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Linear elasticity theory of pentagonal quasicrystals

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We present general solutions of the inhomogeneous linear elastic equations for pentagonal quasicrystals. The equations are those obtained by minimizing the harmonic elastic energy which includes a nontrivial coupling between the phason and displacement variables. Our solutions are presented in terms of the Green's functions for the elastic equations and allow the solution of any inhomogeneous linear elastic problem for pentagonal quasicrystals. They are also applicable to thin icosahedral plates, where the plane of the plate has pentagonal symmetry. We use our general solutions to find the displacement and phason fields surrounding a dislocation, and then derive the interaction energy of dislocations.

I. INTRODUCTION

The apparent experimental discovery of quasicrystalline materials has stimulated a flurry of investigations into the properties of these systems which are characterized by quasiperiodic translational order and noncrystallographic orientational symmetry.[1] The first step towards gaining a theoretical understanding of the mechanical properties was taken by several groups of workers[2] who constructed the harmonic elastic energies for pentagonal and icosahedral quasicrystals. The presence of incommensurate length scales in quasicrystals lead to additional elastic degrees of freedom not found in conventional crystals. (These degrees of freedom have been termed phasons.) Elastic energies that respect the appropriate symmetries were constructed in terms of these phason variables and the conventional displacement fields. In addition, Levine *et al.*[2(b)] considered the geometry of dislocations and found the allowed Burger's vectors.

To further develop the quantitative elastic theory, solutions of the linear elastic equations obtained from minimizing the energies must be found. We present solutions in this paper for the inhomogeneous equations associated with pentagonal quasicrystals. Our solutions are phrased in terms of the Green's functions of the elastic equations. The Green's functions can be used to solve in principal any inhomogeneous linear elastic problem for pentagonal quasicrystals, such as those involving well-defined forces, or those specifying inhomogeneous boundary conditions (i.e., not everywhere zero). The forces for instance, can be externally applied forces, or they can be the forces associated with singularities in the strain fields, e.g., those produced by dislocations or disclinations. The Green's functions should also be valid for thin icosahedral plates where the plane of the plate has pentagonal symmetry and negligible deformations occur perpendicular to this plane of symmetry. It should be emphasized that the elastic equations we are solving assume that the phason degrees of freedom have reached equilibrium.[3]

To illustrate the utility of the Green's function solutions, we calculate here the displacement and phason fields caused by a dislocation in a pentagonal quasicrystal. We further calculate the interaction energy of an arbitrary complexion of dislocations.

This paper is organized as follows. In the next section we review the main results of Ref. 2 which we need here. In Sec. III we derive the Green's functions for the elastic equations. The results are stated in (3.32a)–(3.23j). In Sec. IV we use the Green's functions to calculate the displacement and phason fields surrounding a single dislocation, located at the origin of a pentagonal quasicrystal. The expressions for these are stated in (4.9a)–(4.9d). Finally in (4.16), we display the form for the interaction energy of an arbitrary distribution of such dislocations.

II. ELASTIC ENERGY AND BURGER'S VECTORS FOR PENTAGONAL QUASICRYSTALS

In this section we review and elaborate upon the results of Ref. 2, in order to develop the background information needed for the remainder of the paper.[4] In developing a continuum elastic theory for quasicrystals, the density wave description is a natural choice. As we wish to focus on general elastic properties, i.e., those which depend on symmetries and not specific physical details (such as atomic species), we can expand the mass density $\rho(\mathbf{r})$ in a Fourier series involving a minimal set of $\{G\}$ reciprocal vectors:

$$\rho(\mathbf{r})=\sum_{\mathbf{G}}\rho_{\mathbf{G}}\exp(i\mathbf{G}\cdot\mathbf{r}) . \tag{2.1}$$

For the pentagonal case, $\{G\}$ comprises the five vectors,

$$\mathbf{G}_n=G\left[\cos\frac{2\pi n}{5},\sin\frac{2\pi n}{5}\right],\quad n=0,\ldots,4 ,$$

and their reflected images $-\mathbf{G}_n$ (the latter are included to ensure a real density). Of the five vectors $\mathbf{G}_n$, only four are independent since $\sum_{n=0}^{4}\mathbf{G}_n=0$. This statement is a special case of a general result, namely, the minimum number of vectors $\mathbf{G}_n$ required is $n_i d$ where n_i is the number of relatively incommensurate lengths, and d is the spatial dimensionality. For the pentagonal case, $n_i=d=2$.

Each $\rho_{\mathbf{G}_n}$ appearing in (2.1) is a complex number that may be written as $|\rho_{\mathbf{G}}|e^{i\phi_G}$. Minimization of the free energy with respect to the ϕ_G's leaves four (i.e., $n_i d$) of them unspecified and these are the hydrodynamic variables of the theory. The four degrees of freedom are best parametrized by two two-dimensional vectors, $\mathbf{u}$ and $\mathbf{w}$, as follows:

$$\phi_{\mathbf{G}_n}(\mathbf{r})=\mathbf{G}_n\cdot\mathbf{u}(\mathbf{r})+a\mathbf{G}_{\langle 3n\rangle_5}\cdot\mathbf{w}(\mathbf{r})+\frac{\gamma}{5}\ , \tag{2.2}$$

where $\langle 3n\rangle_5$ means $3n$ mod 5. The parameter a is an arbitrary scale factor, and γ is the value of $\sum_n \phi_{\mathbf{G}_n}$ in the minimum-energy state.

As shown in Refs. 2 and 4, the $\mathbf{u}$ field corresponds to translations of the system, while $\mathbf{w}$ is analogous to the phason degree of freedom in incommensurate systems. The latter variable shifts the density waves relative to each other (in the Penrose tiling picture of quasicrystals, a uniform shift in $\mathbf{w}$ rearranges the unit cells). A phenomenological harmonic elastic energy is readily constructed in terms of $\mathbf{u}$ and $\mathbf{w}$ from their behavior under the operations of the tenfold point group. This group consists of rotations by $2\pi n/10$, $n=0,\ldots,9$, and reflections across the ten mirror planes which bisect the edges of a decagon. Under rotations of the crystal by $2\pi n/10$, $\mathbf{u}$ rotates by $2\pi n/10$, while $\mathbf{w}$ rotates by $6\pi n/10$. The reflections correspond to the transformations $\mathbf{r}\to\overleftrightarrow{\mathbf{B}}\cdot\mathbf{r}$, $\mathbf{u}\to\overleftrightarrow{\mathbf{B}}\cdot\mathbf{u}$, and $\mathbf{w}\to\overleftrightarrow{\mathbf{B}}^1\cdot\mathbf{w}$, where

$$B=\begin{bmatrix}\cos\dfrac{2\pi l}{10} & \sin\dfrac{2\pi l}{10}\\ \sin\dfrac{2\pi l}{10} & -\cos\dfrac{2\pi l}{10}\end{bmatrix},$$
$$B^1=\begin{bmatrix}\cos\dfrac{6\pi l}{10} & \sin\dfrac{6\pi l}{10}\\ \sin\dfrac{6\pi l}{10} & -\cos\dfrac{6\pi l}{10}\end{bmatrix}, \tag{2.3}$$

where $l=0,\ldots,9$, indexes the ten mirror planes. The harmonic elastic energy density has the form

$$F=\tfrac{1}{2}\lambda u_{ii}u_{ii}+\mu u_{ij}u_{ij}+\tfrac{1}{2}K_1 w_{ij}w_{ij}+K_2(w_{xx}w_{yy}-w_{xy}w_{yx})$$
$$+K_3[(u_{xx}-u_{yy})(w_{xx}+w_{yy})+2u_{xy}(w_{xy}-w_{yx})]-\tilde f\tilde u\ , \tag{2.4}$$

where $u_{ij}\equiv\frac{1}{2}(\partial_i u_j+\partial_j u_i)$ is the strain tensor and $w_{ij}\equiv\partial_i w_j$. An additional term coupling $\mathbf{u}$ and $\mathbf{w}$ is present in Ref. 2(b); however, this term can readily be shown to violate the mirror plane symmetry described above.[2(a)] (An energy containing this latter term would describe a "chiral" pentagonal quasicrystal.)[5] In the absence of dislocations, the term proportional to K_2 may be integrated by parts to zero. A stability analysis requires that in the absence of dislocations $\mu+\lambda>0$, $\mu>0$, $K_1>0$, and $\mu K_1>K_3^2$, in order that a state with uniform $\mathbf{u}$ and $\mathbf{w}$ fields correspond to minimum energy.[6]

Note that the first two terms on the right-hand side of (2.4) describe a two-dimensional isotropic solid,[7] while the third term can be viewed as a sum of the energy densities of two XY models, with polar angles w_x and w_y, respectively. The last term in (2.4) represents a general coupling of $\tilde u=\mathbf{u}\oplus\mathbf{w}$, the four-dimensional elastic field, to a generalized four-dimensional force $\tilde f$. In Sec. IV we give a specific example of $\tilde f$ appropriate to dislocations.

