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Extended objects in crystals

M. Wadati
Institute of Applied Physics, Tsukuba University, Ibaraki, 300-31 Japan

H. Matsumoto and H. Umezawa
Theoretical Physics Institute, The University of Alberta, Edmonton, Alberta, Canada T6G 2J1
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A microscopic derivation of the theory of extended objects in crystals is presented. The extended object is the classically behaving macroscopic object created through the boson condensation of phonons, which is mathematically expressed by the boson transformation. A general method for constructing extended objects with topological singularities is summarized. The extended object is classified by a topological singularity of boson transformation functions (or the displacement fields) which satisfy the phonon equation. As examples, dislocations, grain boundaries, and point defects are studied in detail. While the dislocation correspond to a line singularity, the grain boundaries and point defects are expressed as surface singularities in crystals. In particular, it is shown that a point defect, which is defined by the closed-surface singularity with the size of the lattice parameter, gives a reasonable estimate of the energy for a vacancy, i.e., 1 eV. Furthermore, based on a new theory of boundary surfaces, a novel derivation of surface waves is presented. Finally, the improvements over the conventional phenomenological theory of materials (the theory of elasticity) are pointed out.

I. INTRODUCTION

Recently, we developed the quantum field theory of crystals and dislocations[1] by applying a quantum field-theoretical technique (called the boson method) to the system of interacting molecules. The theory consists of two steps. In the first step, we derive the perfect crystal from the Lagrangian which is translationally invariant. As a result of spontaneous breakdown of symmetry, we obtain three quantum modes with gapless energy spectrum, which are identified as acoustic phonons. This is an example of the Goldstone theorem and acoustic phonons are Goldstone bosons. It is shown that the crystal lattice structure is consistent with the translational invariance of the theory, since the phonons play the role of recovering the original symmetry (the dynamical rearrangement of symmetry). In the second step, we create extended objects in crystals through the boson condensation of phonons. Here extended objects means classically behaving macroscopic objects in a quantum ordered state, sometimes called simply macroscopic objects. Throughout the paper, we shall mainly employ the words "extended objects." In this step the boson transformation method, which was first applied to the study of superconductivity, was effectively used. When the number of the condensed bosons is very large, the objects created in the system behave classically and one can develop the theory of extended objects in the quantum ordered state. We have formulated a general method to construct extended objects with topological singularities. Specially, we found that line singularities correspond to dislocations and that the Burgers vectors should be quantized.

The aim of this paper is to present a detailed account of the application of our general formalism to the study of various extended objects in crystals such as dislocations, grain boundaries, point defects, etc. The dislocations correspond to the line singularities, as was pointed out previously. It will be shown that the grain boundaries and point defects are expressed by the surface singularities. Since the boundary surface of a crystal is self-consistently maintained, it can be regarded as a macroscopic singularity. This viewpoint opens a new way of calculating the quantities associated with the crystal surface.

The plan of the paper is as follows. In Sec. II we briefly review our formalism for extended objects in crystals which was derived in the papers in Ref. 1. In Sec. III we summarize a general method for treating extended objects with topological singularities. The relations summarized in this section are the basic tools for our discussion in later sections. A detailed study of dislocations is presented in Sec. IV. Besides the general discussions on the properties of dislocations, an explicit expression for the displacement fields induced by the straight dislocation is obtained. In Sec. V we study the grain boundaries. Our result shows that the boundary generally accompanies some amount of expansion (or contraction) in addition to the change in orientation across the surface. Frank's formula for grain boundaries is found to be valid under the condition that the expansion (or contraction) is negligibly small in the vicinity of the boundary or the misorientation is small enough to ignore the expansion (or contraction). When we have a static surface singularity, calculation shows that the force per unit area normal to the surface is zero, implying that the surface is a free surface. This result is consistent with our view point that the boundary surface is self-consistently maintained. As will be shown in Secs. IV and V, we have continuity relations both for dislocations and grain boundaries. In Sec. VI we study an extended object, the singularity of which is confined into a domain enclosed by a closed surface. It is shown that this object can be regarded as the point defect. Explicit expressions for the field, volume expansion, and stress tensor associated with the point defect are presented. Calculation of the total strain energy gives the reasonable value of 1 eV which is roughly same as the energy for the formation of a lattice vacancy. Section VII is devoted to the analysis of surface sound waves. When we consider an oscillating free surface singularity, we find a new derivation of surface waves in crystal. The dispersion relation for the surface sound wave in isotropic media agrees with the Rayleigh's relation when the amplitude is small. Our theory of surface waves can be readily applied to other physical systems, such as surface magnons and surface properties of superconductors. In Sec. VIII we comment on the relationship between the conventional phenomenological theory of crystals and our formalism.

Although the theory is nonrelativistic, we shall sometimes use four-dimensional notation for convenience:

$$g^{\mu\nu} = g_{\mu\nu} = \begin{pmatrix} -1 & 0 \\ 0 & I \end{pmatrix},$$

$$x_\mu = (x_0, x_1, x_2, x_3) = (t, x_1, x_2, x_3),$$

$$x^\mu = g^{\mu\nu} x_\nu = (-t, x_1, x_2, x_3),$$

$$\partial^\mu = (\partial/\partial t, \partial/\partial x_1, \partial/\partial x_2, \partial/\partial x_3),$$

$$xp = x^\mu p_\mu = x_\mu p^\mu = \vec{x}\cdot\vec{p} - x_0 p_0,$$

and $\epsilon_{\mu\nu\lambda\rho}$ is the totally antisymmetric tensor with $\epsilon_{0123} = 1$.

II. QUANTUM FIELD THEORY OF CRYSTALS

In this section we briefly summarize a quantum field-theoretical formulation of crystals,[1] from which follows the phenomenological theory of materials. The phenomenological theory of materials which describes classical behavior of crystals is usually called the theory of elasticity.[2] In the derivation of this phenomenological theory a key role is played by the boson transformation method.

Our starting point is the Lagrangian $\mathfrak{L}(x)$ which consists of a molecule field $\psi(x)$: $\mathfrak{L}(x) = \mathfrak{L}(\psi(x))$. It is straightforward to extend our consideration to a system of many kinds of molecule fields and electrons. In our consideration, any specific form of the Lagrangian will not be assigned. We only assume that: (a) the Lagrangian is translationally invariant;

$$\int d^4x\, \mathfrak{L}(\psi(x)) = \int d^4x\, \mathfrak{L}(\psi(x+\alpha)), \tag{2.1}$$

where $\vec{\alpha}$ is an arbitrary c-number vector, and that (b) the interaction is such that it can create the crystal with lattice vectors $\vec{a}_i$ ($i = 1, 2, 3$), that is,

$$v(\vec{x} + \vec{a}_i) = v(\vec{x}), \tag{2.2}$$

where $v(\vec{x})$ is the ground-state expectation value of the density operator $n(x) = \psi^\dagger(x)\psi(x)$;

$$v(\vec{x}) = \langle n(x) \rangle . \tag{2.3}$$

We introduce a complete set of orthonormalized real periodic functions $\{\varphi_\lambda(\vec{x}); \lambda = -1, 0, 1, 2, \dots\}$ with the lattice periodicity $\varphi_\lambda(\vec{x} + \vec{a}_i) = \varphi_\lambda(\vec{x})$. Our choice is

$$\{\varphi_\lambda(\vec{x})\} = \{\varphi_{-1}(\vec{x}) = 1, \varphi_0(\vec{x}), \varphi_i(\vec{x}), \dots\}, \tag{2.4}$$

where $\varphi_\lambda(x)$ with $\lambda = 0, 1, 2, 3$ are related to $v(\vec{x})$ through the relation

$$\begin{aligned} v(\vec{x}) &= v_{-1} + v_0 \varphi_0(\vec{x}), \\ \varphi_i(\vec{x}) &= \sum_{j=1}^{3} (V^{-1/2})_{ij} \nabla_j v(\vec{x}), \quad i = 1, 2, 3 . \end{aligned} \tag{2.5}$$

Here v_{-1} and v_0 are constant and V_{ij} is defined by

$$\Omega V_{ij} \equiv \int_\Omega d^3x\, \nabla_i v(\vec{x}) \nabla_j v(\vec{x}), \tag{2.6}$$

with Ω being the volume of the unit cell of the crystal.

