

## Group-theoretical derivation of the numbers of independent physical constants of quasicrystals

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Formulas for calculating the characters of the representation matrices and the number of independent components of any physical-property tensor of quasicrystals have been derived by using group-representation theory, where the internal symmetry of the physical-property tensor was considered. As an example of their application, we have calculated the number of independent elastic constants up to cubic order for many of the quasicrystals discovered to date.

### I. INTRODUCTION

As is well known, the number of independent components of a physical-property tensor in a certain structure is determined by the point-group symmetry which the structure possesses. It follows that the number of independent components of all kinds of physical-property tensors can be obtained with group-representation theory. For periodic structures, systematic results have already been given.<sup>1</sup>

Since the discovery of icosahedral quasicrystals in Al-Mn alloys,<sup>2</sup> other quasicrystals with ten-,<sup>3</sup> twelve-,<sup>4</sup> and eightfold<sup>5</sup> symmetries have been obtained in succession. Additionally, Feng and co-workers<sup>6,7</sup> have discovered an incommensurate structure with cubic point-group symmetry in V-Ni-Si alloys. Recently, Janssen<sup>8</sup> gave a clear theoretical explanation for quasiperiodic structures, which may have either crystallographic or noncrystallographic point-group symmetry. They can be obtained by projecting a higher-dimensional periodic structure upon the physical space or by cutting a higher-dimensional structure.<sup>9,10</sup>

Quasicrystals possess various point-group symmetries. Moreover, in the process of the group-theoretical derivation of the numbers of independent physical constants, the internal symmetry of the physical-property tensor must be considered.<sup>11</sup> In the case of quasicrystals, a vector in the complementary subspace may transform under nonequivalent irreducible representation compared with that for the vector in the physical subspace. These special properties of quasicrystals make it more complicated to derive the number of independent physical constants.

In this paper, we will apply group-representation theory to derive formulas for calculating the characters of the representation matrices and the number of independent components for any possible physical-property tensor in a quasicrystal (Sec. II). As an example we will also calculate the number of independent elastic constants up to cubic order for many of the quasicrystals discovered to date.

### II. THE FUNDAMENTAL THEORY

#### A. The basic formula for calculating the number of independent components

In a periodic structure, let  $F_{ij\dots l}$  represent a component of a tensor of rank  $n$  in three-dimensional space; the total number of such components is  $3^n$ . In general, they are independent of each other. If  $\hat{A}$  is a coordinate-transformation matrix, the relationship between components  $F'_{i'j'k'\dots l'}$  and  $F_{ijk\dots l}$  is

$$F'_{i'j'k'\dots l'} = (\hat{A} \times \hat{A} \times \dots \times \hat{A})_{ijk\dots l, i'j'k'\dots l'} F_{ijk\dots l}, \quad (1)$$

where  $F_{ijk\dots l}$  are related to the old coordinate system and  $F'_{i'j'k'\dots l'}$  to the new system. In addition, the direct product  $\hat{\Gamma}(g) = \hat{A} \times \dots \times \hat{A}$  spans a  $3^n$ -dimensional representation space of the symmetry group  $G$ . In general, it is reducible. The character of this tensor representation can be calculated by the following formula:

$$\chi(g) = \text{Tr} \hat{\Gamma}(g) = [\text{Tr} \hat{A}(g)]^n, \quad (2)$$

where  $\hat{\Gamma}(g)$  and  $\hat{A}(g)$  are the representation matrices corresponding to element  $g$  in  $G$ . The representation can also be reduced to the direct sum of some irreducible representations. The number  $a_i$  of the  $i$ th irreducible representation  $\Gamma^{(i)}$  is determined by:

$$a_i = \frac{1}{|G|} \sum_{g \in G} \chi(g) \overline{\text{Tr} \Gamma^{(i)}(g)}, \quad (3)$$

where  $|G|$  is the order of group  $G$  and the overbar means the complex conjugate.

