

Multidimensional inverse lattice problem and a uniformly sampled arithmetic Fourier transform

Chen Nan-xian, Chen Zhao-dou, and Wei Yu-chuan

China Center of Advanced Science and Technology (World Laboratory), P.O. Box 8730, Beijing 100080, China
and Institute of Applied Physics, Beijing University of Science and Technology, Beijing 100083, China*

(Received 3 January 1996; revised manuscript received 30 May 1996)

The present work develops a unified and concise solution for inverse lattice problems. Also, a uniformly sampled arithmetic Fourier transform is presented in this work which uses Ramanujan's sum rule.
[S1063-651X(96)51911-2]

PACS number(s): 05.50.+q, 02.10.Nj, 02.20.Mp, 02.30.Nw

In the present time of facing the rapid spread of large scale digital computation and parallel information processing, it is expected that numerous facilities in number theory could be of increasing importance in science and technology. This paper develops two useful formulas. The first is a universal *multidimensional* Möbius inversion formula for wide applications to inverse lattice problems in condensed matter physics. The second is an application of the *Ramanujan's sum* to parallel signal processing.

I. MÖBIUS INVERSION FOR MULTIDIMENSIONAL LATTICES

The classical Möbius inversion formula [1,2] has been given wide attention in the last decade for its successful applications to inverse problems in the physical sciences [3-6]. However, a more demanding question is whether it will be feasible to extend the trick to problems that are not simply one dimensional. On the face of things that might seem a mere formality, but it takes only a little effort to find problems essentially tied up with the multiple connectedness of all but one-dimensional spaces [7].

This section provides a unified solution to multidimensional inverse lattice problems with all different kinds of lattice structures based on a generalized Dirichlet inverse. For convenience and clarity, the concise and unified solution is developed and illustrated through the inversive cohesion problem. In general, the cohesive energy $E(x)$ for each atom in a multidimensional crystal lattice can be expressed as a sum of interatomic pair potentials $\Phi(x)$ such that

$$E(x) = \frac{1}{2} \sum_{\mathbf{R} \neq 0} \Phi(\mathbf{R}), \quad (1)$$

where x is the nearest neighbor distance, \mathbf{R} is the lattice vector. For convenience, the absolute value of \mathbf{R} can be expressed as $b_0(n)x$ such that

$$E(x) = \frac{1}{2} \sum_{n=1}^{\infty} r_0(n) \Phi(b_0(n)x), \quad (2)$$

where $b_0(n)$ in a monotonically increasing series represents the distance between the origin on which the reference atom is located and the n th set of lattice points, $r_0(n)$ is the num-

ber of the n th set of lattice points. For example, $b_0(1)=1$ corresponds to the nearest neighbor distance. The inverse lattice problem is to determine $\Phi(x)$ from the fitting curve $E(x)$, which can be obtained from the *ab initio* calculation. The trick here is to extend the series $\{b_0(n)\}$ to $\{b(n)\}$ to achieve multiplicative closeness. Thus, for any m and n , there exist k such that

$$b(k) = b(m)b(n). \quad (3)$$

In other words, $\{b_0(n)\}$ can always be replaced by a multiplicative semigroup $\{b(n)\}$. Therefore, Eq. (2) is equivalent to the following:

$$E(x) = \frac{1}{2} \sum_{n=1}^{\infty} r(n) \Phi(b(n)x), \quad (4)$$

in which

$$r(n) = \begin{cases} r_0(b_0^{-1}[b(n)]), & \text{if } b(n) \in \{b_0(n)\}, \\ 0, & \text{if } b(n) \notin \{b_0(n)\}. \end{cases} \quad (5)$$

The lattice point shell is called *vertural* when $r(n)=0$.

Then the solution to Eq. (4) is given by

$$\Phi(x) = 2 \sum_{n=1}^{\infty} I(n) E(b(n)x), \quad (6)$$

in which the inversion coefficient or the generalized Möbius function $I(n)$ is given by

$$\sum_{b(n)|b(k)} I(n) r \left[b^{-1} \left(\frac{b(k)}{b(n)} \right) \right] = \delta_{k1}. \quad (7)$$

This indicates that $I(n)$ and $r(n)$ are the modified Dirichlet inverse of each other, which is a generalization of common Dirichlet inverse in number theory. The following proves that Eq. (6) is the solution to Eq. (4), as well as to Eq. (2).

$$\begin{aligned} & 2 \sum_{n=1}^{\infty} I(n) E(b(n)x) \\ &= \sum_{k=1}^{\infty} \left\{ \sum_{b(n)|b(k)} I(n) r \left[b^{-1} \left(\frac{b(k)}{b(n)} \right) \right] \right\} \Phi(b(k)x) \\ &= \sum_{k=1}^{\infty} \delta_{k1} \Phi(b(k)x) = \Phi(b(1)x) = \Phi(x). \end{aligned}$$

*Mailing address.