Since the Lagrangian is translationally invariant, we specify the choice of the reference coordinate system by adding the small symmetry-breaking term $\epsilon v(\vec{x})\psi^\dagger(x)\psi(x)$ to the Lagrangian $\mathfrak{L}(x)$. Then, the condition of translational invariance, (2.1), leads to the following Ward-Takahashi relation:

$$\nabla_j v(\vec{x}) = i\epsilon \int d^4y\, \langle \hat{n}(x)\hat{n}(y) \rangle \nabla_j v(\vec{y}), \tag{2.7}$$

where $\hat{n}(x) \equiv n(x) - v(\vec{x})$. On the other hand, the spectral representation of correlation function $\langle \hat{n}(x)\hat{n}(y) \rangle$ can be put in the form

$$\langle \hat{n}(x)\hat{n}(y) \rangle = \frac{i}{(2\pi)^4} \int dk_0 \int_{\Omega_B} d^3k\, e^{ik(x-y)} \times \left(\sum_\alpha \Delta^\alpha(\vec{x}, \vec{y}, k) + \cdots \right), \tag{2.8}$$

where

$$k(x-y) = \vec{k}\cdot(\vec{x} - \vec{y}) - k_0(t_x - t_y), \tag{2.9}$$

and $\Delta^{\alpha}(\vec{x},\vec{y},k)$ denotes a term which has a pole singularity in the following form:

$$\Delta^{\alpha}(\vec{x},\vec{y},k)=\frac{F_{\alpha}(\vec{k},\vec{x})F_{\alpha}^{*}(\vec{k},\vec{y})}{k_0^2-\omega_{\alpha}^2(\vec{k})-\epsilon C_{\alpha}(\vec{k})+i\eta}. \qquad (2.10)$$

Here $F_{\alpha}(\vec{k},\vec{x})$ are functions with lattice periodicity $F_{\alpha}(\vec{k},\vec{x}+\vec{a}_i)=F_{\alpha}(\vec{k},\vec{x})$. The dots in (2.8) stand for the terms with cut singularities and the symbol Ω_B means the volume of the first Brillouin zone.

A detailed account of derivation of (2.7) and (2.8) was presented in Ref. 1, and therefore is not repeated here. For the sake of simplicity, we presented in (2.10) the spectral representation at zero temperature, although our consideration in this paper holds true for system at any temperature. In case of the finite temperature the thermo field dynamics gives a quantum field-theoretical formulation of statistical mechanics for interacting particles.[3]

Expanding the periodic function $F_{\alpha}(\vec{k},\vec{x})$ in terms of $\varphi_{\lambda}(\vec{x})$,

$$F_{\alpha}(\vec{k},\vec{x})=\sum_{\lambda}\gamma_{\lambda}^{\alpha}(\vec{k})\varphi_{\lambda}(\vec{x}), \qquad (2.11)$$

we can rewrite (2.8) and (2.10) as

$$\langle\hat{n}(x)\hat{n}(y)\rangle=\frac{i}{(2\pi)^4}\int dk_0\int_{\Omega_B}d^3k\,e^{ik(x-y)}\times\sum_{\lambda,\lambda'}\varphi_{\lambda}(\vec{x})\Delta_{\lambda\lambda'}(\vec{k})\times\varphi_{\lambda'}(\vec{y}), \qquad (2.12)$$

with

$$\Delta_{\lambda\lambda'}(k)=\sum_{\alpha}\frac{\gamma_{\lambda}^{\alpha}(\vec{k})\gamma_{\lambda'}^{\alpha *}(\vec{k})}{k_0^2-\omega_{\alpha}^2(\vec{k})-\epsilon C_{\alpha}(\vec{k})+i\eta}+\cdots. \qquad (2.13)$$

Let us now eliminate the symmetry-breaking term by considering the limit $\epsilon\to 0$. Performing this limit in Eq. (2.7) and using (2.5) and (2.13), we obtain

$$\varphi_j(x)=\lim_{\epsilon\to 0}(-\epsilon)\sum_{\lambda}\varphi_{\lambda}(\vec{x})\Delta_{\lambda j}(0). \qquad (2.14)$$

Since the terms with cut singularities which are denoted by dots in $\Delta_{\lambda\lambda'}(k)$ do not produce any $1/\epsilon$ singularity at the limit $\epsilon\to 0$, we find that

$$\omega_{\alpha}^2(0)=0,\quad \alpha=1,2,3, \qquad (2.15a)$$

$$\delta_{ij}=\sum_{\alpha}\gamma_i^{\alpha}(0)C_{\alpha}^{-1}(0)\gamma_j^{\alpha *}(0), \qquad (2.15b)$$

$$\gamma_{\lambda}^{\alpha}(0)=0 \text{ for } \lambda\neq 1,2,3. \qquad (2.15c)$$

The completeness relation (2.15b) requires at least three kinds ($\alpha=1,2,3$) of bosons whose energies are gapless according to (2.15a). Those Goldstone bosons are the acoustic phonons. Thus the set of quasiparticles consists of three phonons χ_{α}^0 and the quasimolecule ψ^0. They satisfy

$$\lambda_{\alpha}(\partial)\chi_{\alpha}^0(x)=0, \qquad (2.16)$$

$$\lambda(\partial)\psi^0(x)=0, \qquad (2.17)$$

with, in particular,

$$\lambda_{\alpha}(\partial)=-\frac{\partial^2}{\partial t^2}-\omega_{\alpha}^2(-i\vec{\nabla}). \qquad (2.18)$$

The phonon equation (2.16) can be cast into a more familiar form by the help of the polarization vectors denoted by $e_i^{\alpha}(-i\vec{\nabla})$. The polarization vectors satisfy the unitary condition

$$\sum_i e_i^{\alpha *}(\vec{k})e_i^{\beta}(\vec{k})=\delta_{\alpha\beta}, \qquad (2.19a)$$

$$\sum_{\alpha} e_i^{\alpha}(\vec{k})e_j^{\alpha *}(\vec{k})=\delta_{ij}. \qquad (2.19b)$$

Furthermore, when the theory is invariant under the time reversal, we have

$$e_i^{\alpha *}(\vec{k})=e_i^{\alpha}(-\vec{k}). \qquad (2.20)$$

Let us define new phonon field operator by

$$\chi_i^0(x)=\sum_{\alpha}e_i^{\alpha}(-i\vec{\nabla})\chi_{\alpha}^0(x), \qquad (2.21)$$

and introduce the matrix

$$\omega_{ij}^2(\vec{k})=\sum_{\alpha}e_i^{\alpha}(\vec{k})\omega_{\alpha}^2(\vec{k})e_j^{\alpha *}(\vec{k}). \qquad (2.22)$$

Using the unitarity of the polarization vectors, we can then convert (2.16) into

$$\sum_j\lambda_{ij}(\partial)\chi_j^0(x)=0, \qquad (2.23)$$

with

$$\lambda_{ij}(\partial)=-\delta_{ij}\frac{\partial^2}{\partial t^2}-\omega_{ij}^2(-i\vec{\nabla}). \qquad (2.24)$$

We express the molecule field $\psi(x)$ in terms of the quasiphonon field $\chi_i^0(x)$ and the quasimolecule field $\psi^0(x)$;

$$\psi(x)=\psi(x;\chi_i^0(x),\psi^0(x)). \qquad (2.25)$$

The right-hand side of this relation is a sum of normal products of χ_i^0 and ψ^0. Precisely speaking, this relation means the equality of matrix elements of both sides, i.e., weak relation.