Finally, we review the geometry of the dislocations derived in Ref. 2(b). Dislocations are defined as topologically stable point defects which leave the phases $\phi_{\mathbf{G}_n}$ invariant modulo 2π. In a pentagonal quasicrystal the dislocations are described by four-dimensional Burger's vectors $\tilde b=\mathbf{b}\oplus\mathbf{d}$ where

$$\oint d\mathbf{u}=\mathbf{b},\quad \oint d\mathbf{w}=\mathbf{d}\ . \tag{2.5}$$

The line integrals in (2.5) are along a closed contour surrounding the core of the defect. The Burger's vector $\tilde b$ belongs to the set of all vectors formed from integral linear combinations of the vectors $\tilde R=\mathbf{R}_n\oplus b\mathbf{R}_{\langle 3n\rangle_5}$, where

$$\mathbf{R}_n=R\left[-\sin\frac{2\pi n}{5},\cos\frac{2\pi n}{5}\right],\quad n=0,\ldots,4\ .$$

The invariance of the phases modulo 2π imposes the constraints

$$GR=\frac{8\pi}{5}\sin\frac{4\pi}{5},\quad ab=\frac{\sin(2\pi/5)}{\sin(4\pi/5)}\ . \tag{2.6}$$

As in Ref. 2(b), we choose $b=1$, which yields the simplest geometry of the Burger's vector lattice. Note that no Burger's vector lies either in the $\mathbf{u}=\mathbf{0}$ or $\mathbf{w}=\mathbf{0}$ planes.

III. ELASTIC EQUATIONS AND THEIR SOLUTIONS

In this section we solve the inhomogeneous elastic equations (i.e., the equations of static equilibrium) associated with the harmonic energy (2.4). These equations are generated by the usual Euler-Lagrange procedure, extremizing F with respect to small variables δu_x, δu_y, δw_x, and δw_y. We then find the following system of equations:

$$\mu\nabla^2 u_x+K\frac{\partial}{\partial x}\nabla\cdot\mathbf{u}+K_3\left[\frac{\partial^2 w_x}{\partial x^2}+2\frac{\partial^2 w_y}{\partial x\,\partial y}-\frac{\partial^2 w_x}{\partial y^2}\right]=-\tilde f_1\ , \tag{3.1a}$$

$$\mu\nabla^2 u_y+K\frac{\partial}{\partial y}\nabla\cdot\mathbf{u}+K_3\left[\frac{\partial^2 w_y}{\partial x^2}-2\frac{\partial^2 w_x}{\partial x\,\partial y}-\frac{\partial^2 w_y}{\partial y^2}\right]=-\tilde f_2\ , \tag{3.1b}$$

$$K_1\nabla^2 w_x+K_3\left[\frac{\partial^2 u_x}{\partial x^2}-2\frac{\partial^2 u_y}{\partial x\,\partial y}-\frac{\partial^2 u_x}{\partial y^2}\right]=-\tilde f_3\ , \tag{3.1c}$$

$$K_1\nabla^2 w_y+K_3\left[\frac{\partial^2 u_y}{\partial x^2}+2\frac{\partial^2 u_x}{\partial x\,\partial y}-\frac{\partial^2 u_y}{\partial y^2}\right]=-\tilde f_4\ , \tag{3.1d}$$

where $K=\mu+\lambda$ is the two-dimensional bulk modulus. For notational convenience we will refer to (3.1a)–(3.1d) as $L_i[\tilde u]=-\tilde f_i$ with $i=1,2,3,4$, respectively. Here the L_i are the linear differential operators defined via (3.1). The most convenient way to solve these inhomogeneous equations is to calculate the associated sixteen-component Green's tensor $\overleftrightarrow{\mathbf{G}}(\mathbf{r}-\mathbf{r}')$ defined such that[8]

$$\tilde{u}(\mathbf{r})=\int d\mathbf{r}'\overleftrightarrow{G}(\mathbf{r}-\mathbf{r}')\tilde{f}(\mathbf{r}') \ . \tag{3.2}$$

Thus, the four elements of the jth column of $\overleftrightarrow{G}$ are the solutions of the four equations $L_i[\tilde{u}]=-\tilde{f}_i$, $i=1,2,3,4$ with $\tilde{f}_i=\delta_{ij}\delta(\mathbf{r})$. For notational convenience we write $\overleftrightarrow{G}$ in terms of four 2×2 matrices as follows:

$$G=\begin{bmatrix}\overleftrightarrow{\alpha} & \overleftrightarrow{\beta}\\ \overleftrightarrow{\gamma} & \overleftrightarrow{\delta}\end{bmatrix}=\begin{bmatrix}\alpha_{11} & \alpha_{12} & \beta_{11} & \beta_{12}\\ \alpha_{21} & \alpha_{22} & \beta_{21} & \beta_{22}\\ \gamma_{11} & \gamma_{12} & \delta_{11} & \delta_{12}\\ \gamma_{21} & \gamma_{22} & \delta_{21} & \delta_{22}\end{bmatrix} . \tag{3.3}$$

Then, e.g., α_{11}, α_{21}, γ_{11}, and γ_{21} yield the solutions u_x, u_y, w_x, and w_y of (3.1a)–(3.1d) for a force $\tilde{f}_i=\delta_{i1}\delta(\mathbf{r})$. Analogous statements hold for the remaining components of $\overleftrightarrow{G}$.

We solve for $\overleftrightarrow{G}$ iteratively in powers of the parameter K_3 which couples $\mathbf{u}$ and $\mathbf{w}$ in (3.1). When $K_3=0$, (3.1) reduces to the following simpler set of equations:

$$\mu\nabla^2 u_x+K\frac{\partial}{\partial x}(\nabla\cdot\mathbf{u})=-\tilde{f}_1 \ , \tag{3.4a}$$

$$\mu\nabla^2 u_y+K\frac{\partial}{\partial y}(\nabla\cdot\mathbf{u})=-\tilde{f}_2 \ , \tag{3.4b}$$

$$K_1\nabla^2 w_x=-\tilde{f}_3 \ , \tag{3.4c}$$

$$K_1\nabla^2 w_y=-\tilde{f}_4 \ . \tag{3.4d}$$

The first two equations above are those of an isotropic, two-dimensional crystal,[7] in the presence of a force $(\tilde{f}_1,\tilde{f}_2)$, while the last two are two-dimensional Poisson equations. We denote the components of $\overleftrightarrow{G}$ corresponding to the solutions of (3.4) by zero superscripts. Since $\mathbf{u}$ and $\mathbf{w}$ are decoupled, we know immediately that $\overleftrightarrow{\beta}^{(0)}=\overleftrightarrow{\gamma}^{(0)}=0$. In order to calculate $\overleftrightarrow{\alpha}^{(0)}$ we need only consider (3.4a) and (3.4b); likewise to find $\overleftrightarrow{\delta}^{(0)}$ we need only consider (3.4c) and (3.4d).

Our calculation of $\overleftrightarrow{\alpha}^{(0)}$ is the two-dimensional analog of the calculation presented in Ref. 7 for the Green's tensor for a three-dimensional isotropic crystal. Equations (3.4a) and (3.4b) can be rewritten compactly as follows:

$$\nabla^2\mathbf{u}+\frac{K}{\mu}\nabla(\nabla\cdot\mathbf{u})=-\frac{1}{\mu}\mathbf{F}\delta(\mathbf{r}) \ , \tag{3.5}$$

where $\mathbf{F}=(\tilde{f}_1,\tilde{f}_2)$. If we choose $\mathbf{F}=(1,0)$ then the solutions u_x and u_y equal $\alpha_{11}^{(0)}$ and $\alpha_{21}^{(0)}$, respectively. Choosing $F=(0,1)$ will similarly yield $\alpha_{12}^{(0)}$ and $\alpha_{22}^{(0)}$. We look for solutions of the form $\mathbf{u}=\mathbf{v}+\mathbf{z}$ where $\mathbf{z}$ satisfies the two-dimensional Poisson equation:

$$\nabla^2\mathbf{z}=-\frac{1}{\mu}\mathbf{F}\delta(\mathbf{r}) \ . \tag{3.6}$$

Equation (3.6) has the solution[9]

$$\mathbf{z}=-\frac{\mathbf{F}}{2\pi\mu}\ln(r/a) \tag{3.7}$$

in polar coordinates, where a is a short-distance cutoff, e.g., the lattice spacing. Using (3.7) in (3.5) we find that $\mathbf{v}$ must satisfy

$$\nabla^2\mathbf{v}+\frac{K}{\mu}\nabla(\nabla\cdot\mathbf{v})=\frac{K}{2\pi\mu^2}\nabla\mathbf{F}\cdot\nabla\ln(r/a) \ . \tag{3.8}$$

Taking the z component of the curl of this equation we find that

$$\nabla^2\left[\frac{\partial v_x}{\partial y}-\frac{\partial v_y}{\partial x}\right]=0 \ . \tag{3.9}$$

Since at infinity we must have $\partial v_x/\partial y-\partial v_y/\partial x=0$, then throughout the two-dimensional space this harmonic quantity must equal zero. Thus, we may write $\mathbf{v}=\nabla\phi$. In terms of ϕ, (3.8) reads

$$\nabla^2\phi=\frac{K}{2\pi\mu(2\mu+\lambda)}\mathbf{F}\cdot\nabla\ln(r/a) \ . \tag{3.10}$$

Since the function $\psi=(r^2/4)[\ln(r/a)-1]$ satisfies $\nabla^2\psi=\ln(r/a)$ and has no singularities, then up to an arbitrary harmonic function, the solution ϕ of (3.10) is

$$\phi=\frac{K}{2\pi\mu(2\mu+\lambda)}\mathbf{F}\cdot\mathbf{r}\left[\frac{r}{2}\ln\left[\frac{r}{a}\right]-\frac{r}{4}\right] . \tag{3.11}$$

Using (3.11) and (3.7), and choosing $\mathbf{F}$ as described following (3.5) we find that up to additive constants, the matrix elements of $\overleftrightarrow{\alpha}^{(0)}$ are

$$\alpha_{11}^{(0)}=-\frac{3\mu+\lambda}{4\pi\mu(2\mu+\lambda)}\ln\frac{r}{a}+\frac{K}{4\pi\mu(2\mu+\lambda)}\frac{x^2}{r^2} \ , \tag{3.12a}$$

$$\alpha_{12}^{(0)}=\alpha_{21}^{(0)}=\frac{K}{4\pi\mu(2\mu+\lambda)}\frac{xy}{r^2} \ , \tag{3.12b}$$

$$\alpha_{22}^{(0)}=-\frac{3\mu+\lambda}{4\pi\mu(2\mu+\lambda)}\ln\frac{r}{a}+\frac{K}{4\pi\mu(2\mu+\lambda)}\frac{y^2}{r^2} \ . \tag{3.12c}$$

We are allowed to ignore additive constants in calculating the elements of $\overleftrightarrow{G}$, since these constants will yield spatially uniform shifts of $\tilde{u}(\mathbf{r})$ [cf. (3.2)] which do not cost energy. However, these constants would be important in the situation where the value of $\tilde{u}(\mathbf{r})$ was specified on the boundary.