As we know, the symmetry of a physical-property tensor is decided by the macro-symmetry of the material considered, so the number of independent components of the tensor is fixed for a given material. In other words, every independent component will transform under identity representation. This means that the number of independent components is just the number  $a_1$  of the identity representation ( $\Gamma_1$ ) in the direct representation. Therefore, the basic formula for calculating the number

of independent components is:

$$a_1 = \frac{1}{|G|} \sum_{g \in G} \chi(g). \quad (4)$$

### B. The principal characteristics of physical-property tensors in quasicrystals

A quasicrystal can be obtained by projecting a higher-dimensional periodic structure onto a three- or lower-dimensional physical subspace.<sup>9,10</sup> Let  $\tilde{\mathbf{r}}$  be a position vector in the higher-dimensional space,  $\mathbf{r}_{\parallel}$  and  $\mathbf{r}_{\perp}$  its projections in the parallel (physical) subspace  $P^{\parallel}$  and the perpendicular (complementary) subspace  $P^{\perp}$ , respectively; hence

$$\tilde{\mathbf{r}} = \mathbf{r}_{\parallel} \oplus \mathbf{r}_{\perp}. \quad (5)$$

As we know, for  $d$ -dimensional quasicrystals with a noncrystallographic point group there exist at least two  $d$ -dimensional nonequivalent irreducible representations.  $\mathbf{r}_{\parallel}$  transforms under a  $d$ -dimensional irreducible representation  $\Gamma_i$  whereas  $\mathbf{r}_{\perp}$  transforms under a different  $d$ -dimensional representation  $\Gamma'_i$ . Moreover, the action of a given element of such a noncrystallographic point group on  $\mathbf{r}_{\parallel}$  and  $\mathbf{r}_{\perp}$  gives a certain intrinsic relation  $\hat{A}'(g)\mathbf{r}_{\perp} = [\hat{A}(g)\mathbf{r}_{\parallel}]_{\perp}$ . For example, we have  $(\mathbf{r}_{\perp})_n = (\mathbf{r}_{\parallel})_{(3n) \pmod{5}}$  for the pentagonal structure. However, it should be noted here that, for some quasicrystals with crystallographic point symmetry, such as cubic quasicrystals, these two representations are equivalent<sup>12</sup> (both of them are  $\Gamma_3$ ), so the difference discussed above disappears.

As an example, we will analyze the transformation

$$F_i, F_{ij}, F_{ijk}, F_{ijkl}, F_{ijklmn}, \dots, F_{\alpha i}, F_{\alpha ij}, F_{\alpha ik\beta l}, F_{\alpha j\beta l}, F_{\alpha j\beta l\gamma n}, F_{ij\beta l\gamma n}, F_{ijkl\gamma n}, \dots$$

It is very important to point out that, as in periodic structures, physical-property tensors have some internal symmetry because of physical definitions or thermodynamics, even if macrosymmetry is not considered. Such an internal symmetry implies that some subscripts are commutable, and the number of independent components of this physical-property tensor reduces. Now we use the notation  $\{\dots\}$  to represent that the subscripts in  $\{\dots\}$  can commute with each other. For quasicrystals with the  $n$ -dimensional point group, the representation space of which can be reduced to the direct sum of two equivalent irreducible subspaces, the two types of subscripts  $i$  and  $\alpha$  are also commutable, unlike those for quasicrystals with noncrystallographic point-group symmetry (in this case, the two irreducible subspaces are non-equivalent).

$$[\hat{\Gamma}(g)]_{ijkl, i'j'k'l'} = \{ \{ A \times A \} \times \{ A \times A \} \}_{ijkl, i'j'k'l'}$$

$$= \frac{1}{2} [ (\{ A \times A \} \times \{ A \times A \})_{ijkl, i'j'k'l'} + (\{ A \times A \} \times \{ A \times A \})_{ijkl, k'l'i'j'} ]$$

$$= \frac{1}{8} (A_{ii'} A_{jj'} + A_{ij'} A_{ji'}) (A_{kk'} A_{ll'} + A_{kl'} A_{lk'}) + \frac{1}{8} (A_{ik'} A_{jl'} + A_{il'} A_{jk'}) (A_{ki'} A_{lj'} + A_{kj'} A_{li'}), \quad (8)$$

TABLE I. Characters of icosahedral symmetry [ $\tau = (1 + \sqrt{5}/2)$ ].  $a_1$  is the number of independent components of the elastic-constant tensor.