As was proved in Ref. 1, the spatial translation of the Heisenberg operator

$$\psi(x)\to\psi(x+\alpha) \qquad (2.26)$$

is induced by the transformation of the quasifields

$$\chi_i^0(x)\to\chi_i^0(\vec{\alpha};x)\equiv\chi_i^0(x+\alpha)+\sum_j(N^{-1}V^{1/2})_{ij}[\vec{\alpha}]_j, \qquad (2.27a)$$

$$\psi^0(x) \to \psi^0([\vec{\alpha}];x) \equiv \psi^0(x+\alpha), \tag{2.27b}$$

where $[\vec{\alpha}]$ is a vector reduced from $\vec{\alpha}$ in such a manner that it belongs to the first cell Ω by adjusting integers n_i in

$$\vec{\alpha} = [\vec{\alpha}] + \sum_i n_i \vec{a}_i, \tag{2.28}$$

and the matrix N is given by

$$N_{ij} = \sum_\alpha \gamma_i^\alpha(0) e_j^{\alpha *}(0). \tag{2.29}$$

The dynamical map (2.25) thus implies

$$\psi(x+\alpha) = \psi(x; \chi_i^0([\vec{\alpha}];x), \psi^0([\vec{\alpha}], x)). \tag{2.30}$$

This relation tells us how the spatial translation is dynamically rearranged and restricts severely the functional form (2.25).

The property (2.30) for the dynamical map is true for any Heisenberg operator consisting of $\psi(x)$. Let $O_H(x)$ stand for such an operator. If we expand O_H by means of the complete set $\{\varphi_\lambda(\vec{x})\}$, we have

$$O_H(x) = \sum_\lambda \varphi_\lambda(\vec{x}) O_\lambda(x; \chi_i^0(x), \psi^0(x)). \tag{2.31}$$

Here, O_λ is the expansion coefficient whose momentum support is Ω_B. Since the transformation (2.27) induces (2.26), Eq. (2.31) can be rewritten in the form

$$O_H(x) = \sum_\lambda \varphi_\lambda(\vec{x} + \eta^{-1}(-i\vec{\nabla})\vec{\chi}^0(x)) \times \hat{O}_\lambda(x; \partial\chi_i^0(x), \psi^0(x)), \tag{2.32}$$

where $\eta(-i\vec{\nabla})$ is a derivative matrix operator satisfying

$$\eta_{ij}(0) = (N^{-1}V^{1/2})_{ij}. \tag{2.33}$$

The quantity $\partial\chi_i^0$ in (2.32) stands for χ_i^0 carrying any positive number of derivatives. The operator $\hat{O}_\lambda$ has the property; $\hat{O}_\lambda(x) \to \hat{O}_\lambda(x+\alpha)$ under the transformation (2.27).

In general, the Lagrangian for interacting molecule field has the form

$$\mathcal{L}(x) = \frac{i}{2}\left(\psi^\dagger \frac{\partial\psi}{\partial t} - \frac{\partial\psi^\dagger}{\partial t}\psi\right) - \frac{1}{2M}\vec{\nabla}\psi^\dagger \cdot \vec{\nabla}\psi - V(\psi, \psi^\dagger). \tag{2.34}$$

Here V is a functional of ψ and $\psi^\dagger$. We then find that the molecule current $\vec{j}(x)$ and density $n(x)$ satisfy the conservation law

$$\frac{\partial}{\partial t} n(x) + \vec{\nabla} \cdot \vec{j}(x) = 0, \tag{2.35}$$

where

$$n(x) = \psi^\dagger(x)\psi(x), \tag{2.36a}$$

$$\vec{j}(x) = -\frac{i}{2M}[\psi^\dagger(x)\vec{\nabla}\psi(x) - \vec{\nabla}\psi^\dagger(x) \cdot \psi(x)]. \tag{2.36b}$$

The conservation law among the canonical energy-stress tensor $T_{\mu\nu}$ reads as

$$\frac{\partial}{\partial t} P_i(x) + \sum_j \nabla_j T_{ji}(x) = 0, \tag{2.37}$$

where

$$P_i(x) = T_{0i}(x) = m j_i(x), \tag{2.38a}$$

$$T_{ij}(x) = \frac{1}{2M}(\nabla_i\psi^\dagger \cdot \nabla_j\psi + \nabla_j\psi^\dagger \cdot \nabla_i\psi) + \delta_{ij}\mathcal{L}. \tag{2.38b}$$

The operators P_i and T_{ij} are called the momentum density and stress tensor. When we put $P_i(x)$ and $T_{ij}(x)$ in the forms

$$P_i(x) = -\sum_j \eta_{ij}^\dagger(-i\vec{\nabla})\dot{\chi}_j^0(x) + \sum_{\lambda \neq -1}\sum_j \varphi_\lambda(\vec{x})\gamma_{i\lambda j}(-i\vec{\nabla})\dot{\chi}_j^0(x) + \cdots, \tag{2.39}$$

$$T_{ij}(x) = \sum_{k,l,m} C_{il}^{jm}(-i\vec{\nabla})\nabla_m \eta_{lk}^{-1}(-i\vec{\nabla})\chi_k^0(x) + \sum_{\lambda \neq -1}\sum_l \varphi_\lambda(\vec{x})\Gamma_{ij\lambda}^l(-i\vec{\nabla})\chi_l^0(x) + \cdots, \tag{2.40}$$

then we can prove[1] that $\eta_{ij}(-i\vec{\nabla})$ defined by (2.39) satisfies the relation (2.33). Therefore, without loss of generality, we can identify η in (2.32) with η in (2.39). The coefficients $C_{il}^{jm}(\vec{k})$ in (2.40) are usually called the elastic constants, although they depend on $\vec{k}$. The conservation law (2.37) together with the phonon equation (2.33) leads to the following relations among coefficients:

$$\Phi_{ij}(\vec{k}) \equiv \sum_{l,m} C_{ij}^{lm}(\vec{k}) k_l k_m = [\eta^\dagger(\vec{k})\omega^2(\vec{k})\eta(\vec{k})]_{ij}, \tag{2.41}$$

$$\sum_{\lambda \neq -1}\sum_{j,l} \nabla_j[\varphi_\lambda(\vec{x})\Gamma_{ij\lambda}^l(-i\vec{\nabla})\chi_l^0(x)] = \sum_{\lambda \neq -1}\sum_{j,k} \varphi_\lambda(\vec{x})\gamma_{i\lambda j}(-i\vec{\nabla})\omega_{jk}^2(-i\vec{\nabla})\chi_k^0(x). \tag{2.42}$$

The dots in (2.39) and (2.40) stand either for the higher-order normal products of χ^0 or for the terms which contain ψ^0.

Equation (2.41) relates the elastic constants to the phonon energy and shows again that $\omega_{ij}(\vec{k})$ vanishes at $\vec{k} = 0$.