To find $\overleftrightarrow{\delta}^{(0)}$ we rewrite (3.4c) and (3.4d) as

$$\nabla^2\mathbf{w}=-\frac{1}{K_1}\mathbf{F}'\delta(\mathbf{r}) \ , \tag{3.13}$$

where $\mathbf{F}'=(\tilde{f}_3,\tilde{f}_4)$. This equation has the solution

$$\mathbf{w}=-\frac{\mathbf{F}'}{2\pi K_1}\ln(r/a) \ . \tag{3.14}$$

If we choose $\mathbf{F}'=(1,0)$, then the solutions w_i equal the matrix elements $\delta_{i1}^{(0)}$, $i=1,2$, respectively; similarly, with $\mathbf{F}'=(0,1)$, $w_i=\delta_{i2}^{(0)}$, $i=1,2$. Thus, we obtain

$$\delta_{11}^{(0)}=\delta_{22}^{(0)}=-\frac{1}{2\pi K_1}\ln(r/a) \ , \tag{3.15a}$$

$$\delta_{12}^{(0)}=\delta_{21}^{(0)}=0 \ . \tag{3.15b}$$

Solving (3.1) when $K_3\neq 0$ is considerably more complicated since the equations are coupled in $\mathbf{u}$ and $\mathbf{w}$. We solve (3.1) in that case iteratively, in powers of K_3 and then sum the results to all orders obtaining a closed form expression for the Green's tensor. In general this procedure is rather cumbersome, so we limit our presentation to an outline of the calculation of the matrix elements α_{11}, α_{21}, γ_{11}, and γ_{21}. Similar manipulations yield the remaining elements.

The elements α_{11}, α_{21}, γ_{11}, and γ_{21} are those in the first column of $\overleftrightarrow{G}$. As such they obey the operator equations [cf. (3.1) and the discussion following (3.3)]; $L_i[\alpha_{11},\alpha_{21},\gamma_{11},\gamma_{21}]=-\delta_{i1}\delta(\mathbf{r})$. However, we found it more convenient (for reasons indicated below) to rescale all components of the Green's tensor $\overleftrightarrow{G}$ by the factor

$$\left[1-\frac{K_3^2}{(2\mu+\lambda)K_1}\right],$$

i.e.,

$$\overleftrightarrow{\overline{G}}=\left[1-\frac{K_3^2}{(2\mu+\lambda)K_1}\right]\overleftrightarrow{G}\ . \tag{3.16}$$

We write the components of $\overleftrightarrow{\overline{G}}$ as $\overline{\alpha}_{11}$, $\overline{\alpha}_{21}$, etc., in which case $\overline{\alpha}_{11}$, $\overline{\alpha}_{21}$, $\overline{\gamma}_{11}$, and $\overline{\gamma}_{21}$ correspond respectively to the solutions u_x, u_y, w_x, and w_y which satisfy

$$L_i[\overline{u}]=-\left[1-\frac{K_3^2}{(2\mu+\lambda)K_1}\right]\delta_{i1}\delta(\mathbf{r})\ .$$

Explicitly, this set of equations is [cf. (3.1)]

$$\mu\nabla^2\overline{\alpha}_{11}+K\frac{\partial}{\partial x}\left[\frac{\partial\overline{\alpha}_{11}}{\partial x}+\frac{\partial\overline{\alpha}_{21}}{\partial y}\right]+K_3\left[\frac{\partial^2\overline{\gamma}_{11}}{\partial x^2}+\frac{2\partial^2\overline{\gamma}_{21}}{\partial x\,\partial y}-\frac{\partial^2\overline{\gamma}_{11}}{\partial y^2}\right]=-\left[\frac{(\mu+\lambda)K_1+(\mu K_1-K_3^2)}{(2\mu+\lambda)K_1}\right]\delta(\mathbf{r})\ , \tag{3.17a}$$

$$\mu\nabla^2\overline{\alpha}_{21}+K\frac{\partial}{\partial y}\left[\frac{\partial\overline{\alpha}_{11}}{\partial x}+\frac{\partial\overline{\alpha}_{21}}{\partial y}\right]+K_3\left[\frac{\partial^2\overline{\gamma}_{21}}{\partial x^2}-\frac{2\partial^2\overline{\gamma}_{11}}{\partial x\,\partial y}-\frac{\partial^2\overline{\gamma}_{21}}{\partial y^2}\right]=0\ , \tag{3.17b}$$

$$K_1\nabla^2\overline{\alpha}_{11}+K_3\left[\frac{\partial^2\overline{\alpha}_{11}}{\partial x^2}-\frac{2\partial^2\overline{\alpha}_{21}}{\partial x\,\partial y}-\frac{\partial^2\overline{\alpha}_{11}}{\partial y^2}\right]=0\ , \tag{3.17c}$$

$$K_1\nabla^2\overline{\alpha}_{21}+K_3\left[\frac{\partial^2\overline{\alpha}_{21}}{\partial x^2}+\frac{2\partial^2\overline{\alpha}_{11}}{\partial x\,\partial y}-\frac{\partial^2\overline{\alpha}_{21}}{\partial y^2}\right]=0\ . \tag{3.17d}$$

If $K_3=0$, (3.17a)–(3.17d) have solutions $\overline{\alpha}_{11}^{(0)}=\alpha_{11}^{(0)}$, $\overline{\alpha}_{21}^{(0)}=\alpha_{21}^{(0)}$, $\overline{\gamma}_{11}^{(0)}=\gamma_{11}^{(0)}=0$, $\overline{\gamma}_{21}^{(0)}=\gamma_{21}^{(0)}=0$, with $\alpha_{11}^{(0)}$ and $\alpha_{21}^{(0)}$ given by (3.12a) and (3.12b).

Writing $\overline{\gamma}_{11}=\gamma_{11}^{(0)}+\overline{\gamma}_{11}^{(1)}+\overline{\gamma}_{11}^{(2)}+\cdots$ and similar expressions for the other components [where $\overline{\gamma}_{11}^{(i)}$ is the contribution of $O(K_3^i)$ to $\overline{\gamma}_{11}$], we find from (3.17c) and (3.17d) that $\overline{\gamma}_{11}^{(1)}$ and $\overline{\gamma}_{21}^{(1)}$ are given, respectively, by

$$\overline{\gamma}_{11}^{(1)}=\frac{K_3}{4\pi\mu(2\mu+\lambda)K_1}\left[(3\mu+\lambda)\frac{x^2}{r^2}-2K\frac{x^2y^2}{r^4}\right], \tag{3.18a}$$

$$\overline{\gamma}_{21}^{(1)}=\frac{K_3}{4\pi\mu(2\mu+\lambda)K_1}\left[(3\mu+\lambda)\frac{xy}{r^2}+K\frac{xy(x^2-y^2)}{r^4}\right]. \tag{3.18b}$$

Substituting (3.18a) and (3.18b) into (3.17a) and (3.17b) we find that $\overline{\alpha}_{11}^{(1)}=\overline{\alpha}_{21}^{(1)}=0$, and the corresponding $O(K_3^2)$ contributions satisfy the following coupled equations:

$$\mu\nabla^2\overline{\alpha}_{11}^{(2)}+K\frac{\partial}{\partial x}\left[\frac{\partial\overline{\alpha}_{11}^{(2)}}{\partial x}+\frac{\partial\overline{\alpha}_{21}^{(2)}}{\partial y}\right]=-\frac{2K_3^2K}{4\pi\mu(2\mu+\lambda)K_1}\frac{(x^2-y^2)}{r^4}+\frac{K_3^2}{(2\mu+\lambda)K_1}\delta(\mathbf{r})-\frac{(3\mu+\lambda)K_3^2}{2\mu(2\mu+\lambda)K_1}\delta(\mathbf{r}) \tag{3.19a}$$

and

$$\mu\nabla^2\overline{\alpha}_{21}^{(2)}+K\frac{\partial}{\partial y}\left[\frac{\partial\overline{\alpha}_{11}^{(2)}}{\partial x}+\frac{\partial\overline{\alpha}_{21}^{(2)}}{\partial y}\right]=-\frac{4K_3^2K}{4\pi\mu(2\mu+\lambda)K_1}\frac{xy}{r^4}\ . \tag{3.19b}$$

The last term on the right-hand side of (3.19a), which we have not combined with the preceding term, arises from the combination

$$K_3\left[\frac{\partial^2\overline{\gamma}_{11}^{(1)}}{\partial x^2}+2\frac{\partial^2\overline{\gamma}_{21}^{(1)}}{\partial x\,\partial y}-\frac{\partial^2\overline{\gamma}_{11}^{(1)}}{\partial y^2}\right]$$

appearing in (3.17a).