	1E	12C <sub>5</sub>	12C <sub>5</sub> <sup>2</sup>	20C <sub>3</sub>	15C <sub>2</sub>	$a_1$
$\Gamma_1$	1	1	1	1	1	
$^*\Gamma_3$	3	$\tau$	$1 - \tau$	0	-1	
$^{\dagger}\Gamma_3'$	3	$1 - \tau$	$\tau$	0	-1	
$\Gamma_4$	4	-1	-1	1	0	
$\Gamma_5$	5	0	0	-1	1	
$C_{ijkl}$	21	1	1	0	5	2
$K_{ijkl}$	45	0	0	0	5	2
$R_{ijkl}$	54	-1	-1	0	2	1
$C_{ijklmn}$	56	1	1	2	8	4
$K_{ijklmn}$	165	0	0	3	5	5
$R_{ijklmn}$	189	-1	-1	0	5	4
$R_{ijklmn}^2$	270	0	0	0	10	7

characteristics of the elastic-coefficient tensors in quasicrystals with the above theory. The elastic deformation in quasicrystals is described by the phonon strain tensor  $E_{ij} = (\partial_j U_i + \partial_i U_j)/2$  and the phason strain tensor  $W_{ij} = \partial_j W_i$ . Here,  $E_{ij}$  is the gradient of phonon displacement  $U(\mathbf{r}_{\parallel})$ ; hence both  $\partial_j$  and  $U_i$  transform under the same operator  $\hat{A}(g)$ .  $W_{ij}$  is the gradient of phason displacement  $W(\mathbf{r}_{\parallel})$ , so  $\partial_j$  and  $W_i$  transform under the operators  $\hat{A}(g)$  and  $\hat{A}'(g)$ , respectively.<sup>13</sup> From now on we use subscripts  $i, j, k, l, m, n, \dots$ , for coordinate components in  $P^{\parallel}$ , and subscripts  $\alpha, \beta, \gamma, \dots$ , for coordinate components in  $P^{\perp}$ . It follows that the physical-property tensors in quasicrystals may be classified as follows

### C. The representation matrices and character formulas

In order to determine the value of  $a_1$  in Eq. (4), we will give the formulas for calculating the representation matrices and the corresponding characters of various kinds of tensors below. For each operator, we use  $A$  and  $A'$  for  $\hat{A}(g)$  and  $\hat{A}'(g)$  for convenience

(1) Tensor of rank 2,  $F_{\{ij\}}$ .

$$[\hat{\Gamma}(g)]_{ij, i'j'} = \{ A \times A \}_{ij, i'j'} = \frac{1}{2} (A_{ii'} A_{jj'} + A_{ij'} A_{ji'}), \quad (6)$$

$$\chi(g) = \frac{1}{2} (A_{ii} A_{jj} + A_{ij} A_{ji}) = \frac{1}{2} \{ [\text{Tr} \hat{A}(g)]^2 + \text{Tr} \hat{A}(g^2) \}. \quad (7)$$

(2) Tensor of rank 4,  $F_{\{\{ij\}, \{kl\}\}}$ .

$$\chi(g) = \frac{1}{8} [(\text{Tr } \hat{A}(g))^2 + \text{Tr } \hat{A}(g^2)]^2 + \frac{1}{4} \{ [\text{Tr } \hat{A}(g^2)]^2 + \text{Tr } \hat{A}(g^4) \} . \quad (9)$$

(3) Tensor of rank 6,  $F_{\{ij\},\{kl\},\{mn\}}$ .

$$\begin{aligned} [\hat{F}(g)]_{ijklmn,i'j'k'l'm'n'} &= \{ \{ A \times A \} \times \{ A \times A \} \times \{ A \times A \} \}_{ijklmn,i'j'k'l'm'n'} \\ &= \frac{1}{6} (\{ A \times A \}_{ij,i'j'} \{ A \times A \}_{kl,k'l'} \{ A \times A \}_{mn,m'n'} + \{ A \times A \}_{ij,i'j'} \{ A \times A \}_{kl,m'n'} \{ A \times A \}_{mn,k'l'} \\ &\quad + \{ A \times A \}_{ij,k'l'} \{ A \times A \}_{kl,i'j'} \{ A \times A \}_{mn,m'n'} + \{ A \times A \}_{ij,k'l'} \{ A \times A \}_{kl,m'n'} \{ A \times A \}_{mn,i'j'} \\ &\quad + \{ A \times A \}_{ij,m'n'} \{ A \times A \}_{kl,i'j'} \{ A \times A \}_{mn,k'l'} + \{ A \times A \}_{ij,m'n'} \{ A \times A \}_{kl,k'l'} \{ A \times A \}_{mn,i'j'} ) . \end{aligned} \quad (10)$$

$$\begin{aligned} \chi(g) &= \frac{1}{48} \{ [\text{Tr } \hat{A}(g)]^2 + \text{Tr } \hat{A}(g^2) \}^3 + \frac{1}{8} \{ [\text{Tr } \hat{A}(g)]^2 + \text{Tr } \hat{A}(g^2) \} \{ [\text{Tr } \hat{A}(g^2)]^2 + \text{Tr } \hat{A}(g^4) \} \\ &\quad + \frac{1}{6} \{ [\text{Tr } \hat{A}(g^3)]^2 + \text{Tr } \hat{A}(g^6) \} . \end{aligned} \quad (11)$$