TABLE I. The generalized Möbius function $I(n)$ for a fcc structure.

n	1	2	3	4	5	6	7	8	9	10
$[b(n)]^2$	1	2	3	4	5	6	7	8	9	10
$r(n)$	12	6	24	12	24	8	48	6	36	24
$I(n)$	1/12	-1/24	-1/6	-1/6	-1/6	1/9	-1/3	1/32	1/12	0
n	11	12	13	14	15	16	17	18	19	
$[b(n)]^2$	11	12	13	14	15	16	17	18	19	
$r(n)$	24	24	72	0	48	12	48	30	72	
$I(n)$	-1/6	7/72	-1/2	1/3	-1/64	-1/3	-17/72	-1/2		

In the case where $[b(n)]^2$ are not integers, the least common multiple of all the denominators can be used in the recursive procedure. The solution in Eqs. (6) and (7) can be applied to any lattice structure of interest in condensed matter physics or statistical physics including fcc, $L1_2$, $L1_0$, Diamond, bcc, hcp, DO_3 , and Fibonacci structure. Several examples are provided as follows.

A. Example: fcc structure

The binding energy can be expressed as

$$\begin{aligned}
 E(x) &= \frac{1}{2} \sum_{\{i,j,k\} \neq 0} \Phi[\sqrt{2(i^2+j^2+k^2)}x] \\
 &\quad + \frac{3}{2} \sum_{i,j,k} \Phi\{\sqrt{2[(i-\frac{1}{2})^2+(j-\frac{1}{2})^2+k^2]}x\} \\
 &= \sum_{n=1}^{\infty} r_0(n) \Phi(b_0(n)x), \tag{8}
 \end{aligned}$$

in which the distribution $\{b_0(n)\}$ adding a small fraction of terms is simply equal to $\{\sqrt{n}\}$. The latter is closed under multiplication. Thus, let $b(n) = \{\sqrt{n}\}$, Eqs. (6) and (7) can be applied directly to obtain the solution. Note that in this case we have

$$b(mn) = b(m)b(n), \quad b^{-1}\left(\frac{b(k)}{b(n)}\right) = \frac{k}{n}.$$

Here, the condition of sum over $b(n)|b(k)$ in Eq. (7) can be simplified to $n|k$, or

$$\sum_{n|k} I(n)r\left(\frac{k}{n}\right) = \delta_{k1}. \tag{9}$$

The left-hand side of Eq. (10) is just the common Dirichlet product of $I(n)$ and $r(n)$. Therefore,

$$I(1) = \frac{1}{r(1)} = \frac{1}{12},$$

$$I(2) = -\frac{I(1)r(2)}{r(1)} = -\frac{\frac{1}{12} \times 6}{12} = -\frac{1}{24}, \dots$$

The inversion coefficient or the Möbius function $I(n)$ for a fcc structure are listed in Table I. It is noted that the values of inversion coefficients $I(n)$ are no longer 1, -1, and 0 as for the usual Möbius function.

B. Example: bcc structure

The binding energy per atom in a bcc lattice can be expressed as

$$\begin{aligned}
 E(x) &= \frac{1}{2} \sum_{(l,m,n) \neq (0,0,0)} [\Phi(\sqrt{\frac{4}{3}\{l^2+m^2+n^2\}}x) \\
 &\quad + \Phi(\sqrt{\frac{4}{3}\{(l-\frac{1}{2})^2+(m-\frac{1}{2})^2+(n-\frac{1}{2})^2\}}x)] \\
 &= \frac{1}{2} \sum_{n=1}^{\infty} \Phi(b(n)x), \tag{10}
 \end{aligned}$$

with the distribution $b_0(n)$ and $r_0(n)$ as seen in Table II.