We find that (3.19a) and (3.19b) can be decoupled, i.e., we can obtain self-consistent solutions satisfying $\partial\overline{\alpha}_{11}^{(2)}/\partial x+\partial\overline{\alpha}_{21}^{(2)}/\partial y=0$. These solutions are

$$\overline{\alpha}_{11}^{(2)}=\frac{K_3^2K}{4\pi\mu^2(2\mu+\lambda)K_1}\left[\frac{x^2}{r^2}-\ln\frac{r}{a}\right], \tag{3.20a}$$

$$\overline{\alpha}_{21}^{(2)}=\frac{K_3^2K}{4\pi\mu^2(2\mu+\lambda)K_1}\frac{xy}{r^2}\ . \tag{3.20b}$$

This decoupling would *not* be possible had we worked with the original $\overleftrightarrow{G}$, and is our motivation for the rescaling (3.16). (Recall that the rescaling factor depends on

K_3; thus $\bar{\alpha}_{11}^{(2)}$ is not proportional to $\alpha_{11}^{(2)}$, but also involves $\alpha_{11}^{(0)}$.)

Using (3.20), we can find $\bar{\gamma}_{11}^{(3)}$ and $\bar{\gamma}_{21}^{(3)}$ from (3.17c) and (3.17d) with the results

$$\bar{\gamma}_{11}^{(3)}=\frac{K_3^3K}{4\pi\mu^2(2\mu+\lambda)K_1^2}\left[\frac{x^2}{r^2}-\frac{2x^2y^2}{r^4}\right], \tag{3.21a}$$

$$\bar{\gamma}_{21}^{(3)}=\frac{K_3^3K}{4\pi\mu^2(2\mu+\lambda)K_1^2}\left[\frac{xy}{r^2}+\frac{xy(x^2-y^2)}{r^4}\right]. \tag{3.21b}$$

If we now substitute $\bar{\gamma}_{11}^{(3)}$ and $\bar{\gamma}_{21}^{(3)}$ into the equations for $\bar{\alpha}_{11}$ and $\bar{\alpha}_{21}$, we find that $\bar{\alpha}_{11}^{(3)}=\bar{\alpha}_{21}^{(3)}=0$, and $\bar{\alpha}_{11}^{(4)}$ and $\bar{\alpha}_{21}^{(4)}$ satisfy equations that are identical to the ones satisfied by $\bar{\alpha}_{11}^{(2)}$ and $\bar{\alpha}_{21}^{(2)}$ except that the right-hand sides are multiplied by a factor of $K_3^2/\mu K_1$. So $\bar{\alpha}_{i1}^{(4)}$, $i=1,2$ are related to $\bar{\alpha}_{i1}^{(2)}$ by $\bar{\alpha}_{i1}^{(4)}=(K_3^2/\mu K_1)\bar{\alpha}_{i1}^{(2)}$. This implies that $\bar{\gamma}_{i1}^{(5)}=(K_3^2/\mu K_1)\bar{\gamma}_{i1}^{(3)}$; $i=1,2$. By this procedure we can generate corrections to all orders in K_3. For example, the expression for $\bar{\alpha}_{11}$ is of the form

$$\bar{\alpha}_{11}=-\frac{2\mu}{4\pi\mu(2\mu+\lambda)}\ln\frac{r}{a}+\frac{K}{4\pi\mu(2\mu+\lambda)}\left[\frac{x^2}{r^2}-\ln\frac{r}{a}\right]\left[1+\frac{K_3^2}{\mu K_1}+\frac{K_3^4}{\mu^2K_1^2}+\frac{K_3^6}{\mu^3K_1^3}+\cdots\right], \tag{3.22}$$

which can be written in closed form as

$$\bar{\alpha}_{11}=-\frac{1}{2\pi(2\mu+\lambda)}\ln\frac{r}{a}+\frac{KK_1}{4\pi(2\mu+\lambda)(\mu K_1-K_3^2)}\left[\frac{x^2}{r^2}-\ln\frac{r}{a}\right]. \tag{3.23a}$$

Following this procedure for the remaining components of $\overleftrightarrow{G}$, we find

$$\bar{\alpha}_{12}=\bar{\alpha}_{21}=\frac{KK_1}{4\pi(2\mu+\lambda)(\mu K_1-K_3^2)}\frac{xy}{r^2}, \tag{3.23b}$$

$$\bar{\alpha}_{22}=-\frac{1}{2\pi(2\mu+\lambda)}\ln\frac{r}{a}+\frac{KK_1}{4\pi(2\mu+\lambda)(\mu K_1-K_3^2)}\left[\frac{y^2}{r^2}-\ln\frac{r}{a}\right], \tag{3.23c}$$

$$\bar{\gamma}_{11}=\bar{\beta}_{11}=\frac{K_3}{2\pi K_1(2\mu+\lambda)}\frac{x^2}{r^2}+\frac{KK_3}{4\pi(2\mu+\lambda)(\mu K_1-K_3^2)}\frac{x^2(x^2-y^2)}{r^4}, \tag{3.23d}$$

$$\bar{\gamma}_{21}=\bar{\beta}_{12}=\frac{K_3}{2\pi K_1(2\mu+\lambda)}\frac{xy}{r^2}+\frac{KK_3}{4\pi(2\mu+\lambda)(\mu K_1-K_3^2)}\frac{2x^3y}{r^4}, \tag{3.23e}$$

$$\bar{\gamma}_{12}=\bar{\beta}_{21}=-\frac{K_3}{2\pi K_1(2\mu+\lambda)}\frac{xy}{r^2}-\frac{KK_3}{4\pi(2\mu+\lambda)(\mu K_1-K_3^2)}\frac{2xy^3}{r^4}, \tag{3.23f}$$

$$\bar{\gamma}_{22}=\bar{\beta}_{22}=-\frac{K_3}{2\pi K_1(2\mu+\lambda)}\frac{y^2}{r^2}+\frac{KK_3}{4\pi(2\mu-\lambda)(\mu K_1-K_3^2)}\frac{y^2(x^2-y^2)}{r^4}, \tag{3.23g}$$

$$\bar{\delta}_{11}=-\frac{1}{2\pi K_1}\ln\frac{r}{a}+\frac{KK_3^2}{4\pi K_1(2\mu+\lambda)(\mu K_1-K_3^2)}\left[\frac{x^2(x^2-3y^2)^2}{3r^6}-\ln\frac{r}{a}\right], \tag{3.23h}$$

$$\bar{\delta}_{12}=\bar{\delta}_{21}=\frac{KK_3^2}{4\pi K_1(2\mu+\lambda)(\mu K_1-K_3^2)}\frac{xy(3x^2-y^2)(x^2-3y^2)}{3r^6}, \tag{3.23i}$$

$$\bar{\delta}_{22}=-\frac{1}{2\pi K_1}\ln\frac{r}{a}+\frac{KK_3^2}{4\pi K_1(2\mu+\lambda)(\mu K_1-K_3^2)}\left[\frac{y^2(3x^2-y^2)^2}{3r^6}-\ln\frac{r}{a}\right]. \tag{3.23j}$$

The elements of the Green's tensor $\overleftrightarrow{G}$ may be found from the corresponding ones above by multiplying by the factor $(2\mu+\lambda)K_1/[KK_1+(\mu K_1-K_3^2)]$. It is straightforward though tedious to check that (3.23) when rescaled by this factor satisfy the Green's tensor equations described in the text following (3.2).

IV. ELASTIC FIELDS SURROUNDING DISLOCATIONS AND THE DISLOCATION INTERACTION ENERGY

A. Elastic fields surrounding a single dislocation

Our solution for the Green's tensor $\overleftrightarrow{G}$ presented in the preceding section is used readily to obtain the form of the elastic fields surrounding a dislocation in the pentagonal quasicrystal. Typically, one regards the displacement fields surrounding a dislocation as being multivalued [cf. (2.5)]. However, as suggested in Ref. 7 for the case of crystalline solids, we can choose the **u** and **w** fields satisfying (2.5), as single-valued functions which undergo a fixed discontinuity as they cross a cut line. This discontinuity introduces a singular strain at the cut line which can be written as

$$u_{ij}^s=\tfrac{1}{2}(n_ib_j+n_jb_i)\delta(\xi)\ , \tag{4.1a}$$

$$w_{ij}^s=n_id_j\delta(\xi)\ , \tag{4.1b}$$

where $\hat{\mathbf{n}}$ is the normal to the cut line, and ξ is a coordinate measured along $\hat{\mathbf{n}}$ from the cut. The Burger's vector of the dislocation is the four-vector $(\mathbf{b},\mathbf{d})$.