(4) Tensor of rank 2,  $F_{ai}$ .

$$[\hat{F}(g)]_{ai,\alpha'i'} = (A' \times A)_{ai,\alpha'i'} = A'_{\alpha\alpha'} A_{ii'} , \quad (12)$$

$$\chi(g) = A_{\alpha\alpha'} A_{ii'} = \text{Tr } \hat{A}'(g) \cdot \text{Tr } \hat{A}(g) . \quad (13)$$

(5) Tensor of rank 4,  $F_{\{ai,\beta j\}}$ .

$$\begin{aligned} [\hat{F}(g)]_{ai\beta j,\alpha'i'\beta'j'} &= [ \{ (A' \times A) \times (A' \times A) \} ]_{ai\beta j,\alpha'i'\beta'j'} \\ &= \frac{1}{2} [ (A' \times A \times A' \times A)_{ai\beta j,\alpha'i'\beta'j'} + (A' \times A \times A' \times A)_{ai\beta j,\beta'j'\alpha'i'} ] , \end{aligned} \quad (14)$$

$$\chi(g) = \frac{1}{2} [ \text{Tr } \hat{A}'(g) \cdot \text{Tr } \hat{A}(g) ]^2 + \frac{1}{2} \text{Tr } \hat{A}'(g^2) \cdot \text{Tr } \hat{A}(g^2) . \quad (15)$$

(6) Tensor of rank 6,  $F_{\{ai,\beta j,\gamma k\}}$ .

$$\begin{aligned} [\hat{F}(g)]_{ai\beta j\gamma k,\alpha'i'\beta'j'\gamma'k'} &= [ \{ (A' \times A) \times (A' \times A) \times (A' \times A) \} ]_{ai\beta j\gamma k,\alpha'i'\beta'j'\gamma'k'} \\ &= \frac{1}{6} [ (A' \times A \times A' \times A \times A' \times A)_{ai\beta j\gamma k,\alpha'i'\beta'j'\gamma'k'} + (A' \times A \times A' \times A \times A' \times A)_{ai\beta j\gamma k,\alpha'i'\gamma'k'\beta'j'} \\ &\quad + (A' \times A \times A' \times A \times A' \times A)_{ai\beta j\gamma k,\beta'j'\alpha'i'\gamma'k'} + (A' \times A \times A' \times A \times A' \times A)_{ai\beta j\gamma k,\beta'j'\gamma'k'\alpha'i'} \\ &\quad + (A' \times A \times A' \times A \times A' \times A)_{ai\beta j\gamma k,\gamma'k'\alpha'i'\beta'j'} + (A' \times A \times A' \times A \times A' \times A)_{ai\beta j\gamma k,\gamma'k'\beta'j'\alpha'i'} ] , \end{aligned} \quad (16)$$

$$\chi(g) = \frac{1}{6} [ \text{Tr } \hat{A}'(g) \cdot \text{Tr } \hat{A}(g) ]^3 + \frac{1}{2} \text{Tr } \hat{A}'(g) \cdot \text{Tr } \hat{A}(g) \cdot \text{Tr } \hat{A}'(g^2) \cdot \text{Tr } \hat{A}(g^2) + \frac{1}{3} \text{Tr } \hat{A}'(g^3) \cdot \text{Tr } \hat{A}(g^3) . \quad (17)$$

(7) Tensor of rank 4,  $F_{\{ij\},\beta l}$ .

$$[\hat{F}(g)]_{ij\beta l,i'j'\beta'l'} = \frac{1}{2} (A_{ii'} A_{jj'} + A_{ij'} A_{ji'}) A'_{\beta\beta'} A_{ll'} , \quad (18)$$

$$\chi(g) = \frac{1}{2} \{ [\text{Tr } \hat{A}(g)]^2 + \text{Tr } \hat{A}(g^2) \} \cdot \text{Tr } \hat{A}'(g) \cdot \text{Tr } \hat{A}(g) . \quad (19)$$