The hermiticity of $P_i(x)$ gives

$$\eta_{ji}^*(-i\vec{\nabla}) = \eta_{ji}(i\vec{\nabla}) = \eta_{ij}^\dagger(-i\vec{\nabla}). \tag{2.43}$$

The elastic constants defined by (2.40) have the following symmetries:

$$C_{il}^{jm}(\vec{k}) = C_{jl}^{im}(\vec{k}), \quad (2.44a)$$

$$C_{il}^{mj}(\vec{k}) = C_{li}^{jm*}(\vec{k}), \quad (2.44b)$$

$$C_{il}^{jm*}(\vec{k}) = C_{il}^{jm}(-\vec{k}), \quad (2.44c)$$

The properties (2.44a), (2.44b), and (2.44c) follow from the symmetry of T_{ij}, the Hermiticity of $\Phi_{ij}(\vec{k})$ and (2.20) and (2.43). It is clear that at $\vec{k} = 0$, the elastic constants are real and only 21 of them are independent.

We are now in a position to derive classical equations. It is convenient to introduce at this stage the phonon fields defined by

$$X_i^0(x) = \sum_j \eta_{ij}^{-1}(-i\vec{\nabla})\chi_j^0(x). \quad (2.45)$$

From (2.23), (2.24), and (2.39), we find that

$$\sum_j \Lambda_{ij}(\partial) X_j^0(x) = 0, \quad (2.46)$$

with

$$\Lambda_{ij}(\partial) = -\rho_{ij}(-i\vec{\nabla})\frac{\partial^2}{\partial t^2} - \Phi_{ij}(-i\vec{\nabla}), \quad (2.47)$$

where

$$\rho_{ij}(-i\vec{\nabla}) = \sum_k \eta_{ik}^{\dagger}(-i\vec{\nabla})\eta_{kj}(-i\vec{\nabla}) \quad (2.48)$$

is called the effective density. It should be noted that $X_i^0(x)$ is the canonical conjugate of the first term of (2.39). For this reason, we shall call $\vec{X}^0(x)$ the displacement field. On account of (2.43), the displacement field is Hermitian.

The boson transformation is now performed on the displacement field

$$X_i^0(x) \to X_i^0(x) + u_i(x), \quad (2.49)$$

where $u_i(x)$ is a c-number field satisfying the phonon equation

$$\sum_j \Lambda_{ij}(\partial) u_j(x) = 0. \quad (2.50)$$

It has been proved that the boson transformation does not change the Heisenberg equation (the boson transformation theorem).

In terms of the displacement field $\vec{u}(x)$, the change of the ground-state energy and the total momentum are

$$W[\vec{u}] = \frac{1}{2}\sum_{i,j}\int d^3x \Big(\dot{u}_i(x)\rho_{ij}(-i\vec{\nabla})\dot{u}_j(x) + \sum_{l,m}[\nabla_l u_i(x)] C_{ij}^{lm}(-i\vec{\nabla})[\nabla_m u_j(x)]\Big). \quad (2.51)$$

$$K_i[\vec{u}] = -\sum_j \rho_{ij}(0)\int d^3x\, \dot{u}_j(x) - \sum_{j,k}\int d^3x\, \dot{u}_j(x)\rho_{jk}(-i\vec{\nabla})\nabla_i u_k(x). \quad (2.52)$$

And the ground-state expectation values of momentum density $\vec{P}(x)$, molecule density $n(x)$, and the stress tensor T_{ij} are

$$P_i^u(x) = -\sum_j \rho_{ij}(-i\vec{\nabla})\dot{u}_j(x) + \sum_{\lambda\neq -1}\sum_{j,k}\varphi_\lambda(\vec{x})\gamma_{i\lambda j}(-i\vec{\nabla}) \times \eta_{jk}(-i\vec{\nabla})\dot{u}_k(x) + \cdots, \quad (2.53)$$

$$n^u(x) = v(x) + \frac{1}{M}\sum_{i,j}\nabla_i\rho_{ij}(-i\vec{\nabla})u_j(x) + \sum_{\lambda\neq -1}\sum_{i,j}\varphi_\lambda(\vec{x})\gamma_{\lambda i}(-i\vec{\nabla}) \times \eta_{ij}(-i\vec{\nabla})u_j(x) + \cdots, \quad (2.54)$$

$$T_{ij}^u(x) = \sum_{k,l} C_{il}^{jk}(-i\vec{\nabla})\nabla_k u_l(x) + \sum_{\lambda\neq -1}\sum_{k,l}\varphi_\lambda(\vec{x})\Gamma_{ij\lambda}^k(-i\vec{\nabla}) \times \eta_{kl}(-i\vec{\nabla})u_l(x) + \cdots. \quad (2.55)$$

These equations can be used to improve the conventional theory of elasticity. The detail of the discussion will be given in Sec. VIII.

III. TOPOLOGICAL SINGULARITIES

The macroscopic objects (extended objects) in crystal are described by the displacement, which is a c-number function satisfying the equation

$$\sum_{j=1}^{3}\Lambda_{ij}(\partial)u_j(x) = 0, \quad (3.1)$$

with

$$\Lambda_{ij}(\partial) = -\rho_{ij}(-i\vec{\nabla})\frac{\partial^2}{\partial t^2} + \sum_{l,m} C_{ij}^{lm}(-i\vec{\nabla})\nabla_l\nabla_m. \quad (3.2)$$

In this section we shall develop a systematic method for constructing the displacement $u_i(x)$ with topological singularities.

The dynamical map between a Heisenberg operator $O_H(x)$ and the displacement field $\vec{X}^0(x)$ has the form [cf. (2.32)]

$$O_H(x) = \sum_\lambda \varphi_\lambda(\vec{x} + \vec{X}^0(x))\hat{O}_\lambda(x;\partial\vec{X}^0(x),\psi^0(x)). \quad (3.3)$$

The effect of the boson transformation

$$X_i^0(x) \to X_i^0(x) + u_i(x) \quad (3.4)$$

on (3.3) is

$$O_H^u(x)=\sum_\lambda \varphi_\lambda(\vec{x}+\vec{X}^0(x)+\vec{u}(x))\times\hat{O}_\lambda(x;\partial\vec{X}^0(x)+\partial\vec{u}(x),\psi^0(x)). \quad (3.5)$$

Let us consider a closed loop described by $\vec{x}_c(s)$ $(0\leq s\leq 1)$ with $\vec{x}_c(0)=\vec{x}_c(1)$. Since the observables are single valued and the functions $\varphi_\lambda(\vec{x})$ are periodic, we find that $\partial_\mu\vec{u}(x)$ is single valued and that when $\vec{u}(x)$ is multivalued, it should satisfy

$$\vec{u}(x_c(1))-\vec{u}(x_c(0))=\sum_i n_i^c\,\vec{a}_i, \quad (3.6)$$

where n_i^c $(i=1,2,3)$ are integers. The above relation can be written in terms of the Burgers vector $\vec{B}^c$ as

$$\vec{B}^c\equiv\oint_C ds_\mu\,\partial_\mu\vec{u}(x)=\sum_i n_i^c\,\vec{a}_i, \quad (3.7)$$

which implies that the Burgers vectors are quantized. The integration is carried out along the closed loop C. It is to be remarked that (3.7) is not necessarily valid if the path C crosses the region where $\vec{u}(x)$ is not single valued.

