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# Functions of two-dimensional Bravais lattices

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The symmetries of a function are considered that takes as its argument an arbitrary two-dimensional Bravais lattice, represented by a  $2 \times 2$  matrix. Rotating the lattice corresponds to multiplying its matrix on the right by an element of  $SO(2)$ . Matrices related by left multiplication of an element of  $SL(2, \mathbb{Z})$  also refer to the same lattice. Functions of matrices having these two symmetries possess an expansion known as the Roelcke–Selberg decomposition. This decomposition characterizes the function in terms of a set of coefficients (the discrete spectrum) and a function defined on a line in the complex plane (the continuous spectrum). When the function of the lattice refers to its energy, the continuous spectrum can be related to an interatomic potential between the atoms of the lattice. The decomposition can be considered a Landau theory of a strained two-dimensional Bravais lattice, valid for arbitrarily large strains, expanded about any structure. This type of theory may be useful in determining the energies of a material for many different lattice configurations from a knowledge of the energy at only a few of them.

## I. INTRODUCTION

It is often desirable to know how some physical quantity associated with a crystal varies as the structure itself is varied. To analyze a discontinuous structural phase transition, for example, one might want to know what the free-energy surface between the two structures looked like. The inadequacies of conventional Landau theory for describing such surfaces for reconstructive transitions (no group–subgroup relation between the two structures) are well known.<sup>1</sup> This paper considers functions defined on crystalline configurations that are Bravais lattices. I first discuss the symmetries of such functions in terms of matrix groups. The problem of their proper parametrization is then solved, in two dimensions, by using mathematical techniques of harmonic analysis on the relevant group cosets.<sup>2</sup>

With respect to the traditional Landau theory of a strained Bravais lattice, this theory has two important advantages. First, it is consistent with all Bravais lattice symmetries. Traditional Landau theory handles symmetry correctly only in the limit of infinitesimal deviations from a particular reference structure. Second, some of the parameters occurring in the expansion can, when the function refers to the energy of a lattice, be related to microscopic physical quantities. Ordinary Landau theory is purely phenomenological.

## II. SYMMETRY CONSTRAINTS

The  $n$  Bravais lattice vectors  $\mathbf{t}_i$  of an  $n$ -dimensional Bravais lattice can be defined<sup>3</sup> in terms of orthonormal basis vectors  $\mathbf{e}_j$  as,

$$\mathbf{t}_i = g_{ij} \mathbf{e}_j, \quad i, j = 1, \dots, n. \quad (1)$$

This equation gives a correspondence between the Bravais lattice generated by the  $\mathbf{t}_i$  and an  $n \times n$  matrix  $g$ . (The simple cubic lattice in three dimensions, for example, is just the  $3 \times 3$  identity matrix.) The volume of the unit cell of the lattice  $g$  can be shown to be  $\det g$ , so that the physically

meaningful Bravais lattices are those  $g \in GL(n, \mathbb{R})$ , the group of real  $n \times n$  matrices with nonzero determinant.

Let  $f(g)$  be any real-valued function of  $g$ , for example its energy or free-energy, which is independent of the lattices' orientation. There are two symmetry constraints such a function must obey. The first arises from its invariance under rotations of the lattice, the second from the fact that there are an infinite number of sets of Bravais lattice vectors, and hence matrices  $g$ , which generate the same Bravais lattice. To discuss the first, imagine that the  $\mathbf{t}_i$  are all rotated by a common angle, and/or inverted. The new lattice vectors are then  $\mathbf{t}'_i = k \mathbf{t}_i$ , where  $k \in O(n)$ , the group of orthogonal  $n \times n$  matrices. The rotated lattice corresponding to the  $\mathbf{t}'_i$  can then be represented by the matrix  $gk$ , since

$$\mathbf{t}'_i = k \mathbf{t}_i = k g_{ij} \mathbf{e}_j = g_{ij} k \mathbf{e}_j = g_{ij} k_{jl} \mathbf{e}_l. \quad (2)$$