(8) Tensor of rank 6,  $F_{\{ij\},\{kl\},\gamma n}$ .

$$\begin{aligned} [\hat{F}(g)]_{ijkl\gamma n,i'j'k'l'\gamma'n'} &= \frac{1}{8} [ (A_{ii'} A_{jj'} + A_{ij'} A_{ji'}) (A_{kk'} A_{ll'} + A_{kl'} A_{lk'}) \\ &\quad + (A_{ik'} A_{jl'} + A_{il'} A_{jk'}) (A_{ki'} A_{ij'} + A_{kj'} A_{ii'}) ] A'_{\gamma\gamma'} A_{nn'} , \end{aligned} \quad (20)$$

$$\chi(g) = \frac{1}{8} \{ [\text{Tr } \hat{A}(g)]^2 + \text{Tr } \hat{A}(g^2) \}^2 + 2 \{ [\text{Tr } \hat{A}(g^2)]^2 + \text{Tr } \hat{A}(g^4) \} \cdot \text{Tr } \hat{A}'(g) \cdot \text{Tr } \hat{A}(g) . \quad (21)$$

(9) Tensor of rank 6,  $F_{\{ij\},\{\beta l,\gamma n\}}$ .

$$[\hat{F}(g)]_{ij\beta l\gamma n,i'j'\beta'l'\gamma'n'} = \frac{1}{4} (A_{ii'} A_{jj'} + A_{ij'} A_{ji'}) [ (A' \times A \times A' \times A)_{\beta l\gamma n,\beta'l'\gamma'n'} + (A' \times A \times A' \times A)_{\beta l\gamma n,\gamma'n'\beta'l'} ] , \quad (22)$$

$$\chi(g) = \frac{1}{4} \{ [\text{Tr } \hat{A}'(g) \cdot \text{Tr } \hat{A}(g)]^2 + \text{Tr } \hat{A}'(g^2) \cdot \text{Tr } \hat{A}(g^2) \} \cdot \{ [\text{Tr } \hat{A}(g)]^2 + \text{Tr } \hat{A}(g^2) \} . \quad (23)$$

In a similar manner, the representation matrices and the characters of tensors of higher ranks and other kinds can be obtained.

### III. APPLICATION: CALCULATION OF THE NUMBER OF INDEPENDENT COMPONENTS OF THE ELASTIC-CONSTANT TENSOR IN QUASICRYSTALS

The elastic energy density  $f$  of a quasicrystal is a function of phonon strain field  $E_{ij}$  and phason strain field  $W_{ij}$ , and can be expanded in terms of a Taylor series in the vicinity of  $E_{ij}=0$  and  $W_{ij}=0$  to the third order:

TABLE II. Characters of  $C_{8v}$  symmetry.

	$\epsilon$	$2\alpha$	$2\alpha^2$	$2\alpha^3$	$\alpha^4$	$4\beta$	$4\alpha\beta$	$a_1$
$\Gamma_1$	1	1	1	1	1	1	1	
$\Gamma_2$	1	1	1	1	1	-1	-1	
$\Gamma_3$	1	-1	1	-1	1	1	-1	
$\Gamma_4$	1	-1	1	-1	1	-1	1	
$^*\Gamma_5$	2	$\sqrt{2}$	0	$-\sqrt{2}$	-2	0	0	
$\Gamma_6$	2	0	-2	0	2	0	0	
$^\dagger\Gamma_7$	2	$-\sqrt{2}$	0	$\sqrt{2}$	-2	0	0	
$C_{ijkl}$	6	0	2	0	6	2	2	2
$K_{ijkl}$	10	2	2	2	10	2	2	3
$R_{ijkl}$	12	-2	0	-2	12	0	0	1
$C_{ijklmn}$	10	0	-2	0	10	2	2	2
$K_{ijklmn}$	20	-2	0	-2	20	0	0	2
$R_{ijklmn}^1$	24	0	0	0	24	0	0	3
$R_{ijklmn}^2$	30	2	-2	2	30	2	2	5
$C'_{ijkl}$	21	$3+2\sqrt{2}$	1	$3-2\sqrt{2}$	5	5	5	5
$C'_{ijklmn}$	56	$4+2\sqrt{2}$	0	$4-2\sqrt{2}$	8	8	8	9
$R'_{ijkl}$	24	$-4-2\sqrt{2}$	0	$-4+2\sqrt{2}$	8	0	0	1
$R'_{ijklmn}$	84	$-6-4\sqrt{2}$	0	$-6+4\sqrt{2}$	20	0	0	5
$R''_{ijklmn}$	60	$4+2\sqrt{2}$	0	$4-2\sqrt{2}$	20	4	4	8

TABLE III. Characters of  $C_{10v}$  symmetry [ $\tau=(1+\sqrt{5})/2$ ].