When $\vec{u}(x)$ is multivalued, its topological structure is determined by the function $G_{\mu\nu}^\dagger(x)$ defined by

$$G_{\mu\nu}^{\dagger(i)}(x)=(\partial_\mu\partial_\nu-\partial_\nu\partial_\mu)u_i(x). \quad (3.8)$$

The domains in which some components of $G_{\mu\nu}^{\dagger(i)}(x)$ do not vanish are the domains of topological singularity. To simplify the expression we introduce the notations

$$C_{ij}^{00}(\partial)=-\rho_{ij}(-i\vec{\nabla}),$$
$$C_{ij}^{lm}(\partial)=C_{ij}^{lm}(-i\vec{\nabla}), \quad (3.9)$$
$$C_{ij}^{l0}(\partial)=C_{ij}^{0l}(\partial)=0,$$

in terms of which we can write

$$\Lambda_{ij}(\partial)=\sum_{\mu,\nu}C_{ij}^{\mu\nu}(\partial)\partial_\mu\partial_\nu\,. \quad (3.10)$$

Since $\partial_\rho\vec{u}(x)$ is single valued, we have

$$(\partial_\mu\partial_\nu-\partial_\nu\partial_\mu)\partial_\rho\vec{u}(x)=0. \quad (3.11)$$

Let us operate $C_{li}^{\lambda\mu}(\partial)\partial_\lambda$ on both sides of (3.8). Using (3.11) we have

$$\sum_j\Lambda_{ij}(\partial)\partial_\nu u_j(x)=\sum_j\sum_{\lambda,\mu}C_{ij}^{\lambda\mu}(\partial)\partial_\lambda G_{\mu\nu}^{\dagger(j)}(x). \quad (3.12)$$

Therefore, when we introduce the Green's function $\Delta_{jk}(x)$ by

$$\sum_j\Lambda_{ij}(\partial)\Delta_{jk}(x)=\delta_{ik}\delta^{(4)}(x), \quad (3.13)$$

we obtain

$$\partial_\nu u_j(x)=\sum_{k,l}\sum_{\lambda,\rho}\int d^4x'\,\Delta_{jk}(x-x')C_{kl}^{\lambda\rho}(\partial')\times\partial_\lambda' G_{\rho\nu}^{\dagger(l)}(x'). \quad (3.14)$$

In order to construct $G_{\mu\nu}^{\dagger(j)}$ explicitly, it is convenient to introduce its dual conjugate defined by

$$G_{\mu\nu}^{(j)}(x)=\tfrac{1}{2}\epsilon_{\mu\nu}^{\lambda\rho}G_{\lambda\rho}^{\dagger(j)}(x). \quad (3.15)$$

The relation (3.15), in turn gives

$$G_{\mu\nu}^{\dagger(j)}(x)=-\tfrac{1}{2}\epsilon_{\mu\nu}^{\lambda\rho}G_{\lambda\rho}^{(j)}(x). \quad (3.16)$$

Making use of (3.8) and (3.11), we find that

$$\partial^\mu G_{\mu\nu}^{(j)}(x)=0. \quad (3.17)$$

It can be readily shown that the condition (3.17) is sufficient for the relation (3.14) to reproduce (3.8).

Making use of above relations, we can develop a systematic method for constructing the displacement $u_i(x)$ with topological singularities.[4] First, look for $G_{\mu\nu}^{(i)}$ which satisfies the divergenceless condition (3.17), and then construct $G_{\mu\nu}^{\dagger(i)}$ according to (3.16). By means of (3.14), $\partial_\nu u_j(x)$ can be evaluated. The multivalued function $u_j(x)$ is obtained through a path integral of $\partial_\nu u_j$. Existence of the path integral is guaranteed by (3.8) as long as the path does not cross the singularities. In fact, $G_{\mu\nu}^{\dagger(i)}(x)=0$ is the integrability condition for $u_j(x)$ outside of the singular domain. Although $u_j(x)$ is path dependent, an explicit expression of the function $u_j(x)$ for x outside of the topologically singular domain can be obtained.

Let us consider a case in which the topological singularity is given by a world sheet $y_\mu(\tau,\sigma)$ which depends on two parameters τ and σ. Since $G_{\mu\nu}^{\dagger(\alpha)}$ does not vanish only on this worldsheet, it has the form

$$G_{\mu\nu}^{\dagger(\alpha)}(x)=M^\alpha\int dS_{\mu\nu}\,\delta^{(4)}(x-y), \quad (3.18)$$

where the surface integration is made over the worldsheet. Making use of the notation

$$\frac{\partial[y_\mu,y_\nu]}{\partial[\tau,\sigma]}=\frac{\partial y_\mu}{\partial\tau}\frac{\partial y_\nu}{\partial\sigma}-\frac{\partial y_\nu}{\partial\tau}\frac{\partial y_\mu}{\partial\sigma}, \quad (3.19)$$

we can rewrite (3.18) in the following form:

$$G_{\mu\nu}^{(\alpha)}=M^\alpha\int\int d\tau\,d\sigma\frac{\partial[y_\mu,y_\nu]}{\partial[\tau,\sigma]}\delta^{(4)}(x-y(\tau,\sigma)). \quad (3.20)$$

This leads to

$$\partial^\mu G_{\mu\nu}^{(\alpha)}(x)=M^\alpha\int\int d\tau\,d\sigma\left(-\frac{\partial y_\nu}{\partial\sigma}\frac{\partial}{\partial\tau}+\frac{\partial y_\nu}{\partial\tau}\frac{\partial}{\partial\sigma}\right)\times\delta^{(4)}(x-y(\tau,\sigma)). \quad (3.21)$$

The right-hand side of the above expression should vanish according to the divergenceless condition

(3.17). This condition restricts the choice of surface $y(\tau,\sigma)$. When we assume that τ is the timelike parameter;

$$y_0(\tau,\sigma)=\tau\,, \tag{3.22}$$

$y_\mu(\tau,\sigma)$ appears to be a line at each instance τ. The divergenceless condition (3.17) requires that the line expressed by $\vec{y}=\vec{y}(\sigma)$ should not have any boundary; infinitely long or closed on itself. We shall see in Sec. IV that this singular line corresponds to the dislocation and M^α is the Burgers vector.

Next we consider a worldsheet $y_\mu(\tau,\sigma_1,\sigma_2)$ which depends on three parameters τ, σ_1, and σ_2. Making use of the notation

$$\frac{\partial[y_\mu,y_\nu,y_\beta]}{\partial[\tau,\sigma_1,\sigma_2]}=\frac{\partial y_\mu}{\partial\tau}\frac{\partial[y_\nu,y_\beta]}{\partial[\sigma_1,\sigma_2]}-\frac{\partial y_\mu}{\partial\sigma_1}\frac{\partial[y_\nu,y_\beta]}{\partial[\tau,\sigma_2]}+\frac{\partial y_\mu}{\partial\sigma_2}\frac{\partial[y_\nu,y_\beta]}{\partial[\tau,\sigma_1]}\,, \tag{3.23}$$

we construct

$$G^{(\alpha)}_{\mu\nu}=\sum_\beta M^{\alpha\beta}\iiint d\tau\,d\sigma_1\,d\sigma_2\frac{\partial[y_\mu,y_\nu,y_\beta]}{\partial[\tau,\sigma_1,\sigma_2]}\times\delta^{(4)}(x-y(\tau,\sigma_1,\sigma_2))\,. \tag{3.24}$$

This leads to

$$\partial^\mu G^{(\alpha)}_{\mu\nu}(x)=M^{\alpha\beta}\iiint d\tau\,d\sigma_1\,d\sigma_2\left(-\frac{\partial[y_\nu,y_\beta]}{\partial[\sigma_1,\sigma_2]}\frac{\partial}{\partial\tau}+\frac{\partial[y_\nu,y_\beta]}{\partial[\tau,\sigma_2]}\frac{\partial}{\partial\sigma_1}-\frac{\partial[y_\nu,y_\beta]}{\partial[\tau,\sigma_1]}\frac{\partial}{\partial\sigma_2}\right)\delta^{(4)}(x-y(\tau,\sigma_1,\sigma_2))\,. \tag{3.25}$$

Therefore, when $y_\mu(\tau,\sigma_1,\sigma_2)$ does not have any boundary, $G^{(\alpha)}_{\mu\nu}$ given by (3.24) satisfies the divergenceless condition (3.17). The surface singularities which extend infinitely will be identified as grain boundaries in Sec. V, while closed surfaces with small size will be found to be point defects in Sec. VI. It is easy to generalize (3.24) into

$$G^{(\alpha)}_{\mu\nu}(x)=\sum_\beta M^{\alpha\beta}\iiiint d\tau\,d\sigma_1\,d\sigma_2\,d\eta\times\frac{\partial[y_\mu,y_\nu,y_\beta]}{\partial[\tau,\sigma_1,\sigma_2]}\rho(\eta)\times\delta^{(4)}(x-y(\tau,\sigma_1,\sigma_2,\eta)) \tag{3.26}$$

by introducing the weight function $\rho(\eta)$. In this case, the singularity at each instance τ is a closed volume which is an accumulation of surface singularities (parametrized by η and σ) with the weight function $\rho(\eta)$. The divergenceless condition (3.17) is satisfied when, for fixed η, $y_\mu(\tau,\sigma_1,\sigma_2,\eta)$ forms a closed surface.