We use $\{b_0(n)\}$ as a generator to produce a series $\{b(n)\}$ with weights $\{r(n)\} \cdot \{b(n)\}$ as a multiplicative semigroup, which is closed under multiplication. Now the solution is given in Table III.

$$\begin{aligned}
 \Phi(x) &= 2 \left[\frac{1}{8} E(x) - \frac{3}{32} E(\sqrt{\frac{4}{3}}x) + \frac{9}{128} E(\frac{4}{3}x) \right. \\
 &\quad \left. - \frac{27}{512} E\left(\sqrt{\frac{64}{27}}x\right) + \dots \right].
 \end{aligned}$$

Thus the effective pair potentials can be easily evaluated based on the cohesive energy curve $E(x)$, which can be calculated using the *ab initio* data for real or virtual structures [8–11]. This method is also available for improving the embedded atom method (EAM) potentials [12]. Obviously, the solutions to inverse lattice problems are useful for all types of multidimensional problems in physical science. Note that the technique can be replaced by the method based on algebraic rings of integers for two-dimensional inverse lattice problems [13], then the inversion coefficient takes values only of 1, -1, 0.

In conclusion, Eqs. (6) and (7) have provided a resolution to Maddox's challenge [7].

II. RAMANUJAN'S SUM AND UNIFORM SAMPLING FOURIER EXPANSION

Ramanujan's sum $C(m,n)$ is defined as

$$C(m,n) = \sum_{\substack{h \in [0,n-1] \\ (h,n)=1}} e^{2\pi i h m/n}, \tag{11}$$

TABLE II. The coefficients $b_0(n)$ and $r_0(n)$ of a bcc structure.

$b_0(n)^2$	1	4/3	8/3	11/3	4	16/3	19/3	20/3	8	9
$r_0(n)$	8	6	12	24	8	6	24	24	32	12
$b_0(n)^2$	32/3	35/3	12	40/3	43/3	44/3	16			
$r_0(n)$	12	48	30	24	24	24	8			

where h runs only over values less than n and prime to n . Also, there is an interesting theorem on Ramanujan's sum [1,2]. The theorem states that

$$\sum_{\substack{h \in [0, n-1] \\ (h, n) = 1}} e^{2\pi i h m / n} = \sum_{d|(m, n)} d \mu(n/d), \quad (12)$$

where d runs over the common divisors of m and n . Equation (13) implies that the Ramanujan's sum $C(m, n)$ is always an integer. Maddox was interested in the application of this strange formula.

Now let us introduce a uniform sampling arithmetic Fourier transform (USAFT). The simplest theorem of USAFT states that if

$$f(x) = \sum_{n|N} a_n \cos nx, \quad (13)$$

then

$$a_n = \frac{1}{N} \sum_{s=1}^N C\left(s, \frac{N}{n}\right) f\left(\frac{2\pi s}{N}\right). \quad (14)$$

This theorem indicates that the coefficients of USAFT are simply equal to Ramanujan's sum, which sum can be evaluated by addition and subtraction of some integers, which is suitable for parallel processing.

Proof. Let

$$\tilde{f}(x) = \sum_{n|N} a_n e^{inx},$$

then

$$\begin{aligned} & \frac{1}{N} \sum_{s=1}^N C\left(s, \frac{N}{n}\right) f\left(\frac{2\pi s}{N}\right) \\ &= \frac{1}{N} \sum_{s=1}^N \sum_{\substack{h \in [1, N/n] \\ (h, N/n) = 1}} e^{i2\pi h(s/N/n)} f\left(\frac{2\pi s}{N}\right) \\ &= \frac{1}{N} \sum_{s=1}^N \sum_{\substack{h \in [1, N/n] \\ (h, N/n) = 1}} e^{-2\pi h(s/N/n)} \sum_{m|N} a_m e^{2\pi i m s / N} \\ &= \sum_{m|N} a_m \frac{1}{N} \sum_{\substack{h \in [1, N/n] \\ (h, N/n) = 1}} \sum_{s=1}^N e^{(2\pi i s / N)(m + nh)} \\ &= \sum_{m|N} a_m \delta_{mn} = a_n, \end{aligned} \quad (15)$$

or

TABLE III. Inversion function of a bcc structure.

n	1	2	3	4	5	6	7	8	9	10
$[b(n)]^2$	1	$\frac{4}{3}$	$\frac{16}{9}$	$\frac{64}{27}$	$\frac{8}{3}$	$\frac{256}{81}$	$\frac{32}{9}$	$\frac{11}{3}$	4	$\frac{1024}{243}$
$r(n)$	8	6	0	0	12	0	0	24	8	0
$I(n)$	$\frac{1}{8}$	$-\frac{3}{32}$	$\frac{9}{128}$	$-\frac{27}{512}$	$-\frac{3}{16}$	$\frac{81}{2048}$	$\frac{9}{32}$	$-\frac{3}{8}$	$-\frac{1}{8}$	$-\frac{243}{8192}$

$$a_n = \frac{1}{N} \sum_{s=1}^N C\left(s, \frac{N}{n}\right) \tilde{f}\left(\frac{2\pi s}{N}\right). \quad (16)$$