	$\epsilon$	$2\alpha$	$2\alpha^2$	$2\alpha^3$	$2\alpha^4$	$\alpha^5$	$5\beta$	$5\alpha\beta$	$a_1$
$\Gamma_1$	1	1	1	1	1	1	1	1	
$\Gamma_2$	1	1	1	1	1	1	-1	-1	
$\Gamma_3$	1	-1	1	-1	1	-1	1	-1	
$\Gamma_4$	1	-1	1	-1	1	1	1	-1	
$^*\Gamma_5$	2	$\tau$	$\tau-1$	$1-\tau$	$-\tau$	-2	0	0	
$\Gamma_6$	2	$\tau-1$	$-\tau$	$-\tau$	$\tau-1$	2	0	0	
$^\dagger\Gamma_7$	2	$1-\tau$	$-\tau$	$\tau$	$\tau-1$	-2	0	0	
$\Gamma_8$	2	$-\tau$	$\tau-1$	$\tau-1$	$-\tau$	2	0	0	
$C_{ijkl}$	6	1	1	1	1	6	2	2	2
$K_{ijkl}$	10	0	0	0	0	10	2	2	2
$R_{ijkl}$	12	$-\tau$	$\tau-1$	$\tau-1$	$-\tau$	12	0	0	1
$C_{ijklmn}$	10	0	0	0	0	10	2	2	2
$K_{ijklmn}$	20	0	0	0	0	20	0	0	2
$R_{ijklmn}^1$	24	-1	-1	-1	-1	24	0	0	2
$R_{ijklmn}^2$	30	0	0	0	0	30	2	2	4
$C'_{ijkl}$	21	$3+4\tau$	1	$7-4\tau$	1	5	5	5	5
$C'_{ijklmn}$	56	$5+6\tau$	1	$11-6\tau$	1	8	8	8	9
$R'_{ijkl}$	24	$-1-2\tau$	-1	$-3+2\tau$	-1	8	0	0	1
$R'_{ijklmn}$	84	$-3-4\tau$	-1	$-7+4\tau$	-1	20	0	0	4
$R''_{ijklmn}$	60	0	0	0	0	20	4	4	6

$$\begin{aligned}
 f(E_{pq}, W_{pq}) = & \frac{1}{2} \frac{\partial^2 f}{\partial E_{ij} \partial E_{kl}} \Big|_0 E_{ij} E_{kl} + \frac{1}{2} \frac{\partial^2 f}{\partial W_{ij} \partial W_{kl}} \Big|_0 W_{ij} W_{kl} + \frac{\partial^2 f}{\partial E_{ij} \partial W_{kl}} \Big|_0 E_{ij} W_{kl} + \frac{1}{6} \frac{\partial^3 f}{\partial E_{ij} \partial E_{kl} \partial E_{mn}} \Big|_0 E_{ij} E_{kl} E_{mn} \\
 & + \frac{1}{6} \frac{\partial^3 f}{\partial W_{ij} \partial W_{kl} \partial W_{mn}} \Big|_0 W_{ij} W_{kl} W_{mn} + \frac{1}{2} \frac{\partial^3 f}{\partial E_{ij} \partial E_{kl} \partial W_{mn}} \Big|_0 E_{ij} E_{kl} W_{mn} \\
 & + \frac{1}{2} \frac{\partial^3 f}{\partial E_{ij} \partial W_{kl} \partial W_{mn}} \Big|_0 E_{ij} W_{kl} W_{mn} + \dots,
 \end{aligned}
 \tag{24}$$

TABLE IV. Characters of  $C_{12v}$  symmetry.