Here we have considered only those extended objects which exist at all the time. When a singular domain has no end points in the four-dimensional space time, the divergenceless condition (3.17) is still satisfied. Therefore, considering a worldsheet confined in certain time interval, we can deal with the extended objects which exist only for this time interval. Those instantaneous or finite-lifetime singularities supply us with a powerful method for study of time-dependent macroscopic phenomena in crystals; however, in this paper we do not pursue this direction.

As will be seen in subsequent sections, the fundamental properties of dislocations, grain boundaries and point defects can be analyzed without any approximation. However, we frequently employ low-momentum approximation and isotropic approximation in order to compare our theory with the conventional theory. In those approximations, we have

$$C^{00}_{ij}(k)=-\rho_0\delta_{ij},\quad C^{l0}_{ij}(\partial)=C^{0l}_{ij}(\partial)=0\,,$$
$$C^{lm}_{ij}(\vec{k})=C^{lm}_{ij}(0)=C_{iljm}=\mu(\delta_{ij}\delta_{lm}+\delta_{im}\delta_{jl})+\lambda\delta_{il}\delta_{jm}\,, \tag{3.27}$$

where ρ_0 is the density, and λ and μ are the Lame constant and the shear modulus, respectively. With (3.27), (3.2) reads as

$$\Lambda_{ij}(ip)=\rho_0p_0^2\delta_{ij}-\mu\vec{p}^2\delta_{ij}-(\lambda+\mu)p_ip_j\,. \tag{3.28}$$

Therefore Green's function in momentum space $\Delta_{jk}[p]$ defined by $\sum_j\Lambda_{ij}(ip)\Delta_{jk}[p]=\delta_{ik}$, is

$$\Delta_{jk}[p]=\frac{(p_0^2-v_l^2|\vec{p}|^2)\delta_{jk}+(v_l^2-v_t^2)p_jp_k}{\rho_0(p_0^2-v_t^2|\vec{p}|^2)(p_0^2-v_l^2|\vec{p}|^2)}\,, \tag{3.29}$$

where v_t and v_l are velocity of transverse and logitudinal sound waves in isotropic media;

$$v_t=(\mu/\rho_0)^{1/2},\quad v_l=[(\lambda+2\mu)/\rho_0]^{1/2}. \tag{3.30}$$

In static cases, it is sometimes more convenient to work with Green's function in coordinate space. Substituting

$$\Delta_{jk}[\vec{p}]\equiv\Delta_{jk}[p]\,|_{p_0}=0=-\frac{1}{\mu}\frac{1}{|\vec{p}|^2}\delta_{jk}+\frac{\lambda+\mu}{\mu(\lambda+2\mu)}\frac{1}{|\vec{p}|^4}p_jp_k \tag{3.31}$$

into the relation

$$\Delta_{jk}(\vec{x})=\frac{1}{(2\pi)^3}\int d^3p\,e^{i\vec{p}\cdot\vec{x}}\Delta_{jk}[\vec{p}]\,, \tag{3.32}$$

we obtain

$$\Delta_{jk}(\vec{x})=-\frac{\lambda+3\mu}{\mu(\lambda+2\mu)}\frac{1}{8\pi r}\delta_{jk}-\frac{\lambda+\mu}{\mu(\lambda+2\mu)}\frac{x_jx_k}{8\pi r^3}\,. \tag{3.33}$$

Feeding (3.33) and (3.27) into (3.14), we arrive at the useful formula for static case;

$$\frac{\partial u_j(x)}{\partial x_m} = \sum_{l,b} \int \frac{d^3x'}{4\pi} \left[\frac{\mu}{\lambda+2\mu} \left(\frac{x_b - x_b'}{|\vec{r}-\vec{r}'|^3} \delta_{jl} + \frac{x_l - x_l'}{|\vec{r}-\vec{r}'|^3} \delta_{jb} - \frac{x_j - x_j'}{|\vec{r}-\vec{r}'|^3} \delta_{lb} \right) + \frac{\lambda+\mu}{\lambda+2\mu} \frac{3(x_j - x_j')(x_l - x_l')(x_b - x_b')}{|\vec{r}-\vec{r}'|^5} \right] G_{bm}^{\dagger(l)}(\vec{x}'). \tag{3.34}$$

IV. DISLOCATIONS

In Sec. III we have shown that a line singularity is expressed by

$$G_{\mu\nu}^{(\alpha)}(x) = M^\alpha \iint d\tau\, d\sigma \frac{\partial[y_\mu, y_\nu]}{\partial[\tau, \sigma]} \delta^{(4)}(x - y(\tau, \sigma)). \tag{4.1}$$

Using this expression we now discuss the salient features of dislocations.[5]

First we shall show that M^α in (4.1) which specifies the strength of a line singularity is nothing but the Burgers vector. To do this, consider a static line singularity

$$y_0(\tau, \sigma) = \tau, \quad y_i(\tau, \sigma) = y_i(\sigma), \quad i = 1, 2, 3. \tag{4.2}$$

Equations (4.1) and (4.2) show that the nonvanishing components of $G_{\mu\nu}^{(\alpha)}(x)$ are

$$G_{0k}^{(\alpha)}(x) = M^\alpha \int d\sigma \frac{dy_k(\sigma)}{d\sigma} \delta^{(3)}(\vec{x} - \vec{y}(\sigma)). \tag{4.3}$$

Applying the Stokes theorem to (3.7), we have

$$B^{(l)} \equiv \oint_C ds_k \partial^k u_l(x) = \int_{S_C} dS_{ij}\, G_{ij}^{\dagger(l)}(x), \tag{4.4}$$

where S_C is the area enclosed by path C, and $dS_{ij} = \frac{1}{2} dx_i \Lambda\, dx_j$. Since $G_{ij}^{\dagger(l)}(x) = \epsilon_{0ijk} G_{0k}^{(l)}(x)$, (4.4) is rewritten as

$$B^{(l)} = \int_{S_C} dS_k G_{0k}^{(l)}(x), \tag{4.5}$$

where $dS_k = \epsilon_{kij} \frac{1}{2} dx_i \Lambda\, dx_j$. We parametrize space coordinates $\vec{x} = \vec{x}(\xi_1, \xi_2, \xi_3)$ such that a line specified by $\xi_2 = \xi_3 = 0$ coincides with the line $\vec{y}(\sigma)$. Substituting

$$\frac{dy_k(\sigma)}{d\sigma} \delta^{(3)}(\vec{x} - \vec{y}(\sigma)) = \frac{\partial x_k}{\partial \xi_1} \frac{\partial[\xi_1, \xi_2, \xi_3]}{\partial[x_1, x_2, x_3]} \times \delta(\xi_1 - \sigma)\delta(\xi_2)\delta(\xi_3) \tag{4.6}$$

into (4.3), we obtain

$$G_{0k}^{(l)}(x) = M^l \frac{\partial x_k}{\partial \xi_1} \frac{\partial[\xi_1, \xi_2, \xi_3]}{\partial[x_1, x_2, x_3]} \delta(\xi_2)\delta(\xi_3). \tag{4.7}$$