Taking the real part of Eq. (16), we get Eq. (14) immediately. The last step of Eq. (15) is equivalent to

$$\frac{1}{N} \sum_{\substack{h \in [1, N/n] \\ (h, N/n) = 1}} \sum_{s=1}^N e^{(2\pi i s / N)(m + nh)} = \delta_{mn} = \begin{cases} 1, & m = n \\ 0, & m \neq n. \end{cases} \quad (17)$$

In fact, in the case of $m = n$, there exists only one h such that $(h+1)n = N$, thus $\frac{1}{N} \sum_{s=1}^N \exp\{i\frac{2\pi s}{N}(h+1)n\} = 1$. In all other cases, the contribution from h 's and n 's to the sum vanishes because

$$\frac{1}{N} \sum_{s=1}^N e^{2\pi i s i(M/N)} = \begin{cases} 1, & N|M \\ 0, & N \nmid M. \end{cases} \quad (18)$$

The corresponding coefficient for odd component is

$$b_n(N) = \frac{(-1)^k}{N} \sum_{s=1}^N C\left(s - \frac{N}{2q+2}, \frac{N}{n}\right) f\left(\frac{2\pi s}{N}\right) \text{ for } n| \frac{N}{4}, \quad (19)$$

where k and q satisfy

$$n = 2^q(2k+1), \quad q, k = 0, 1, 2, 3, \dots \quad (20)$$

The proof is similar as before. In conclusion, a practical explanation of Ramanujan's sum is discovered.

A. Example for $N=4$

$$\begin{aligned} \begin{pmatrix} a_1 \\ a_2 \\ a_4 \\ b_1 \end{pmatrix} &= \frac{1}{4} \begin{pmatrix} C(1,4) & C(2,4) & C(3,4) & C(4,4) \\ C(1,2) & C(2,2) & C(3,2) & C(4,2) \\ C(1,1) & C(2,1) & C(3,1) & C(4,1) \\ C(0,4) & C(1,4) & C(2,4) & C(3,4) \end{pmatrix} \begin{pmatrix} f(\frac{1}{4}2\pi) \\ f(\frac{2}{4}2\pi) \\ f(\frac{3}{4}2\pi) \\ f(\frac{4}{4}2\pi) \end{pmatrix} \\ &= \frac{1}{4} \begin{pmatrix} 0 & -2 & 0 & 2 \\ -1 & 1 & -1 & 1 \\ 1 & 1 & 1 & 1 \\ 2 & 0 & -2 & 0 \end{pmatrix} \begin{pmatrix} f(\frac{1}{4}2\pi) \\ f(\frac{2}{4}2\pi) \\ f(\frac{3}{4}2\pi) \\ f(\frac{4}{4}2\pi) \end{pmatrix}. \end{aligned} \quad (21)$$

B. Example for $N=8$

$$\begin{pmatrix} a_1 \\ a_2 \\ a_4 \\ a_8 \\ b_1 \\ b_2 \end{pmatrix} = \frac{1}{8} \begin{pmatrix} C(1,8)C(2,8)C(3,8)C(4,8)C(5,8)C(6,8)C(7,8)C(8,8) \\ C(1,4)C(2,4)C(3,4)C(4,4)C(5,4)C(6,4)C(7,4)C(8,4) \\ C(1,2)C(2,2)C(3,2)C(4,2)C(5,2)C(6,2)C(7,2)C(8,2) \\ C(1,1)C(2,1)C(3,1)C(4,1)C(5,1)C(6,1)C(7,1)C(8,1) \\ C(7,8)C(0,8)C(1,8)C(2,8)C(3,8)C(4,8)C(5,8)C(6,8) \\ C(0,4)C(1,4)C(2,4)C(3,4)C(4,4)C(5,4)C(6,4)C(7,4) \end{pmatrix} \begin{pmatrix} f(\frac{1}{8}2\pi) \\ f(\frac{2}{8}2\pi) \\ f(\frac{3}{8}2\pi) \\ f(\frac{4}{8}2\pi) \\ f(\frac{5}{8}2\pi) \\ f(\frac{6}{8}2\pi) \\ f(\frac{7}{8}2\pi) \\ f(\frac{8}{8}2\pi) \end{pmatrix}$$

$$= \frac{1}{8} \begin{pmatrix} 0 & 0 & 0 & -4 & 0 & 0 & 0 & 4 \\ 0 & -2 & 0 & 2 & 0 & -2 & 0 & 2 \\ -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 4 & 0 & 0 & 0 & 4 & 0 & 0 \\ 2 & 0 & -2 & 0 & 2 & 0 & -2 & 0 \end{pmatrix} \begin{pmatrix} f(\frac{1}{8}2\pi) \\ f(\frac{2}{8}2\pi) \\ f(\frac{3}{8}2\pi) \\ f(\frac{4}{8}2\pi) \\ f(\frac{5}{8}2\pi) \\ f(\frac{6}{8}2\pi) \\ f(\frac{7}{8}2\pi) \\ f(\frac{8}{8}2\pi) \end{pmatrix} \quad (22)$$

Note that in the above equation a nonsquare 6×8 matrix is used.