	$\epsilon$	$2\alpha$	$2\alpha^2$	$2\alpha^3$	$2\alpha^4$	$2\alpha^5$	$\alpha^6$	$6\beta$	$6\alpha\beta$	$a_1$
$\Gamma_1$	1	1	1	1	1	1	1	1	1	
$\Gamma_2$	1	1	1	1	1	1	1	-1	-1	
$\Gamma_3$	1	-1	1	-1	1	-1	1	1	-1	
$\Gamma_4$	1	-1	1	-1	1	-1	1	-1	1	
$^*\Gamma_5$	2	$\sqrt{3}$	1	0	-1	$-\sqrt{3}$	-2	0	0	
$\Gamma_6$	2	1	-1	-2	-1	1	2	0	0	
$\Gamma_7$	2	0	-2	0	1	0	-2	0	0	
$\Gamma_8$	2	-1	-1	2	-1	-1	2	0	0	
$^\dagger\Gamma_9$	2	$-\sqrt{3}$	1	0	-1	$\sqrt{3}$	-2	0	0	
$C_{ijkl}$	6	2	0	2	0	2	6	2	2	2
$K_{ijkl}$	10	5	1	2	1	5	10	2	2	3
$R_{ijkl}$	12	-6	0	0	0	-6	12	0	0	0
$C_{ijklmn}$	10	1	1	-2	1	1	10	2	2	2
$K_{ijklmn}$	20	-6	2	0	2	-6	20	0	0	1
$R_{ijklmn}^1$	24	-6	0	0	0	-6	24	0	0	1
$R_{ijklmn}^2$	30	10	0	-2	0	10	30	2	2	5
$C'_{ijkl}$	21	$7+3\sqrt{3}$	2	1	0	$7-3\sqrt{3}$	5	5	5	5
$C'_{ijklmn}$	56	$12+6\sqrt{3}$	2	0	2	$12-6\sqrt{3}$	8	8	8	9
$R'_{ijkl}$	24	$-9-3\sqrt{3}$	2	0	0	$-9+3\sqrt{3}$	8	0	0	0
$R'_{ijklmn}$	84	$-21-9\sqrt{3}$	2	0	0	$-21+9\sqrt{3}$	20	0	0	1
$R''_{ijklmn}$	60	$15+5\sqrt{3}$	2	0	0	$15-5\sqrt{3}$	20	4	4	8

with the conditions  $f(0,0)=0$ ,  $\partial f/\partial E_{ij}|_0=0$ ,  $\partial f/\partial W_{ij}|_0=0$ , where  $|_0$  means  $E_{pq}=0$  and  $W_{pq}=0$ .

The definitions of the fourth-order and sixth-order elastic-constant tensors are:

$$\begin{aligned} C_{ijkl} &= \frac{\partial^2 f}{\partial E_{ij} \partial E_{kl}} \Big|_0, & K_{ijkl} &= \frac{\partial^2 f}{\partial W_{ij} \partial W_{kl}} \Big|_0, & R_{ijkl} &= \frac{\partial^2 f}{\partial E_{ij} \partial W_{kl}} \Big|_0, \\ C_{ijklmn} &= \frac{\partial^3 f}{\partial E_{ij} \partial E_{kl} \partial E_{mn}} \Big|_0, & K_{ijklmn} &= \frac{\partial^3 f}{\partial W_{ij} \partial W_{kl} \partial W_{mn}} \Big|_0, \\ R_{ijklmn}^1 &= \frac{\partial^3 f}{\partial E_{ij} \partial E_{kl} \partial W_{mn}} \Big|_0, & R_{ijklmn}^2 &= \frac{\partial^3 f}{\partial E_{ij} \partial W_{kl} \partial W_{mn}} \Big|_0. \end{aligned} \quad (25)$$

According to the analyses of physical-property tensors in quasicrystals in Sec. II,  $C_{ijkl}$  corresponds to  $F_{\{\{ij\},\{kl\}\}}$ ,  $K_{ijkl}$  corresponds to  $F_{\{\alpha j, \beta l\}}$  and so on, i.e.,

$$\begin{aligned} C_{ijkl} &\rightarrow F_{\{\{ij\},\{kl\}\}}, & K_{ijkl} &\rightarrow F_{\{\alpha j, \beta l\}}, \\ R_{ijkl} &\rightarrow F_{\{ij\}, \beta l}, \\ C_{ijklmn} &\rightarrow F_{\{\{ij\},\{kl\},\{mn\}\}}, & K_{ijklmn} &\rightarrow F_{\{\alpha j, \beta l, \gamma n\}}, \\ R_{ijklmn}^1 &\rightarrow F_{\{\{ij\},\{kl\}\}, \gamma n}, & R_{ijklmn}^2 &\rightarrow F_{\{ij\}, \{\beta l, \gamma n\}}. \end{aligned} \quad (26)$$

Obviously, once the point symmetry group of the quasicrystal is given, the representation matrices and corresponding characters of the above seven types of elastic-constant tensors can be derived, and then the number of independent components  $a_1$  can easily be obtained from Eq. (4). The results for the icosahedral quasicrystal are listed in Table I.