Without loss of generality, we can choose (ξ_2, ξ_3) plane as the integral surface;

$$dS_k = \frac{1}{2} \frac{\partial[x_i, x_j]}{\partial[\xi_2, \xi_3]} \epsilon_{kij} d\xi_2\, d\xi_3. \tag{4.8}$$

Since

$$\frac{1}{2} \epsilon_{kij} \frac{\partial x_k}{\partial \xi_1} \frac{\partial[x_i, x_j]}{\partial[\xi_2, \xi_3]} = \frac{\partial[x_1, x_2, x_3]}{\partial[\xi_1, \xi_2, \xi_3]}, \tag{4.9}$$

we arrive at

$$B^{(l)} = \int_{S_C} d\xi_2\, d\xi_3\, \delta(\xi_2)\delta(\xi_3) M^l = M^l. \tag{4.10}$$

Therefore, M^l is the Burgers vector. Let us denote the unit vector tangent to $\vec{y}(\sigma)$ by $\vec{\eta}(\sigma)$. If

$$\vec{B} \cdot \vec{\eta}(\sigma) = 0 \tag{4.11}$$

happens to hold in a certain domain of σ, this is the edge dislocation in this domain, while

$$\vec{B} \cdot \vec{\eta}(\sigma) = \pm |B| \tag{4.12}$$

corresponds to the right-handed and left-handed screw dislocations, respectively.

We have already mentioned that a line singularity (dislocation) should not have any boundary; infinitely long or closed on itself. This is in accordance with the experimental facts which show that a dislocation line cannot end within an otherwise perfect region of crystal, but must terminate at a free surface, another dislocation line, a grain boundary, or some other defect. When we have an assembly of dislocations, the continuity property of dislocations leads to a dislocation network. Let us consider an assembly of dislocations $\{y_\mu^a\}$, $a = 1, 2, \ldots, N$. We assume that τ is the timelike parameter. We then choose y_0^a as follows:

$$y_0^a(\tau, \sigma) = \tau, \quad a = 1, 2, \ldots, N. \tag{4.13}$$

At each instance τ, $y_\mu^a(\tau, \sigma)$ appears to be a line. In this case, $G_{\mu\nu}^{(\alpha)}(x)$ is given by

$$G_{\mu\nu}^{(\alpha)}(x) = \sum_a M_a^\alpha \iint d\tau\, d\sigma \frac{\partial[y_\mu^a, y_\nu^a]}{\partial[\tau, \sigma]} \delta^{(4)}(x - y^a(\tau, \sigma)). \tag{4.14}$$

This leads to

$$\partial^\mu G_{\mu\nu}^{(\alpha)}(x) = \sum_a M_a^\alpha \iint d\tau\, d\sigma \left(-\frac{\partial y_\nu^a}{\partial\sigma} \frac{\partial}{\partial\tau} + \frac{\partial y_\nu^a}{\partial\tau} \frac{\partial}{\partial\sigma} \right) \times \delta^{(4)}(x - y^a(\tau, \sigma)) = \sum_a M_a^\alpha \int d\tau \frac{\partial y_\nu^a}{\partial\tau} \delta^{(4)}(x - y^a(\tau, \sigma)) \Big|_{\sigma_1^a(\tau)}^{\sigma_2^a(\tau)}, \tag{4.15}$$

where $\sigma_1^a(\tau)$ and $\sigma_2^a(\tau)$ are the end points of the line $y^a(\tau, \sigma)$ at time τ. Using (4.13), we have

$$\partial^\mu G^{(\alpha)}_{\mu 0}(x) = \partial_j G^{(\alpha)}_{j0}(x) = \sum_a M^\alpha_a[\delta^{(3)}(\vec{x} - \vec{y}^a(t, \sigma^a_1)) - \delta^{(3)}(\vec{x} - \vec{y}^a(t, \sigma^a_2))]. \tag{4.16}$$

On the other hand, the divergenceless condition (3.17) with $\nu = 0$ reads as

$$\partial_j G_{j0}(x) = 0, \tag{4.17}$$

which gives

$$\int_V d^3x\, \partial_j G_{j0}(x) = 0. \tag{4.18}$$

Suppose now that a line [say $y^b(\tau, \sigma)$] has an end point at $\sigma = \sigma^b(\tau)$ which is not shared by any other line. When we choose V in such a way that it contains no end points other than $y^{(b)}(\tau, \sigma^b)$, (4.16) gives

$$\int_V d^3x\, \partial_j G^{(\alpha)}_{j0}(x) = M^\alpha_b \quad \text{for } \alpha = 1, 2, 3. \tag{4.19}$$

This contradicts with (4.18). Therefore, assembly of all the lines should form a network which does not have any end point. A joint point of more than two dislocation lines is called the dislocation node. Consider a node denoted by $y(\tau)$. The lines which are joint with each other at $y(\tau)$ will be denoted by $y^b(\tau, \sigma)$ ($b = 1, 2, \ldots, M$). Then, choosing V to contain no other nodes than $y(\tau)$, we obtain from (4.16) and (4.18)

$$\sum_b (\pm M^\alpha_b) = 0, \tag{4.20}$$

where + (−) sign corresponds to the first (second) term in the right-hand side of (4.16). This relation, which means that the strength of the dislocation is conserved at each node, will be referred to as the continuity relation. When we regard a network of dislocations as an electric circuit, the continuity relation corresponds to Kirchhoff's law of electric current. Conversely, the right-hand side in (4.15) for all ν vanishes when (4.20) holds at each node, implying that (4.20) is the complete condition for the divergenceless condition (3.17) to be satisfied. Therefore, the lines $y^{(a)}_\mu(\tau, \sigma)$ ($a = 1, 2, \ldots, N$) at time τ should form a network without any end point and the continuity relation (4.20) should hold at each node of the network. Experimentally, the dislocation networks are observed in various materials.[5,6]

Further application of the divergenceless relation (3.17) shows that the Burgers vector

$$B^{(l)}_c \equiv \oint_C ds_k\, \partial^k u_l(x)$$

has the same value for any two integral paths C_1 and C_2 which can be deformed onto each other without crossing the singularity. In a mathematical terminology, $\vec{B}_{C_1} = \vec{B}_{C_2}$ when paths C_1 and C_2 belong to the same homotopy class.[7] Recently, Kléman *et al.*[8] have used the theory of homotopy groups to classify the defects in crystals.