This implies that  $f(g) = f(gk)$  for all  $k \in O(n)$ . To find the second constraint, suppose that a set  $\mathbf{t}'_i$  can be defined in terms of the set  $\mathbf{t}_j$  by  $\mathbf{t}'_i = \gamma_{ij} \mathbf{t}_j$ , for some matrix  $\gamma \in GL(n, \mathbb{Z})$ . The notation  $GL(n, \mathbb{Z})$  refers to the group of  $n \times n$  matrices with integral entries (such  $\gamma$  have  $\det \gamma = \pm 1$ ). The  $\mathbf{t}'_i$  are then linear combinations of the  $\mathbf{t}_j$  with integral coefficients. Therefore, the lattice the  $\mathbf{t}'_i$  generate will lie within the lattice generated by the  $\mathbf{t}_j$ . But the converse is also true. Since  $GL(n, \mathbb{Z})$  is a group,  $\gamma^{-1} \in GL(n, \mathbb{Z})$  also, and multiplying both sides of  $\mathbf{t}'_i = \gamma_{ij} \mathbf{t}_j$  by  $\gamma_{ii}^{-1}$  gives,

$$\gamma_{ii}^{-1} \mathbf{t}'_i = \gamma_{ii}^{-1} \gamma_{ij} \mathbf{t}_j = \delta_{ij} \mathbf{t}_j = \mathbf{t}_i. \quad (3)$$

Therefore, the lattice generated by the  $\mathbf{t}_i$  lies within the lattice generated by the  $\mathbf{t}'_i$ . The two sets  $\mathbf{t}'_i$  and  $\mathbf{t}_j$  must then refer to the same lattice and hence  $f(g) = f(\gamma g)$  for all  $\gamma \in GL(n, \mathbb{Z})$ .

Functions defined on  $GL(n, \mathbb{R})$  possessing the above symmetries are said to be right  $O(n)$  and left  $GL(n, \mathbb{Z})$  invariant. The harmonic analysis of such functions for the case  $n = 3$  is a difficult mathematical problem that appears to be not yet fully resolved.<sup>4</sup> Therefore, and because two-dimen-

sional Bravais lattices are of intrinsic physical interest, I will from now on restrict attention to the case  $n = 2$ . Further, since there are no symmetries to exploit with respect to isotropic volume changes of a lattice,<sup>5</sup> I will consider only  $g = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \text{SL}(2, \mathbb{R})$ . One then has  $f(g) = f(\gamma g)$  and  $f(g) = f(gk)$ , where now  $\gamma \in \text{SL}(2, \mathbb{Z})$  and  $k \in \text{SO}(2)$  (all groups having unit determinant), and also

$$f\left(\begin{pmatrix} a & b \\ c & d \end{pmatrix}\right) = f\left(\begin{pmatrix} a & -b \\ -c & d \end{pmatrix}\right). \quad (4)$$

This last symmetry comes from multiplying  $g$  on both the right and left by  $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ , which corresponds physically to rotating the lattice by  $\pi$  and inverting  $t_2$ . The value  $f(g)$  assumes at  $g$  is the same as the value it assumes when  $g$  is right multiplied by any member of  $\text{SO}(2)$  or left multiplied by any member of  $\text{SL}(2, \mathbb{Z})$ . This can be summarized by saying that  $f(g)$  is a function of the cosets  $\text{SL}(2, \mathbb{Z}) \backslash \text{SL}(2, \mathbb{R}) / \text{SO}(2)$ . The right  $\text{SO}(2)$  invariance of  $f(g)$  can be dealt with by a transformation that maps  $\text{SL}(2, \mathbb{R}) / \text{SO}(2) \rightarrow H$ , where  $H$  is the upper half complex plane. Define  $z = gi$ , where the action of the matrix  $g$  on  $i$  is given by

$$gi = \begin{pmatrix} a & b \\ c & d \end{pmatrix} i = \frac{ai + b}{ci + d}. \quad (5)$$

This transformation has the property that  $ki = i$ , so that all matrices  $g$  differing only by a rotation are mapped to the same  $z$ . The left  $\text{SL}(2, \mathbb{Z})$  invariance of  $f(g)$  can then be shown to imply that

$$f(z) = f(z + 1) = f(-1/z), \quad (6)$$

while the constraint of Eq. (4) implies that  $f(z)$  is even about the imaginary axis. That is,  $f(z) = f(-\bar{z})$ ,  $\bar{z}$  denoting the complex conjugate of  $z$ .