In Tables II–IV, the tensors  $C_{ijkl}$ ,  $K_{ijkl}$ ,  $R_{ijkl}$ ,  $C_{ijklmn}$ ,  $K_{ijklmn}$ ,  $R_{ijklmn}^1$ ,  $R_{ijklmn}^2$  correspond to planar quasicrystals with eight-, ten-, and twelfold symmetries, the tensors  $C'_{ijkl}$ ,  $K'_{ijkl}$ ,  $R'_{ijkl}$ ,  $C'_{ijklmn}$ ,  $K'_{ijklmn}$ ,  $R'_{ijklmn}^1$ ,  $R'_{ijklmn}^2$  to three-dimensional cases. For cubic quasicrystals, the sub-

scripts of a tensor which refer to the physical space can commute with those which refer to the complementary space, i.e.,  $\alpha i \rightarrow \{ai\}$  and  $F_{\alpha i} \rightarrow F_{\{ai\}}$  for the tensor of rank 2. Similarly, commutation relations between subscripts can be found for other tensors. All the results are listed in Table V.

In Tables I–V, the notations \* and † are used to indicate the transformations in physical space and complementary space of icosahedral, planar quasicrystals with eight-, ten-, and twelfold symmetries and cubic quasicrystals, respectively. For the three-dimensional quasicrystals with eight-, ten-, and twelfold symmetries in Tables II–IV, both  $\partial_j$  and  $U_i$  in  $E_{ij}$  transform under the representation  $(\Gamma_1 + \Gamma^*)$ , but  $\partial_j$  and  $W_i$  in  $W_{ij}$  transform under the representation  $\Gamma^*$  and  $\Gamma^\dagger$  respectively (here,  $\Gamma^*$  and  $\Gamma^\dagger$  are the representations labeled by \* and † respectively in Tables II–IV; hence, in the characteristic formulas in Sec. II, the representation of  $\hat{A}(g)$  under which  $E_{ij}$  transforms is  $(\Gamma_1 + \Gamma^*)$  the representation of  $\hat{A}(g)$  under which  $W_{ij}$  transforms is  $\Gamma^*$ , and the representation of  $\hat{A}'(g)$  takes the representation  $\Gamma^\dagger$  for both planar and three-dimensional cases.<sup>14</sup>

Finally, we would like to make mention of some previous work. Levine *et al.*<sup>15</sup> derived the elastic-constant tensor of rank 4 of icosahedral and pentagonal quasicrystals, Socolar<sup>16</sup> gave those of planar octagonal and dodecagonal quasicrystals, Hu, Ding, and Yang<sup>14</sup> obtained those for three-dimensional eight-, ten-, and twelfold symmetries, Yang *et al.*<sup>12</sup> derived those for cubic quasicrystals, Ishii<sup>17</sup> discussed thoroughly the relation between phase transformations and the cubic-order invariants for the phason strains in icosahedral quasicrystals, Oxborrow and Henley<sup>18</sup> pointed out that there exists only one third-order phason strain constant in the dodecagonal phase, and so on. Our results all agree with theirs. Of course, using the method in the above example, we can easily obtain any higher-order constants of physical-property tensors for quasicrystal structures.

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TABLE V. Characters of cubic quasicrystal point symmetry.

	1E	8C <sub>3</sub>	3C <sub>2</sub> <sup>2</sup>	6C <sub>2</sub>	6C <sub>4</sub>	a <sub>1</sub>
Γ <sub>1</sub>	1	1	1	1	1	
Γ <sub>1</sub> '	1	1	1	-1	-1	
Γ <sub>2</sub>	2	-1	2	0	0	
*†Γ <sub>3</sub>	3	0	-1	-1	1	
Γ <sub>3</sub> '	3	0	-1	1	-1	
C <sub>ijkl</sub>	21	0	5	5	1	3
K <sub>ijkl</sub>	21	0	5	5	1	3
R <sub>ijkl</sub>	36	0	4	4	0	3
C <sub>ijklmn</sub>	56	2	8	8	0	6
K <sub>ijklmn</sub>	56	2	8	8	0	6
R <sub>ijklmn</sub> <sup>1</sup>	126	0	10	10	0	9
R <sub>ijklmn</sub> <sup>2</sup>	126	0	10	10	0	9

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