This singular strain will in turn yield a singular stress which must be compensated by introducing fictitious forces so that the total stress is everywhere continuous. To find the singular stress we rewrite our Euler-Lagrange equations (3.1a)–(3.1d) as

$$\frac{\delta F}{\delta u_j}=A_{ijkl}\frac{\partial u_{kl}}{\partial x_i}+B_{ijkl}\frac{\partial w_{kl}}{\partial x_i}=0,\quad j=1,2 \tag{4.2a}$$

$$\frac{\delta F}{\delta w_j}=C_{ijkl}\frac{\partial u_{kl}}{\partial x_i}+D_{ijkl}\frac{\partial w_{kl}}{\partial x_i}=0,\quad j=1,2 \tag{4.2b}$$

where

$$A_{ijkl}=\lambda\delta_{ij}\delta_{kl}+\mu(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk})\ , \tag{4.3a}$$

$$B_{ijkl}=K_3(\delta_{i1}-\delta_{i2})(\delta_{ij}\delta_{kl}+\delta_{ik}\delta_{jl}-\delta_{il}\delta_{jk})\ , \tag{4.3b}$$

$$C_{ijkl}=K_3(\delta_{k1}-\delta_{k2})(\delta_{ij}\delta_{kl}+\delta_{ik}\delta_{jl}-\delta_{il}\delta_{jk})\ , \tag{4.3c}$$

$$D_{ijkl}=K_1\delta_{ik}\delta_{jl}\ . \tag{4.3d}$$

The stress tensors σ_{ij} and P_{ij} coupling to the **u** and **w** fields are defined, respectively, by the equations of equilibrium

$$\frac{\partial\sigma_{ij}}{\partial x_i}=\frac{\delta F}{\delta u_j}=0,\quad j=1,2 \tag{4.4a}$$

$$\frac{\partial P_{ij}}{\partial x_i}=\frac{\delta F}{\delta w_j}=0,\quad j=1,2\ . \tag{4.4b}$$

Thus, the singular strains (4.1) correspond to singular stresses σ_{ij}^s and P_{ij}^s as follows:

$$\sigma_{ij}^s=A_{ijkl}u_{kl}^s+B_{ijkl}w_{kl}^s\ , \tag{4.5a}$$

$$P_{ij}^s=C_{ijkl}u_{kl}^s+D_{ijkl}w_{kl}^s\ . \tag{4.5b}$$

Corresponding to these stresses are two force fields defined by:

$$f_j^u=\frac{\partial\sigma_{ij}^s}{\partial x_i},\quad j=1,2 \tag{4.6a}$$

$$f_j^w=\frac{\partial P_{ij}^s}{\partial x_i},\quad j=1,2\ . \tag{4.6b}$$

As noted above, to obtain a physical, continuous stress field we must counterbalance these forces by introducing fictitious forces distributed along the cut line which are equal in magnitude, but opposite in sign to those of (4.6). Then, the problem of finding **u** and **w** in the presence of a dislocation is equivalent to that of finding single-valued but discontinuous fields in the presence of these fictitious forces.

Using (3.2), (3.3), and (4.1)–(4.6), we find that the **u** and **w** fields surrounding a dislocation with Burger's vector $(\mathbf{b},\mathbf{d})$ are given by

$$u_i(\mathbf{r})=\int dl'n_l\left[(A_{kjlm}b_m+B_{kjlm}d_m)\frac{\partial\alpha_{ij}(\mathbf{r}-\mathbf{r}')}{\partial x_k'}+(C_{kjlm}b_m+D_{kjlm}d_m)\frac{\partial\beta_{ij}(\mathbf{r}-\mathbf{r}')}{\partial x_k'}\right] \tag{4.7a}$$

and

$$w_i(\mathbf{r})=\int dl'n_l\left[(A_{kjlm}b_m+B_{kjlm}d_m)\frac{\partial\gamma_{ij}(\mathbf{r}-\mathbf{r}')}{\partial x_k'}+(C_{kjlm}b_m+D_{kjlm}d_m)\frac{\partial\delta_{ij}(\mathbf{r}-\mathbf{r}')}{\partial x_k'}\right]\ , \tag{4.7b}$$

where dl' is an infinitesimal segment of the cut line, and the integration is done along the entire length of the cut (which for a single dislocation runs from the core to infinity). Equations (4.7) are generalizations of (27.9) of Ref. 7 to the case of pentagonal quasicrystals.

To evaluate (4.7) for an arbitrary Burger's vector $\tilde{b}=(b_x,b_y,d_x,d_y)$, it is simpler to first consider $\tilde{b}=(b_x,0,d_x,0)$. While this is not an allowed Burger's vector (see the discussion at the end of Sec. II) we can rotate our coordinate system by 90° counterclockwise to obtain **u** and **w** for a dislocation with Burger's vector $\tilde{b}=(0,b_y,0,d_y)$ with $b_y=b_x$, $d_y=-d_x$. (This will be an allowed Burger's vector if $b_y=d_y$.) We can then find the solution for an arbitrary $\tilde{b}=(b_x,b_y,d_x,d_y)$ by adding the two solutions above. We may then impose the geometric constraints discussed at the end of Sec. II, which restrict the choice of allowed values for the components of $\tilde{b}$.

Choosing $\tilde{b}=(b_x,0,d_x,0)$ with the core at the origin, we can choose our cut line to run along the y axis from 0 to infinity. The normal to this cut line is then $\hat{\mathbf{n}}=(1,0)$. Equations (4.7) then reduce to the following, upon using (4.3):

$$u_i(\mathbf{r})=\int_0^\infty dy' \left[[(2\mu+\lambda)b_x+K_3 d_x]\frac{\partial \alpha_{i1}(\mathbf{r}-\mathbf{r}')}{\partial x'}+(\lambda b_x-K_3 d_x)\frac{\partial \alpha_{i2}(\mathbf{r}-\mathbf{r}')}{\partial y'} + (K_3 b_x+K_1 d_x)\frac{\partial \beta_{il}(\mathbf{r}-\mathbf{r}')}{\partial x'}+K_3 b_x\frac{\partial \beta_{i2}(\mathbf{r}-\mathbf{r}')}{\partial y'}\right], \tag{4.8a}$$

$$w_i(\mathbf{r})=\int_0^\infty dy' \left[[(2\mu+\lambda)b_x+K_3 d_x]\frac{\partial \gamma_{i1}(\mathbf{r}-\mathbf{r}')}{\partial x'}+(\lambda b_x-K_3 d_x)\frac{\partial \gamma_{i2}(\mathbf{r}-\mathbf{r}')}{\partial y'} + (K_3 b_x+K_1 d_x)\frac{\partial \delta_{i1}(\mathbf{r}-\mathbf{r}')}{\partial x'}+K_3 b_x\frac{\partial \delta_{i2}(\mathbf{r}-\mathbf{r}')}{\partial y'}\right]. \tag{4.8b}$$

The terms which are of the form $\partial f(\mathbf{r}-\mathbf{r}')/\partial y'$ we then integrate by parts. For the remaining terms which are of the form $\partial f(\mathbf{r}-\mathbf{r}')/\partial x'$, we calculate a function $g(\mathbf{r}-\mathbf{r}')$ such that $\partial f(\mathbf{r}-\mathbf{r}')/\partial x'=\partial g(\mathbf{r}-\mathbf{r}')/\partial y'$ and then integrate by parts. We will not display the final results for $\mathbf{u}$ and $\mathbf{v}$ as they are contained below in the expressions (4.9) for a Burger's vector of arbitrary orientation.

Expressions for $\mathbf{u}$ and $\mathbf{w}$ for $\tilde{b}=(0,b_y,0,d_y)$ can be easily obtained from the results for $\tilde{b}=(b_x,0,d_x,0)$ by rotating the coordinate system by $\pi/2$ counterclockwise. Under such a rotation, $b_x\to b_y$, $u_x\to u_y$, $u_y\to -u_x$. If physical space is rotated by $\pi/2$, the space of $\mathbf{w}$ is rotated by $3\pi/2$ (see the discussion in Sec. II). Therefore $d_x\to -d_y$, $w_x\to -w_y$, and $w_y\to w_x$. So, if to the results obtained for $\tilde{b}=(b_x,0,d_x,0)$ we make the substitutions, $x\to y$, $y\to -x$, $b_x\to b_y$, $d_x\to -d_y$, $u_x\to u_y$, $u_y\to -u_x$, $w_x\to -w_y$, and $w_y\to w_x$, we would obtain the expression for $\mathbf{u}$ and $\mathbf{w}$ for $\tilde{b}=(0,b_y,0,d_y)$.