Note that

$$\begin{pmatrix} \sqrt{y} & x/\sqrt{y} \\ 0 & 1/\sqrt{y} \end{pmatrix} i = x + iy. \quad (7)$$

The Bravais lattice vectors of the matrix on the right are  $t_1 = \sqrt{y}e_1 + x/\sqrt{y}e_2$  and  $t_2 = 1/\sqrt{y}e_2$ . This is the convention where  $t_2$  is aligned with the  $e_2$  axis. Rotating this structure, by multiplying the matrix on the right by an element of  $\text{SO}(2)$ , will of course change the matrix, but not the complex number to which it maps.

The action of  $\text{SL}(2, \mathbb{Z})$  on  $H$  and  $z \rightarrow -\bar{z}$  divides  $H$  into fundamental domains. A domain  $D$  has the property that for every  $z \in H$  there exists a  $\gamma \in \text{SL}(2, \mathbb{Z})$  such that  $\gamma z \in D$  or  $-\overline{\gamma z} \in D$ . The resulting subdivision of  $H$  is shown in Fig. 1. A domain has the physical interpretation that it contains within it all inequivalent two-dimensional Bravais lattices (of a given cell volume). Note the (local) twofold and threefold symmetries about the square and triangular lattices. A Landau expansion in the strains about the square lattice would take into account its twofold symmetry, but not the threefold symmetry about the triangular lattice, or any other symmetry of  $f(z)$ . Hence, a parametrization of  $f(z)$  incorporating all of the symmetries discussed above could be considered a Landau theory valid for strains of arbitrary magnitude, expanded about any structure.

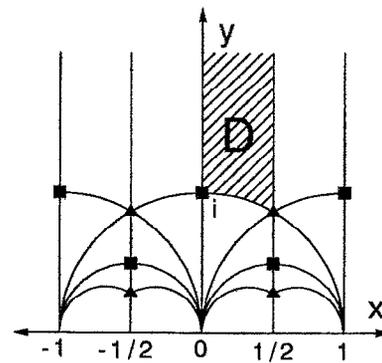


FIG. 1. A division of the upper half complex plane into domains  $D$ . The domains become progressively smaller as you approach the real axis, so those closest to the axis are not shown. Each domain contains within it all possible two-dimensional Bravais lattices of a common value. The square and triangular structures are located at the vertices of the domains and are labeled accordingly. A particular domain has been shaded and labeled  $D$ . The boundary of  $D$  is made up of Bravais lattices having nontrivial point group symmetries, that is, a point group symmetry other than inversion. Structures on the imaginary axis are rectangular, those on the unit circle rhomboidal, and those with  $\text{Re } z = 1/2$  face centered rectangular. Structures with  $y \rightarrow \infty$  have  $|t_2| \rightarrow 0$ . Hence, the physically relevant structures in  $D$  are those near the unit circle.

### III. PARAMETRIZATION OF $f(z)$

The function  $f(z)$  can be parametrized in terms of basis functions of  $H$ . This expansion has both a discrete sum and a continuous integral. The sum involves cusp forms  $v_n(z)$  while the integral is taken over the Eisenstein series  $E_s(z)$ . Both types basis functions have the following two properties. They are eigenfunctions of the non-Euclidean Laplacian

$$\Delta = y^2 \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right)$$

on  $H$  ( $x$  and  $y$  are the real and imaginary parts of  $z$ ). That is,  $\Delta v_n(z) = s_n(s_n - 1)v_n(z)$  and  $\Delta E_s(z) = s(s - 1)E_s(z)$ . The real parts of the  $s_n$  and  $s$  are always equal to  $1/2$ , so that they can be written  $s_n = 1/2 + it_n$  and  $s = 1/2 + it$ . The first three  $t_n$  are<sup>2</sup> approximately 13.78, 17.74, and 19.42, while  $t$  is arbitrary. And second, they are both themselves invariant under  $\text{SL}(2, \mathbb{Z})$ , so that  $v_n(z) = v_n(\gamma z)$  and  $E_s(z) = E_s(\gamma z)$ . A function  $f(z)$  can be expanded in terms of these functions if it belongs to  $L^2(\text{SL}(2, \mathbb{Z}) \backslash H)$ . This is satisfied if, in addition to satisfying Eq. (6) above, its norm  $(f, f)$  is finite, where the inner product of two functions  $f(z)$  and  $g(z)$  is defined as,

