 0. \tag{A2}$$

Then we define

$$S_n = \sum_{k=1}^{\infty}(c_{nk} + c_{-nk}) = \frac{1}{n}\sum_{m=1}^{n} f\left(\frac{2m\pi}{n}\right). \tag{A3}$$

Therefore,

$$c_n + c_{-n} = \sum_{k=1}^{\infty}\mu(k)S_{nk} = \sum_{k=1}^{\infty}\frac{\mu(k)}{nk}\sum_{m=1}^{nk} f\left(\frac{2m\pi}{nk}\right). \tag{A4}$$

Similarly, from

$$f(x+y) = \sum_{n=-\infty}^{\infty} c_n \mathrm{e}^{\mathrm{i}nx}\mathrm{e}^{\mathrm{i}ny} \tag{A5}$$

we have

$$S_n(y) = \sum_{k=1}^{\infty}(c_{nk}\mathrm{e}^{\mathrm{i}nky} + c_{-nk}\mathrm{e}^{-\mathrm{i}nky}) = \frac{1}{n}\sum_{m=1}^{n} f\left(\frac{2m\pi}{n} + y\right) \tag{A6}$$

and

$$c_n\mathrm{e}^{\mathrm{i}ny} + c_{-n}\mathrm{e}^{-\mathrm{i}ny} = \sum_{k=1}^{\infty}\mu(k)S_{nk}(y) = \sum_{k=1}^{\infty}\frac{\mu(k)}{nk}\sum_{m=1}^{nk} f\left(\frac{2m\pi}{nk} + y\right). \tag{A7}$$

Let

$$\begin{cases} c_{nk}\mathrm{e}^{\mathrm{i}nky_1} + c_{-nk}\mathrm{e}^{-\mathrm{i}nky_1} & = W_1 \\ c_{nk}\mathrm{e}^{\mathrm{i}nky_2} + c_{-nk}\mathrm{e}^{-\mathrm{i}nky_2} & = W_2 \end{cases} \tag{A8}$$

then

$$c_n = \frac{\begin{vmatrix} W_1 & \mathrm{e}^{-\mathrm{i}ny_1} \\ W_2 & \mathrm{e}^{-\mathrm{i}ny_2} \end{vmatrix}}{\Delta} = \frac{W_1\mathrm{e}^{-\mathrm{i}ny_2} - W_2\mathrm{e}^{-\mathrm{i}ny_1}}{\Delta} \tag{A9}$$

and

$$c_{-n} = \frac{\begin{vmatrix} \mathrm{e}^{\mathrm{i}ny_1} & W_1 \\ \mathrm{e}^{\mathrm{i}ny_2} & W_2 \end{vmatrix}}{\Delta} = \frac{W_2\mathrm{e}^{\mathrm{i}ny_1} - W_1\mathrm{e}^{\mathrm{i}ny_2}}{\Delta} \tag{A10}$$

where

$$\Delta = \begin{vmatrix} \mathrm{e}^{\mathrm{i}ny_1} & \mathrm{e}^{-\mathrm{i}ny_1} \\ \mathrm{e}^{\mathrm{i}ny_2} & \mathrm{e}^{-\mathrm{i}ny_2} \end{vmatrix} = \mathrm{e}^{\mathrm{i}n(y_1-y_2)} - \mathrm{e}^{-\mathrm{i}n(y_1-y_2)}. \tag{A11}$$

We can select y_1, y_2 such that $y_1 - y_2 \neq \frac{k}{n}\pi$ and $\Delta \neq 0$. If $f(x)$ is real, and $f(x) = \sum_{n=1}^{\infty}[a_n\cos nx + b_n\sin nx]$, then

$$a_n = c_n + c_{-n} \qquad \text{and} \qquad b_n = \mathrm{i}(c_n - c_{-n}). \tag{A12}$$

Therefore

$$\begin{aligned} a_n &= \frac{\begin{vmatrix} W_1 & \mathrm{e}^{-\mathrm{i}ny_1} \\ W_2 & \mathrm{e}^{-\mathrm{i}ny_2} \end{vmatrix} - \begin{vmatrix} W_1 & \mathrm{e}^{\mathrm{i}ny_1} \\ W_2 & \mathrm{e}^{\mathrm{i}ny_2} \end{vmatrix}}{\Delta} \\ &= \frac{\begin{vmatrix} W_1 & \mathrm{e}^{-\mathrm{i}ny_1} - \mathrm{e}^{\mathrm{i}ny_1} \\ W_2 & \mathrm{e}^{-\mathrm{i}ny_2} - \mathrm{e}^{\mathrm{i}ny_2} \end{vmatrix}}{\Delta} \end{aligned}$$

$$= \frac{\begin{vmatrix} W_1 & -\sin ny_1 \\ W_2 & -\sin ny_2 \end{vmatrix}}{\sin n(y_1 - y_2)} = \frac{W_2 \sin ny_1 - W_1 \sin ny_2}{\sin n(y_1 - y_2)} \tag{A13}$$

$$b_n = \mathrm{i}\frac{\begin{vmatrix} W_1 & \mathrm{e}^{-\mathrm{i}ny_1} \\ W_2 & \mathrm{e}^{-\mathrm{i}ny_2} \end{vmatrix} + \begin{vmatrix} W_1 & \mathrm{e}^{\mathrm{i}ny_1} \\ W_2 & \mathrm{e}^{\mathrm{i}ny_2} \end{vmatrix}}{\Delta}$$

$$= \frac{\begin{vmatrix} W_1 & \cos ny_1 \\ W_2 & \cos ny_2 \end{vmatrix}}{\sin n(y_1 - y_2)} = \frac{W_1 \cos ny_2 - W_2 \cos ny_1}{\sin n(y_1 - y_2)}\,. \tag{A14}$$

If only finitely many terms N are taken, or $1 \leqslant n \leqslant N$, then we may have $y_1 = 0$, and $y_2 = \pi/(N+1)$. In this case, we have

$$a_n = W_1 = \sum_{k=1}^{\infty} \mu(k) S_{nk}(0) = \sum_{k=1}^{\infty} \frac{\mu(k)}{nk} \sum_{m=1}^{nk} f\left(\frac{2m\pi}{nk}\right) \tag{A15}$$

and

$$b_n = \frac{W_2 - W_1 \cos\left(\frac{n\pi}{N+1}\right)}{\sin\left(\frac{n\pi}{N+1}\right)} \tag{A16}$$

where

$$W_2 = \sum_{k=1}^{\infty} \frac{\mu(k)}{nk} \sum_{m=0}^{\infty} f\left(\frac{2m\pi}{nk} + \frac{\pi}{N+1}\right)$$

$$= \sum_{k=1}^{\infty} \mu(k) S_{nk}\left(\frac{\pi}{N+1}\right). \tag{A17}$$

In this way, the sampling distribution becomes more convenient for calculation than the existing works, but there still exist practical problems for further study.

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