Adding the results of our expressions for $\mathbf{u}$ and $\mathbf{w}$ when $\tilde{b}=(b_x,0,d_x,0)$ and $\tilde{b}=(0,b_y,0,d_y)$ we find the following expressions for a dislocation $\tilde{b}=(b_x,b_y,d_x,d_y)$ located at the origin:

$$\begin{aligned} u_x(\mathbf{r})= {} & \frac{b_x}{2\pi}\left[\tan^{-1}\frac{y}{x}+\frac{(\mu+\lambda)K_1}{(\mu+\lambda)K_1+(\mu K_1-K_3^2)}\frac{xy}{r^2}\right] \\ & +\frac{b_y}{2\pi}\left[\frac{\mu K_1-K_3^2}{(\mu+\lambda)K_1+(\mu K_1-K_3^2)}\ln\frac{r}{a}-\frac{(\mu+\lambda)K_1}{(\mu+\lambda)K_1+(\mu K_1-K_3^2)}\frac{x^2}{r^2}\right] \\ & +\frac{d_x}{2\pi}\left[\frac{K_3K_1}{\mu K_1-K_3^2}\frac{xy}{r^2}-\frac{K_3K_1^2(\mu+\lambda)}{2(\mu K_1-K_3^2)[(\mu+\lambda)K_1+(\mu K_1-K_3^2)]}\frac{2xy^3}{r^4}\right] \\ & +\frac{d_y}{2\pi}\left[-\frac{K_3K_1}{(\mu+\lambda)K_1+(\mu K_1-K_3^2)}\frac{x^2}{r^2}-\frac{K_3K_1^2(\mu+\lambda)}{2(\mu K_1-K_3^2)[(\mu+\lambda)K_1+(\mu K_1-K_3^2)]}\frac{x^2(x^2-y^2)}{r^4}\right], \end{aligned} \tag{4.9a}$$

$$\begin{aligned} u_y(\mathbf{r})= {} & \frac{b_x}{2\pi}\left[-\frac{(\mu K_1-K_3^2)}{(\mu+\lambda)K_1+(\mu K_1-K_3^2)}\ln\frac{r}{a}+\frac{(\mu+\lambda)K_1}{(\mu+\lambda)K_1+(\mu K_1-K_3^2)}\frac{y^2}{r^2}\right] \\ & +\frac{b_y}{2\pi}\left[\tan^{-1}\frac{y}{x}-\frac{(\mu+\lambda)K_1}{(\mu+\lambda)K_1+(\mu K_1-K_3^2)}\frac{xy}{r^2}\right] \\ & +\frac{d_x}{2\pi}\left[-\frac{K_3K_1}{(\mu+\lambda)K_1+(\mu K_1-K_3^2)}\frac{y^2}{r^2}+\frac{K_3K_1^2(\mu+\lambda)}{2(\mu K_1-K_3^2)[(\mu+\lambda)K_1+(\mu K_1-K_3^2)]}\frac{y^2(x^2-y^2)}{r^4}\right] \\ & +\frac{d_y}{2\pi}\left[\frac{K_3K_1}{\mu K_1-K_3^2}\frac{xy}{r^2}-\frac{K_3K_1^2(\mu+\lambda)}{2(\mu K_1-K_3^2)[(\mu+\lambda)K_1+(\mu K_1-K_3^2)]}\frac{2x^3y}{r^4}\right], \end{aligned} \tag{4.9b}$$

$$w_x(\mathbf{r})=\frac{b_x}{2\pi}\left[\frac{2K_3(\mu+\lambda)}{(\mu+\lambda)K_1+(\mu K_1-K_3^2)}\frac{xy}{r^2}-\frac{K_3(\mu+\lambda)}{(\mu+\lambda)K_1+(\mu K_1-K_3^2)}\frac{2xy^3}{r^4}\right]$$
$$+\frac{b_y}{2\pi}\left[\frac{2K_3(\mu+\lambda)}{(\mu+\lambda)K_1+(\mu K_1-K_3^2)}\frac{x^2}{r^2}-\frac{K_3(\mu+\lambda)}{(\mu+\lambda)K_1+(\mu K_1-K_3^2)}\frac{x^2(x^2-y^2)}{r^4}\right]$$
$$+\frac{d_x}{2\pi}\left[\tan^{-1}\frac{y}{x}+\frac{K_3^2K_1(\mu+\lambda)}{2(\mu K_1-K_3^2)[(\mu+\lambda)K_1+(\mu K_1-K_3^2)]}\frac{xy(x^2-3y^2)(3x^2-y^2)}{3r^6}\right]$$
$$+\frac{d_y}{2\pi}\left[\frac{K_3^2[(\mu+\lambda)K_1+2(\mu K_1-K_3^2)]}{2(\mu K_1-K_3^2)[(\mu+\lambda)K_1+(\mu K_1-K_3^2)]}\ln\frac{r}{a}-\frac{K_3^2K_1(\mu+\lambda)}{2(\mu K_1-K_3^2)[(\mu+\lambda)K_1+(\mu K_1-K_3^2)]}\frac{x^2(x^2-3y^2)^2}{3r^6}\right], \tag{4.9c}$$

$$w_y(\mathbf{r})=\frac{b_x}{2\pi}\left[\frac{2K_3(\mu+\lambda)}{(\mu+\lambda)K_1+(\mu K_1-K_3^2)}\frac{y^2}{r^2}+\frac{K_3(\mu+\lambda)}{(\mu+\lambda)K_1+(\mu K_1-K_3^2)}\frac{y^2(x^2-y^2)}{r^4}\right]$$
$$+\frac{b_y}{2\pi}\left[\frac{2K_3(\mu+\lambda)}{(\mu+\lambda)K_1+(\mu K_1-K_3^2)}\frac{xy}{r^2}-\frac{K_3(\mu+\lambda)}{(\mu+\lambda)K_1+(\mu K_1-K_3^2)}\frac{2x^3y}{r^4}\right]$$
$$+\frac{d_x}{2\pi}\left[\frac{-K_3^2[(\mu+\lambda)K_1+2(\mu K_1-K_3^2)]}{2(\mu K_1-K_3^2)[(\mu+\lambda)K_1+(\mu K_1-K_3^2)]}\ln\frac{r}{a}+\frac{K_3^2K_1(\mu+\lambda)}{2(\mu K_1-K_3^2)[(\mu+\lambda)K_1+(\mu K_1-K_3^2)]}\frac{y^2(3x^2-y^2)^2}{3r^6}\right]$$
$$+\frac{d_y}{2\pi}\left[\tan^{-1}\frac{y}{x}-\frac{K_3^2K_1(\mu+\lambda)}{2(\mu K_1-K_3^2)[(\mu+\lambda)K_1+(\mu K_1-K_3^2)]}\frac{xy(x^2-3y^2)(3x^2-y^2)}{3r^6}\right]. \tag{4.9d}$$

The ultraviolet cutoff a can now be interpreted as the dislocation core size.

B. Energy of a single dislocation at the origin

Using (4.9) we can explicitly calculate the energy of a single dislocation at the origin with Burger's vector $\tilde{b}=(0,a_0,0,a_0)$. The energy, as expected on dimensional grounds, diverges logarithmically with the size of the system, and is of the form

$$E=\frac{a_0^2}{8\pi}\left[\frac{4(\mu+\lambda)(\mu K_1-K_3^2)}{(\mu+\lambda)+(\mu K_1-K_3^2)}+2K_1+(2K_2-K_1)K_3^2\left[\frac{1}{\mu K_1-K_3^2}+\frac{1}{(\mu+\lambda)+(\mu K_1-K_3^2)}\right]\right]\ln\frac{R}{a}. \tag{4.10}$$

Since this energy must be positive, we conclude that in the presence of dislocations, in additions to conditions stated following (2.4), stability also requires that $K_2>0$ and $K_2-K_1>0$.

C. Continuous distributions of dislocations and their interaction energy

For a distribution of dislocations given by a field $\tilde{b}(\mathbf{r})$, the fields $\mathbf{u}$ and $\mathbf{w}$ are given by

$$u_i(\mathbf{r})=\frac{1}{2\pi}\int\frac{d^2r'}{a^2}\tilde{b}_\alpha(\mathbf{r}')W_i^\alpha(\mathbf{r}-\mathbf{r}') \tag{4.10a}$$

and

$$w_i(\mathbf{r})=\frac{1}{2\pi}\int\frac{d^2r'}{a^2}\tilde{b}_\alpha(\mathbf{r}')\overline{W}_i^\alpha(\mathbf{r}-\mathbf{r}'). \tag{4.10b}$$

The Greek indices in (4.10) run from 1 to 4 and $\tilde{b}=(b_x,b_y,d_x,d_y)$. The tensors W_i^α and $\overline{W}_i^\alpha$ are defined via (4.9), requiring that if $\tilde{b}_\alpha(\mathbf{r})/a^2=\tilde{b}_\alpha\delta(\mathbf{r})$ then (4.10) reduces to (4.9). The strains accompanying these fields can then be written in the form

$$u_{ij}(\mathbf{r})=\frac{1}{2\pi}\int\frac{d^2r'}{a^2}\tilde{b}_\alpha(\mathbf{r}')W_{ij}^\alpha(\mathbf{r}-\mathbf{r}') \tag{4.11a}$$

and

$$w_{ij}(\mathbf{r})=\frac{1}{2\pi}\int\frac{d^2r'}{a^2}\tilde{b}_\alpha(\mathbf{r}')\overline{W}_{ij}^\alpha(\mathbf{r}-\mathbf{r}'), \tag{4.11b}$$

where

$$W_{ij}^\alpha(\mathbf{r}-\mathbf{r}')=\frac{1}{2}\left[\frac{\partial W_j^\alpha(\mathbf{r}-\mathbf{r}')}{\partial x_i}+\frac{\partial W_i^\alpha(\mathbf{r}-\mathbf{r}')}{\partial x_j}\right] \tag{4.12a}$$

and

$$\overline{W}_{ij}^\alpha(\mathbf{r}-\mathbf{r}')=\frac{\partial\overline{W}_j^\alpha(\mathbf{r}-\mathbf{r}')}{\partial x_i}. \tag{4.12b}$$

To calculate the interaction energy H_D of a distribution of dislocations we insert (4.11) into the elastic energy density (2.4), with $\tilde{f}=0$, and then integrate over all space.