$$(f, g) = 2 \int_D f(z) \overline{g(z)} y^{-2} dx dy. \quad (8)$$

The integration is over a fundamental domain  $D$ .<sup>6</sup> Although I will return to the physical significance of this later, note now that, due to the measure used in Eq. (8),  $(f, f)$  will be finite if, in particular,  $f(z)$  is bounded on  $D$ . To summarize, an important result from harmonic analysis, known as the Roelcke-Selberg spectral decomposition of  $\Delta$  on  $L^2(\text{SL}(2, \mathbb{Z}) \backslash H)$ , is that such  $f(z)$  can be expanded as

$$f(z) = \sum_{n>0} (f, v_n) v_n(z) + \frac{1}{4\pi i} \int_{\text{Re } s = 1/2} (f, E_s) E_s(z). \quad (9)$$

That is,  $f(z)$  can be parametrized by a set of coefficients  $(f, v_n)$  and a function  $(f, E_s)$ .

Functions in  $L^2(\text{SL}(2, \mathbb{Z}) \backslash \mathbb{H})$  are not required to be even about the imaginary axis. Since there are, in general, both even and odd cusp forms, the sum in Eq. (9) should be considered to be over the even  $v_n(z)$  only. The Eisenstein series are even<sup>7</sup> so that no additional restriction is placed on the continuous part of the expansion.

In most physical applications,  $f(z)$  will be real. This constraint can be shown to imply that  $(f, E_s) = (f, E_{\bar{s}})$ , so that this function need only be known on  $\text{Re } s = 1/2$  for  $\text{Im } s > 0$  or  $\text{Im } s < 0$ . The even cusp forms are apparently<sup>8</sup> real, so that one can expect the  $(f, v_n)$  to be real also.

The  $n = 0$  cusp form is given by  $v_0 = \sqrt{3/\pi}$ . However, analytic expressions of the  $v_n(z)$  for  $n > 0$  do not exist and their  $s_n = 1/2 + it_n$  are not known exactly. They do however possess expansions in terms of  $K$ -Bessel functions,<sup>9</sup>

$$v_n(z) = \sum_{m>0} c_m y^{1/2} K_{it_n}(2\pi m y) \cos(2\pi m x), \quad (10)$$

and the first few  $c_m$ , as well as the  $t_n$ , for several cusp forms have been numerically calculated.<sup>10</sup>

For  $\text{Re } s > 1$ , the Eisenstein series has the series expansion,<sup>11</sup>

$$E_s(z) = \frac{1}{2} y^s \sum_{(m,n)=1} |mz + n|^{-2s}. \quad (11)$$

The notation  $(m, n)$  refers to those pairs of integers whose greatest common divisor is 1. The  $E_s(z)$  can be analytically continued to  $\text{Re } s < 1$  [the region of the complex  $s$ -plane relevant to Eq. (9)], and has an expansion in terms of  $K$ -Bessel functions similar to that given for the  $v_n(z)$  in Eq. (10). In this case however, the  $c_m$  for each  $s$  are known exactly.

#### IV. RELATION OF $(f, E_s)$ TO THE ATOMIC PAIR POTENTIAL

An important problem is the relation of the parameters  $(f, v_n)$  and the function  $(f, E_s)$  to physical quantities. I show that if  $f(z)$  refers to the energy of lattice  $z$ , then  $(f, E_s)$  can be expressed in terms of a pair potential between the atoms. Assuming the atoms interact solely by a pair potential  $V(r)$ ,  $r$  the distance between them, then the energy per atom is

$$f(z) = \frac{1}{2} \sum'_{\mathbf{r}_{n,m}} V(r). \quad (12)$$

The sum runs over all lattice vectors  $\mathbf{r}_{n,m} = n\mathbf{t}_1 + m\mathbf{t}_2$ , except for the zero vector, with  $r = |\mathbf{r}_{n,m}|$ . Now write  $V(r)$  in terms of its Mellin transform, with transform variable  $2s$ , so that  $f(z)$  becomes,

$$f(z) = \frac{1}{2} \sum'_{\mathbf{r}_{n,m}} \frac{1}{2\pi i} \int_{\text{Re } 2s = 2c} MV(2s) r^{-2s} d2s. \quad (13)$$