III. CONCLUSION

This work is intended for solving some important inverse problems in physics. But it could be also considered as a response to Maddox's two challenge problems [7].

For the universal solution to multidimensional inverse lattice problems we introduce a concept of virtual lattice points and a modified form of a Dirichlet product. Also the present work presents a method for discrete Fourier expansion, in which the coefficients are simply Ramanujan's sum $C(m,n)$. $C(m,n)$ can be evaluated using the Möbius function. Thus it is suitable for parallel processing. Now that the extensive use of large scale digital computation in solving

inverse problems has become popular, the discovery of number theory's applications such as USAFT might be of increasing importance.

ACKNOWLEDGMENTS

Finally, the authors would like to express their thanks to Y.N. Shen, W.Q. Zhang, Q. Xie, and X.J. Ge at Beijing University of Science and Technology, S.J. Liu at Beijing Normal University, C.B. Pan at Peking University, and Y. Wang at Institute of Mathematics of Chinese Science Academy, Z.G. Wang at Key Laboratory of Semiconductor Materials of Chinese Science Academy, for their very helpful discussion and suggestion. This work is supported partly by the Natural Science Foundation of China, and partly by the National Advanced Materials Committee of China.

-
- [1] G. H. Hardy and E. M. Wright, *An Introduction to the Theory of Numbers*, 5th ed. (Oxford University Press, Oxford, 1979).
- [2] M. R. Schroeder, *Number Theory in Science and Communication*, 2nd ed., corrected printing (Springer-Verlag, New York, 1990); T. M. Apostol, *Introduction to Analytic Number Theory* (Springer-Verlag, New York, 1976).
- [3] N. X. Chen, Phys. Rev. Lett. **64**, 1193 (1990); N. X. Chen, Y. Chen, and G. Y. Li, Phys. Lett. A **149**, 357 (1990).
- [4] T. L. Xie, P. F. Goldsmith, and W. Zhou, Astrophys. J. **371**, L81 (1991); T. L. Xie, P. F. Goldsmith, R. L. Shell, and W. Zhou, Astrophys. J. **402**, 216 (1993); H. Rosu, Nuovo Cimento B **108**, 1333 (1993).
- [5] D. W. Tufts and X. Sadasiv, IEEE Acoust. Speech Signal Process. Magazine, Jan. 1988, p. 13; I. S. Reed and D. W. Tufts *et al.*, IEEE Trans. Acoust. Speech Signal Process. **38**, 458 (1990); D. W. Tufts *et al.*, IEEE Trans. Acoust. Speech Signal Process. **41**, 152 (1993).
- [6] D. Spector, Commun. Math. Phys. **127**, 239 (1990).
- [7] J. Maddox, Nature (London) **344**, 377 (1990).
- [8] A. E. Carlsson, C. D. Gelatt, and H. Ehrenreich, Philos. Mag. A **41**, 241 (1980); A. Mookerjee *et al.*, J. Phys. Condens. Matter. **4**, 2439 (1992); M. Li *et al.*, Phys. Lett. A **169**, 364 (1992).
- [9] B. W. Ninham, B. D. Hughes, and N. E. Frankel, Physica A **186**, 441 (1992); N. X. Chen, M. Li, and S. J. Liu, Phys. Lett. A **195**, 135 (1994).
- [10] S. Liu *et al.*, J. Phys. Condens. Matter **5**, 2439 (1993); J. Wang, K. M. Zhang, and X. D. Xie, J. Phys. Condens. Matter **6**, 989 (1994).
- [11] M. Li *et al.*, Phys. Lett. A **177**, 134 (1993); M. Li and N. X. Chen, Phys. Rev. B **52**, 997 (1995).
- [12] Q. Xie and M. C. Huang, Phys. Lett. A **184**, 119 (1994); Q. Xie and N. X. Chen, Phys. Rev. B **51**, 15 856 (1995).
- [13] N. X. Chen *et al.*, J. Phys. A **29**, 5591 (1996).