To carry out all of the integrals and obtain a closed form expression for the pairwise interaction is very tedious. Instead, we use a method presented in Appendix C of Ref. 10. We first evaluate H_D when $K_3=0$. In that case there will be no coupling between **b** and **d**. Furthermore, as noted in Sec. III, with $K_3=0$, the **u** portion of the energy is identical to that of an isotropic two-dimensional crystal. Apart from a boundary term proportional to K_2 the **w** portion is identical to the sum of two XY models. Upon explicit calculation we have found that if $K_3=0$, the term proportional to K_2 equals zero. Thus $H_D^{(0)}$, the value of H_D when $K_3=0$, takes the form

$$H_D^{(0)}=-\frac{1}{8\pi}\int\frac{d^2r}{a^2}\int_{|\mathbf{r}-\mathbf{r}'|>a}\frac{d^2r'}{a^2}\left[M^{(0)}\left[\mathbf{b}(\mathbf{r})\cdot\mathbf{b}(\mathbf{r}')\ln\frac{|\mathbf{r}-\mathbf{r}'|}{a}-\frac{\mathbf{b}(\mathbf{r})\cdot(\mathbf{r}-\mathbf{r}')\mathbf{b}(\mathbf{r}')\cdot(\mathbf{r}-\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|^2}\right]+N^{(0)}\mathbf{d}(\mathbf{r})\cdot\mathbf{d}(\mathbf{r}')\ln\frac{|\mathbf{r}-\mathbf{r}'|}{a}\right]+\int\frac{d^2r}{a^2}[CM^{(0)}|\mathbf{b}(\mathbf{r})|^2+C'N^{(0)}|\mathbf{d}(\mathbf{r})|^2]\,, \quad (4.13)$$

where $M^{(0)}=4\mu K/(2\mu+\lambda)$ and $N^{(0)}=2K_1$. We are assuming that we have charge neutrality $\int d^2r\mathbf{b}(\mathbf{r})=\int d^2r\mathbf{d}(\mathbf{r})=0$, so that the energy is finite for an infinite system. The constants C and C' will depend on the microscopic cutoff used (i.e., the details of the dislocation core).

To calculate H_D when $K_3\neq 0$, we first evaluate $\partial H_D/\partial K_3$. Using (2.4) we have

$$\frac{\partial H_D}{\partial K_3}=\frac{\delta H_D}{\delta u_i}\frac{\partial u_i}{\partial K_3}+\frac{\delta H_D}{\delta w_i}\frac{\partial w_i}{\partial K_3}+\int d^2r\{[u_{xx}(\mathbf{r})-u_{yy}(\mathbf{r})][w_{xx}(\mathbf{r})+w_{yy}(\mathbf{r})]+2u_{xy}(\mathbf{r})[w_{xy}(\mathbf{r})-w_{yx}(\mathbf{r})]\}\,. \quad (4.14)$$

Since we have minimized H_D with respect to $\delta\mathbf{u}$ and $\delta\mathbf{w}$, the first two terms on the right-hand side of (4.14) are identically zero. We are then left with the task of evaluating the integral on the right-hand side of (4.14) which is comparatively easy. In using the Euler-Lagrange equations to simplify $\partial H_D/\partial K_3$, we have however ignored any contribution from the K_2 term. The K_2 term is a boundary term and as such has no effect on the Euler-Lagrange equations, which only considers nonzero variations in the bulk of the material. So, in order to calculate the total dislocation Hamiltonian, we have to explicitly include any contribution from the K_2 term. The final expression for H_D will then be given by

$$H_D=H_D^{(0)}+\int_0^{K_3}dK_3'\frac{\partial H_D}{\partial K_3'}+K_2\int d^2r[w_{xx}(\mathbf{r})w_{yy}(\mathbf{r})-w_{xy}(\mathbf{r})w_{yx}(\mathbf{r})]\,. \quad (4.15)$$

The technical details of evaluating (4.15) are shown in the Appendix. The final result is given by

$$\begin{aligned}H_D=&-\frac{1}{8\pi}\int\frac{d^2r}{a^2}\int_{|\mathbf{r}-\mathbf{r}'|>a}\frac{d^2r'}{a^2}\Bigg\{M\left[\mathbf{b}(\mathbf{r})\cdot\mathbf{b}(\mathbf{r}')\ln\frac{|\mathbf{r}-\mathbf{r}'|}{a}-\frac{\mathbf{b}(\mathbf{r})\cdot(\mathbf{r}-\mathbf{r}')\mathbf{b}(\mathbf{r}')\cdot(\mathbf{r}-\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|^2}\right]+N\mathbf{d}(\mathbf{r})\cdot\mathbf{d}(\mathbf{r}')\ln\frac{|\mathbf{r}-\mathbf{r}'|}{a}\\&+W\left[\frac{(x-x')[(x-x')^2-3(y-y')^2]}{|\mathbf{r}-\mathbf{r}'|^3}d_x(\mathbf{r})+\frac{(y-y')[3(x-x')^2-(y-y')^2]}{|\mathbf{r}-\mathbf{r}'|^3}d_y(\mathbf{r})\right]\\&\times\left[\frac{(x-x')[(x-x')^2-3(y-y')^2]}{|\mathbf{r}-\mathbf{r}'|^3}d_x(\mathbf{r}')+\frac{(y-y')[3(x-x')^2-(y-y')^2]}{|\mathbf{r}-\mathbf{r}'|^3}d_y(\mathbf{r}')\right]\\&+S\Bigg[\frac{1}{4}\frac{(x-x')^2-(y-y')^2}{|\mathbf{r}-\mathbf{r}'|^2}\mathbf{b}(\mathbf{r}')\cdot\mathbf{d}(\mathbf{r})+\frac{1}{2}\frac{(x-x')(y-y')}{|\mathbf{r}-\mathbf{r}'|^2}\epsilon_{ij}b_i(\mathbf{r})d_j(\mathbf{r}')\\&+\frac{1}{2}\frac{\mathbf{b}(\mathbf{r})\cdot(\mathbf{r}-\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\left[\frac{(x-x')[(x-x')^2-3(y-y')^2]}{|\mathbf{r}-\mathbf{r}'|^3}d_x(\mathbf{r})+\frac{(y-y')[3(x-x')^2-(y-y')^2]}{|\mathbf{r}-\mathbf{r}'|^3}d_y(\mathbf{r})\right]\Bigg]\Bigg\}\\&+\int\frac{d^2r}{a^2}[CM|\mathbf{b}(\mathbf{r})|^2+C'N|\mathbf{d}(\mathbf{r})|^2\cdot C''W\mathbf{d}(\mathbf{r})\cdot\mathbf{b}(\mathbf{r})]\,,\end{aligned} \quad (4.16)$$

where

$$M=\frac{4(\mu+\lambda)(\mu K_1-K_3^2)}{(2\mu+\lambda)K_1-K_3^2}\ , \tag{4.17}$$

$$N=2K_1+\frac{2K_3^2(2K_2-K_1)}{(2\mu+\lambda)K_1-K_3^2}+\frac{(\mu+\lambda)K_1K_3^2(2K_2-K_1)}{(\mu K_1-K_3^2)[(2\mu+\lambda)K_1-K_3^2)]}\ , \tag{4.18}$$

$$W=\frac{46(\mu+\lambda)K_1K_3^2(2K_2-K_1)}{3(\mu K_1-K_3^2)[(2\mu+\lambda)K_1-K_3^2]}\ , \tag{4.19}$$

$$S=\frac{4(\mu+\lambda)K_3^2(K_2-K_1)}{[(2\mu+\lambda)K_1-K_3^2]}\ , \tag{4.20}$$

and C'' is again a cutoff-dependent constant.

We have explicitly checked that (4.22) respects the pentagonal quasicrystalline symmetries discussed in Sec. II. In carrying out this check one notes that **b** and **d** transform under rotations like **u** and **w**, respectively. Thus if our coordinates **r** and hence **b** are rotated by an angle θ, symmetry demands that **d** be rotated by 3θ to obtain the same physical system. It is straightforward to check that the expression

$$\frac{(x-x')[(x-x')^2-3(y-y')^2]}{|\mathbf{r}-\mathbf{r}'|^3}d_x(\mathbf{r})+\frac{(y-y')[3(x-x')^2-(y-y')^2]}{|\mathbf{r}-\mathbf{r}'|^3}d_y(\mathbf{r})$$

does indeed remain invariant under such transformations.