The integral is taken over a vertical line in the complex  $s$ -plane intersecting the real axis at some  $c > 1$ . I assume that  $V(r)$  can be written this way, and that  $MV(2s)$  is analytic in the interval  $1/2 \leq \text{Re } s \leq c$ . [This is satisfied, for example, by potentials that remain finite as  $r \rightarrow 0$ , and go to zero faster than  $1/r^2$  as  $r \rightarrow \infty$ . These sorts of potentials also guarantee that  $f(z)$  is bounded on  $D$ .] Interchanging the sum and the

integral in Eq. (13) gives the sum  $\sum'_{\mathbf{r}_{n,m}} r^{-2s}$  inside the integral. Such sums over lattice sites, of powers of distances of the lattice sites from the origin, can be handled using Epstein zeta functions  $Z(Y_z, s)$ . For  $\text{Re } s > 1$ , they are defined<sup>12</sup> as

$$Z(Y_z, s) = \frac{1}{2} \sum_{\mathbf{a} \in \mathbb{Z}^2 - 0} Y_z[\mathbf{a}]^{-s}. \quad (14)$$

Here,  $Y_z[\mathbf{a}]$  refers to the number  $\mathbf{a}' Y_z \mathbf{a}$ ,  $\mathbf{a}$  being a two-component column vector,  $\mathbf{a}'$  its transpose, and  $Y_z$  the  $2 \times 2$  symmetric matrix related to  $z = x + iy$  by<sup>13</sup>

$$Y_z = \begin{pmatrix} (x^2 + y^2)/y & x/y \\ x/y & 1/y \end{pmatrix}. \quad (15)$$

Or alternatively, in terms of  $g$ ,  $Y_z = gg'$ . It can be shown that when  $\mathbf{a} = \begin{pmatrix} n \\ m \end{pmatrix}$ ,  $Y_z[\mathbf{a}] = |\mathbf{r}_{n,m}|^2$ . Hence, Eq. (13) can be rewritten as,

$$f(z) = \frac{1}{\pi i} \int_{\text{Re } s = c} MV(2s) Z(Y_z, s) ds. \quad (16)$$

To relate this expression for  $f(z)$  to the expansion given in Eq. (9), the line of integration must be moved from  $\text{Re } s = c$  to  $\text{Re } s = 1/2$ . The Epstein zeta function can be analytically continued to the whole  $s$ -plane with a unique pole at  $s = 1$  with residue  $\pi/2$ .<sup>14</sup> The Mellin transform  $MV(2s)$  is analytic by assumption in the region  $1/2 \leq \text{Re } s \leq c$ . I will also assume that  $|MV(2\sigma + 2it)Z(Y_z, \sigma + it)| \rightarrow 0$  as  $t \rightarrow \infty$  for  $1/2 \leq \sigma \leq c$  (Ref. 15), so that the end pieces vanish. After moving the integral, substitute the relation  $Z(Y_z, s) = \xi(2s)E_s(z)$  (Ref. 16),  $\xi(2s)$  the Riemann zeta function. Comparing the result with Eq. (9) gives  $(f, v_0) = \sqrt{\pi^3/3} MV(2)$ , coming from the residue, and

$$(f, E_s) = 2MV(2s)\xi(2s). \quad (17)$$

#### V. DISCUSSION

It is not clear how to relate the  $(f, v_n)$  to physical quantities. This is made difficult by the absence of analytic expressions for them. However, it can be hoped that the  $(f, v_n)$  become negligible for large  $n$ . This is because, physically,  $f(z)$  cannot vary too rapidly with  $z$  (similar structures being expected to have similar free energies), and because the  $v_n(z)$  with large  $n$  oscillate rapidly with  $z$  [their eigenvalues  $s_n(s_n - 1)$  increasing with  $n$ ].