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APPENDIX: EVALUATION OF (4.15)

We evaluate the integral in (4.14) by substituting the strain tensors given in (4.11). We will then have an expression of the form

$$\frac{\partial H_D}{\partial K_3}=\int\frac{d^2r}{a^2}\int_{|\mathbf{r}-\mathbf{r}'|>a}\frac{d^2r'}{a^2}\tilde{b}_\alpha(\mathbf{r})\tilde{b}_\beta(\mathbf{r}')E_{\alpha\beta}(\mathbf{r}-\mathbf{r}')\ , \tag{A1}$$

where $E_{\alpha\beta}(\mathbf{r}-\mathbf{r}')$ is given by

$$E_{\alpha\beta}(\mathbf{r}-\mathbf{r}')=\frac{1}{(2\pi)^2}\int d^2r''\{[W^\alpha_{xx}(\mathbf{r}-\mathbf{r}'')-W^\alpha_{yy}(\mathbf{r}-\mathbf{r}'')][\overline{W}^\beta_{xx}(\mathbf{r}'-\mathbf{r}'')+\overline{W}^\beta_{yy}(\mathbf{r}'-\mathbf{r}'')]+2W^\alpha_{xy}(\mathbf{r}-\mathbf{r}'')[\overline{W}^\beta_{xy}(\mathbf{r}'-\mathbf{r}'')-\overline{W}^\beta_{yx}(\mathbf{r}'-\mathbf{r}'')]\}\ . \tag{A2}$$

To carry out the integral in (A2) it is convenient to go to Fourier space, writing

$$E_{\alpha\beta}(\mathbf{R})=\frac{1}{4\pi^2}\int d^2q(-1+e^{-i\mathbf{q}\cdot\mathbf{R}})E_{\alpha\beta}(\mathbf{q})e^{-qa}\ . \tag{A3}$$

The factor e^{-qa} provides an ultraviolet cutoff, while using the factor $(-1+e^{-i\mathbf{q}\cdot\mathbf{R}})$ provides an infrared cutoff and will not affect the energy of a charge neutral system. The Fourier transform $E_{\alpha\beta}(\mathbf{q})$ will then involve a linear combination of products of the form $W^\alpha_{ij}(\mathbf{q})\overline{W}^\beta_{kl}(-\mathbf{q})$. We will not display all of the details of the calculation here, but indicate the techniques used.

The angular portion of the spatial integrals needed in evaluating $W(\mathbf{q})$ or $\overline{W}(-\mathbf{q})$ involves performing integrals of the form

$$G(\mathbf{q})=\int_0^{2\pi}d\theta\frac{\sin^m\theta\cos^n\theta}{q_x\cos\theta+q_y\sin\theta}\ , \tag{A4}$$

where $m+n$ is odd. Defining a complex variable, $z=e^{i\theta}$, we can rewrite $G(\mathbf{q})$ as

$$G(\mathbf{q})=\frac{1}{q_x-iq_y}\left[\frac{1}{i}\right]^{m+1}\left[\frac{1}{2}\right]^{m+n-1}\oint_{\text{unit circle}}dz\left[\frac{1}{z}\right]^{m+n}\frac{(z^2-1)^m(z^2+1)^n}{z^2+z_0}\ , \tag{A5}$$

where $z_0=(q_x+iq_y)/(q_x-iq_y)$. The integrand has two simple poles which lie on the contour and a pole of order $m+n$ at the origin. The integral $G(\mathbf{q})$ will then be proportional to the sum of the principal values of the two simple poles and the residue of the pole at the origin. The general expression for $G(\mathbf{q})$ is

$$G(\mathbf{q})=\frac{\pi}{q_x-iq_y}\left[\frac{1}{i}\right]^m\left[\frac{1}{2}\right]^{m+n-2}\frac{1}{(n+m-1)!}\lim_{z\to 0}\left[\frac{d}{dz}\right]^{n+m-1}\frac{(z^2-1)^m(z^2+1)^n}{z^2+z_0}-2\pi\left[\frac{1}{i}\right]^{2m+1}q_x^m q_y^n\frac{1}{q^{m+n+1}}\ . \tag{A6}$$

Collecting terms in **b** and **d** we find that $\partial H_D/\partial K_3$ may be written as

$$\frac{\partial H_D}{\partial K_3}=\frac{1}{[(\mu+\lambda)K_1+(\mu K_1-K_3^2)]^2}\times\int\frac{d^2r}{a^2}\int_{|\mathbf{r}-\mathbf{r}'|>a}\frac{d^2r'}{a^2}[b_i(\mathbf{r})A_{ij}(\mathbf{r}-\mathbf{r}')b_j(\mathbf{r}')+b_i(\mathbf{r})B_{ij}(\mathbf{r}-\mathbf{r}')d_j(\mathbf{r}')+d_i(\mathbf{r})C_{ij}(\mathbf{r}-\mathbf{r}')d_j(\mathbf{r}')]\ , \tag{A7}$$

where

$$A_{mn}(\mathbf{r}-\mathbf{r}')=\frac{1}{(2\pi)^2}\int d^2q(e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}-1)e^{-qa}\left[-4K_3K_1(\mu+\lambda)^2\left[\frac{1}{q^2}\delta_{mn}-\frac{q_mq_n}{q^4}\right]\right]\ , \tag{A8a}$$

$$B_{mn}(\mathbf{r}-\mathbf{r}')=\frac{1}{(2\pi)^2}\int d^2q(e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}-1)e^{-qa}\times\left\{2(\mu+\lambda)K_1[(2\mu+\lambda)K_1+K_3^2]\left[\left[\frac{q_x}{q^2}\delta_{mx}+\frac{q_y}{q^2}\delta_{my}\right]\left[\frac{q_x(q_x^2-3q_y^2)}{q^4}\delta_{nx}+\frac{q_y(3q_x^2-q_y^2)}{q^4}\delta_{ny}\right]-\frac{(q_x^2-q_y^2)}{q^4}(\delta_{mx}\delta_{nx}+\delta_{my}\delta_{ny})-\frac{2q_xq_y}{q^4}(\delta_{mx}\delta_{ny}-\delta_{my}\delta_{nx})\right]\right\}\ , \tag{A8b}$$

$$C_{mn}(\mathbf{r}-\mathbf{r}')=\frac{1}{(2\pi)^2}\int d^2q(e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}-1)e^{-qa}\times\left[-(2\mu+\lambda)K_3K_1^2\frac{1}{q^2}\delta_{mn}-\frac{K_3K_1^2(\mu+\lambda)[\mu K_1^2(2\mu+\lambda)-K_3^4]}{(\mu K_1-K_3^2)^2}\times\left[\frac{q_x^2(q_x^2-3q_y^2)^2}{q^8}\delta_{mx}\delta_{nx}+\frac{q_y^2(3q_x^2-q_y^2)^2}{q^8}\delta_{my}\delta_{ny}+\frac{2q_xq_y(q_x^2-3q_y^2)(3q_x^2-q_y^2)}{q^8}\delta_{mx}\delta_{ny}\right]\right]\ . \tag{A8c}$$

To perform the integrals over momentum space, we need to calculate integrals of the form

$$F(\mathbf{r})=\frac{1}{2\pi}\int dq\,d\theta\,q(e^{i\mathbf{q}\cdot\mathbf{r}}-1)e^{-qa}\frac{q_x^mq_y^n}{q^{m+n+2}}\ , \tag{A9}$$

where $m+n$ is even.

We can rewrite $F(\mathbf{r})$ as

$$F(\mathbf{r})=\int_0^\infty dq\frac{e^{-qa}}{q}I(q)\ , \tag{A10}$$

where

$$I(q)=\frac{(-1)^m}{\pi}\int_0^\pi d\phi[\cos(qr\sin\phi)-1]\times\sin^m(\phi+\theta)\cos^n(\phi+\theta)\ , \tag{A11}$$

where θ is the polar angle of $\mathbf{r}$. For a specific m and n, $I(q)$ becomes an algebraic expression which involves Bessel functions of many orders. To make such a connection we use the integral representations of Bessel functions:

$$J_n(x)=\frac{x^n}{2^n\sqrt{\pi}\Gamma(n+\frac{1}{2})}\int_0^\pi\cos(x\sin\theta)\cos^{2n}\theta d\theta\ ,\quad n>-\tfrac{1}{2} \tag{A12}$$

where $\Gamma(n+\frac{1}{2})=[1\times3\times5\times\cdots\times(2n-1)/2^n]\sqrt{\pi}$ is the gamma function for half integers.

As the final step in calculating $F(\mathbf{r})$ we use the relations

$$\int_0^\infty dq\frac{e^{-qa}}{q}[J_0(qr)-1]=-\ln\frac{r}{a}+\ln2-C\ , \tag{A13}$$

where C is a cutoff-dependent constant. The above result is valid in the regime $r/a\gg1$. Also in this regime

$$\int_0^\alpha dq\frac{e^{-qa}}{q}J_n(qr)\cong\frac{1}{n},\quad n>0 \tag{A14}$$

is a valid approximation.

Using these techniques and approximations we have obtained a result for $\partial H_D/\partial K_3$. If we integrate over K_3, we obtain the second term on the right-hand side of (4.15). Using an identical procedure we have calculated the third term on the right-hand side of (4.15). By adding these to $H_D^{(0)}$ we obtain the expression for H_D stated in (4.16).

[1] For a thorough discussion, see D. Levine and P. J. Steinhardt, Phys. Rev. B **34**, 596 (1986); J. E. S. Socolar and P. J. Steinhardt, *ibid.* **34**, 617 (1986), and references therein.

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[4]See also J. E. Socolar, T. C. Lubensky, and P. J. Steinhardt, Phys. Rev. B **34**, 345 (1986).

[5]J. Toner (private communication).

[6]In Sec. IV, we discuss the corresponding constraint on K_2 when dislocations are present.

[7]See, e.g., L. D. Landau and E. M. Lifshiftz, *Theory of Elasticity* (Pergamon, Oxford, 1959).

[8]See, e.g., R. Courant and D. Hilbert, *Methods of Mathematical Physics* (Interscience, New York, 1953), Vol. I.

[9]See, e.g., P. M. Morse and H. Feshbach, *Methods of Theoretical Physics*, (McGraw-Hill, New York, 1953), Part II.

[10]D. R. Nelson and B. I. Halperin, Phys. Rev. B **19**, 2457 (1979).