It may be useful to expand  $(f, E_s)$  itself in terms of basis functions. The choice of such basis functions would be dictated by the evenness of  $(f, E_s)$  about the real axis, and physical considerations motivated by its relation to the atomic pair potential, Eq. (17). If, for a crystal, such an expansion were to converge rapidly, and the  $(f, v_n)$  also became negligible for sufficiently large  $n$ , then one could effectively fully characterize  $f(z)$  by a finite number of adjustable parameters. These parameters could then be determined by a best fit if one knew  $f(z)$  at a finite number of structures  $z$ . The variation of  $f(z)$  is represented by an energy landscape in Fig. 2. This landscape would be appropriate when the stable lattice has no particular symmetry. Note however that the symmetries of  $f(z)$  still enforce the energies of the square and triangular lattices to be locally extremal. The atomic displacements of the domain wall shown will be sensitive to the

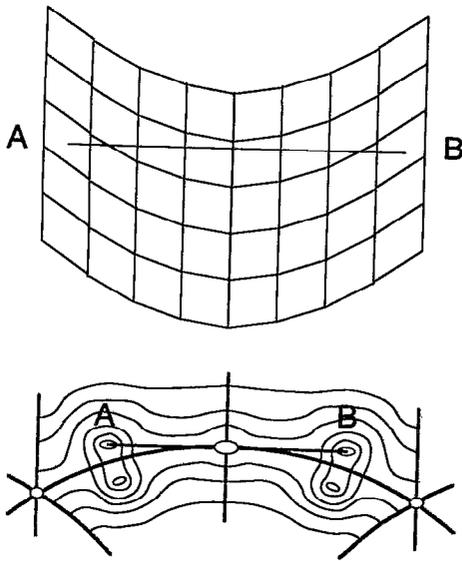


FIG. 2. The top picture is a ferroelastic domain wall. The two domains A and B, and the line between them map to the points A and B and line between them in the complex plane. The midpoint of the line in the complex plane is the square lattice  $i$ . The energy landscape is purely hypothetical but is consistent with the symmetry of  $f(z)$ , and the physical requirement that the global minima of  $f(z)$  be located at A and B. Note the "reflection" symmetries about the unit circle and imaginary axis which always force the rhombohedral and rectangular structures on these lines to be extremal. For short range repulsive forces between the atoms the energy will become progressively bigger the further you get from the unit circle.

details of the energy landscape between the two structures. An extension of the theory given here to the inhomogeneous case, i.e., allowing  $z$  to depend on position, may be able to describe such domain walls. Of course, such an extension would involve contributions to the energy which arise from spatial derivatives of  $z$ . Ordinary elasticity theory, even if carried to arbitrarily high order, is incapable of describing domain walls involving large displacements because it never takes into account the full symmetry of  $f(z)$ .

Suppose that the Bravais lattice with the lowest free-energy of a crystal is square. A rectangular distortion of this structure corresponds to moving away from  $z = i$  up or down the imaginary axis, while moving to the left or right of  $i$  induces a rhombohedral distortion. The lowest order changes in the free-energy associated with these two displacements are given by the two respective elastic constants of the square lattice. These may be determined from  $f(z)$  by evaluating the second derivative of  $f(z)$  with respect to deviations in the real and imaginary parts of  $z$  from  $i$ , evaluated at  $i$ . In general, any crystal's elastic constants can be determined if  $f(z)$  is known. Conversely, knowledge of the elastic constants constrains the  $(f, v_n)$  and  $(f, E_s)$ .

The parametrization of  $f(z)$  discussed here is an extension of a Landau theory of the square to triangular lattice by Horowitz *et al.*<sup>17</sup> These authors consider a transition trajectory in which the angle  $\gamma$  between two equal length lattice vectors is continuously changed from  $\pi/2$  in the square lattice to  $\pi/3$  in the triangular lattice. (This trajectory can be

represented in Fig. 1 by going from  $z = e^{i\pi/2}$  to  $z = e^{i\pi/3}$  along the unit circle.) They define an order parameter for this transition to be  $\eta(\gamma) = 1 - 4 \cos^2 \gamma$ . The free-energy along the trajectory can then presumably be written as

$$f(\eta) = A\eta^2 + B\eta^3 + \dots, \quad (18)$$

where  $A$  and  $B$  are constants. This free-energy obeys two constraints on its variation with  $\gamma$ . The first is evenness about  $\gamma = \pi/2$ , a consequence of  $\eta(\gamma) = \eta(-\gamma + \pi)$ . The second is  $\partial f / \partial \eta|_{\eta=0} = 0$ . These constraints guarantee that the free-energy be extremal with respect to deviations of  $\gamma$  from the square and triangular lattices, respectively. In my parametrization, the first constraint follows from the evenness of  $f(z)$  about the imaginary axis, while the second can be shown to arise from the local threefold symmetry of  $f(z)$  about  $z = e^{i\pi/3}$ . To summarize, although I consider a broader class of structures, and our formalisms are quite different, the symmetries of the two free-energies as a function of the configurations we both consider are identical.

The central result of this paper is that the variation of any function of a two-dimensional Bravais lattice, under the constraint of constant volume, can be fully characterized in terms of a (presumably) finite number of coefficients, and a function defined on line in the upper half complex plane. One application of this characterization may be an attempt to find the energy of all Bravais lattice configurations of a crystal given knowledge of the energy at only a few of them.

## ACKNOWLEDGMENTS

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<sup>1</sup> See V. P. Dmitriev, S. B. Rochal, Yu. M. Gufan, and P. Tolédano, *Phys. Rev. Lett.* **60**, 1958, (1988), and also Ian Folkins and M. B. Walker, *Phys. Rev. Lett.* **65**, 127, (1990).

<sup>2</sup> My basic reference is Audrey Terras, *Harmonic Analysis on Symmetric Spaces and Applications I* (Springer-Verlag, New York, 1985). The Epstein zeta function and Mellin transform are discussed in Chap. 1, the two-dimensional fundamental domain and the Roelcke-Selberg decomposition in Chap. 3.

<sup>3</sup> Similar representations of a Bravais lattice by a matrix, and analyses of which matrices refer to the same lattice can be found elsewhere. See the book discussed in Ref. (4), or J. Neubüser, H. Wondratschoki, and R. Bülow, *Acta Crystall. A* **27**, 517 (1971).

<sup>4</sup> The three-dimensional fundamental domain and progress in extending the Roelcke-Selberg decomposition to three dimensions are discussed in Audrey Terras, *Harmonic Analysis on Symmetric Spaces and Applications II* (Springer-Verlag, New York, 1988).

<sup>5</sup> A full parametrization of  $f(g)$  would take into account changes in volume. However, since there are no symmetries that relate structures of different volume, symmetry considerations do not dictate how to do this.

<sup>6</sup> This expression differs from (3.100) of Ref. 2 by the factor of 2. This is because the evenness of  $f(z)$  about the imaginary axis makes our fundamental domain twice as small as the  $D$  understood in (3.100).

<sup>7</sup> D. Hejhal, in *Recent Progress in Analytic Number Theory*, edited by H. Halberstam and C. Hooley (Academic, London, 1981), p. 95.

<sup>8</sup> The  $c_m$  of Eq. (10) are listed as real in the Tables of  $c_m$  discussed in Ref. 2 and Ref. 7. If this is true in general, then Eq. (10) implies that the even  $v_n(z)$  are real.

<sup>9</sup> The  $K$ -Bessel functions and expansion are referred to on pages 140 and 219, respectively of Ref. 2.

<sup>10</sup> See Refs. 2 and 7. Only the  $c_m$  with  $m$  prime are listed since, from these, all other  $c_m$  can be calculated.

<sup>11</sup> Reference 2, p. 207.

<sup>12</sup> Reference 2, p. 58.

<sup>13</sup> The convention used here for relating  $z$  and  $Y$  is slightly different from that given on p. 206 of Ref. 2.

<sup>14</sup> Reference 2, p. 59.

<sup>15</sup> For  $\frac{1}{2} < \sigma < 1$ ,  $Z(Y, s) = O(|t|^{1-\sigma})$ . See H. S. A. Potter and E. C. Titchmarsh, Proc. London Math. Soc. **39**, 372 (1935).

<sup>16</sup> Reference 2, p. 207.

<sup>17</sup> B. Horowitz, R. J. Gooding, and J. A. Krumhansl, Phys. Rev. Lett. **62**, 843 (1989).