As an example, we shall consider an infinitely long straight dislocation in an isotropic media. Under the low-momentum approximation, the displacement field due to the dislocation is obtained as follows. In the case of a straight-line singularity, we can write

$$y_k(\sigma) = \sigma\delta_{k3}, \quad -\infty < \sigma < \infty \tag{4.21}$$

in the coordinate system in which the singularity lies on the 3rd axis. From (4.3) and (4.21), we find that the nonvanishing components of $G^{(\alpha)}_{\mu\nu}(x)$ and $G^{\dagger(\alpha)}_{\mu\nu}(x)$ are

$$G^{(\alpha)}_{03}(x) = M^\alpha \delta(x_1)\delta(x_2), \tag{4.22}$$

$$G^{\dagger(\alpha)}_{12}(x) = M^\alpha \delta(x_1)\delta(x_2). \tag{4.23}$$

Substituting (4.23) into (3.23), we obtain

$$\begin{aligned}\frac{\partial u_j(x)}{\partial x_1} = &-\frac{1}{4\pi} M^1 \left[\left(\frac{\mu}{\lambda+2\mu}\frac{2x_2}{x_1^2+x_2^2} + \frac{\lambda+\mu}{\lambda+2\mu}\frac{4x_1^2 x_2}{(x_1^2+x_2^2)^2}\right)\delta_{j1} + \left(\frac{\mu}{\lambda+2\mu}\frac{2x_1}{x_1^2+x_2^2} + \frac{\lambda+\mu}{\lambda+2\mu}\frac{4x_1 x_2^2}{(x_1^2+x_2^2)^2}\right)\delta_{j2}\right] \\ &-\frac{1}{4\pi} M^2 \left[\left(-\frac{\mu}{\lambda+2\mu}\frac{2x_1}{x_1^2+x_2^2} + \frac{\lambda+\mu}{\lambda+2\mu}\frac{4x_1 x_2^2}{(x_1^2+x_2^2)^2}\right)\delta_{j1} + \left(\frac{\mu}{\lambda+2\mu}\frac{2x_2}{x_1^2+x_2^2} + \frac{\lambda+\mu}{\lambda+2\mu}\frac{4x_2^3}{(x_1^2+x_2^2)^2}\right)\delta_{j2}\right] \\ &-\frac{1}{2\pi} M^3 \frac{x_2}{x_1^2+x_2^2}\delta_{j3},\end{aligned} \tag{4.24a}$$

$$\begin{aligned}\frac{\partial u_j(x)}{\partial x_2} = &\frac{1}{4\pi} M^1 \left[\left(\frac{\mu}{\lambda+2\mu}\frac{2x_1}{x_1^2+x_2^2} + \frac{\lambda+\mu}{\lambda+2\mu}\frac{4x_1^3}{(x_1^2+x_2^2)^2}\right)\delta_{j1} + \left(-\frac{\mu}{\lambda+2\mu}\frac{2x_2}{x_1^2+x_2^2} + \frac{\lambda+\mu}{\lambda+2\mu}\frac{4x_1^2 x_2}{(x_1^2+x_2^2)^2}\right)\delta_{j2}\right] \\ &+\frac{1}{4\pi} M^2 \left[\left(\frac{\mu}{\lambda+2\mu}\frac{2x_2}{x_1^2+x_2^2} + \frac{\lambda+\mu}{\lambda+2\mu}\frac{4x_1^2 x_2}{(x_1^2+x_2^2)^2}\right)\delta_{j1} + \left(\frac{\mu}{\lambda+2\mu}\frac{2x_1}{x_1^2+x_2^2} + \frac{\lambda+\mu}{\lambda+2\mu}\frac{4x_1 x_2^2}{(x_1^2+x_2^2)^2}\right)\delta_{j2}\right] \\ &+\frac{1}{2\pi} M^3 \frac{x_1}{x_1^2+x_2^2}\delta_{j3},\end{aligned} \tag{4.24b}$$

$$\frac{\partial u_j(x)}{\partial x_3}=0. \tag{4.24c}$$

Therefore, outside of the singularity at $x_1=x_2=0$, the displacement fields are

$$u_1(x)=\frac{1}{2\pi}M^1\left[\tan^{-1}\left(\frac{x_2}{x_1}\right)+\frac{\lambda+\mu}{\lambda+2\mu}\frac{x_1x_2}{x_1^2+x_2^2}\right]+\frac{1}{4\pi}M^2\left(\frac{\mu}{\lambda+2\mu}\ln(x_1^2+x_2^2)-\frac{\lambda+\mu}{\lambda+2\mu}\frac{x_1^2-x_2^2}{x_1^2+x_2^2}\right), \tag{4.25a}$$

$$u_2(x)=-\frac{1}{4\pi}M^1\left(\frac{\mu}{\lambda+2\mu}\ln(x_1^2+x_2^2)+\frac{\lambda+\mu}{\lambda+2\mu}\frac{x_1^2-x_2^2}{x_1^2+x_2^2}\right)+\frac{1}{2\pi}M^2\left[\tan^{-1}\left(\frac{x_2}{x_1}\right)-\frac{\lambda+\mu}{\lambda+2\mu}\frac{x_1x_2}{x_1^2+x_2^2}\right], \tag{4.25b}$$

$$u_3(x)=\frac{1}{2\pi}M^3\tan^{-1}\left(\frac{x_2}{x_1}\right). \tag{4.25c}$$

The integral constants are chosen so as to yield simple expressions for $u_i(x)$. The formula (4.25) reduces to the familiar results when we consider pure screw or pure edge dislocations. For screw dislocation where $M^1=M^2=0$, we have

$$u_1(x)=u_2(x)=0,\quad u_3(x)=(1/2\pi)M^3\tan^{-1}(x_2/x_1). \tag{4.26}$$

For edge dislocation where $M^2=M^3=0$, (4.25) leads to

$$\begin{aligned} u_1(x)&=\frac{1}{2}M^1\left[\tan^{-1}\left(\frac{x_2}{x_1}\right)+\frac{\lambda+\mu}{\lambda+2\mu}\frac{x_1x_2}{x_1^2+x_2^2}\right],\\ u_2(x)&=-\frac{1}{4\pi}M^1\left(\frac{\mu}{\lambda+2\mu}\ln(x_1^2+x_2^2)+\frac{\lambda+\mu}{\lambda+2\mu}\frac{x_1^2-x_2^2}{x_1^2+x_2^2}\right),\\ u_3(x)&=0. \end{aligned} \tag{4.27}$$

V. GRAIN BOUNDARIES

Common material is not a single crystal, but an aggregate of small crystal grains. An interface between two single crystal grains is called a grain boundary. We regard grain boundary as a macroscopic object (extended object) which has certain surface singularity. In Sec. III we have shown that a surface singularity is described by

$$G_{\mu\nu}^{(\alpha)}(x)=M^{\alpha\beta}\iiint d\tau\, d\sigma_1\, d\sigma_2\frac{\partial[y_\mu,y_\nu,y_\beta]}{\partial[\tau,\sigma_1,\sigma_2]}\times\delta^{(4)}(x-y(\tau,\sigma_1,\sigma_2)). \tag{5.1}$$

We shall consider the static case;

$$y_0(\tau,\sigma_1,\sigma_2)=\tau,\quad y_i(\tau,\sigma_1,\sigma_2)=y_i(\sigma_1,\sigma_2)$$
$$(i=1,2,3),\quad M^{\alpha 0}=0. \tag{5.2}$$

Then, the nonvanishing components of $G_{\mu\nu}^{(\alpha)}(x)$ are

$$G_{0k}^{(\alpha)}(x)=\sum_l M^{\alpha l}\iint d\sigma_1\, d\sigma_2\frac{\partial[y_k,y_l]}{\partial[\sigma_1,\sigma_2]}\times\delta^{(3)}(\vec{x}-\vec{y}(\sigma_1,\sigma_2)). \tag{5.3}$$

The topological singularity at each instance is a surface given by $\vec{y}(\sigma_1,\sigma_2)$. As is shown below, the matrix $M^{\alpha l}$ is related to the rotations of the regions separated by a surface.

We introduce the parametrization of the space coordinates $\vec{x}=\vec{x}(\xi_1,\xi_2,\xi_3)$ such that surface specified by $\xi_3=0$ coincides with the surface $\vec{y}(\sigma_1,\sigma_2)$. Substituting the relation

$$\delta^{(3)}(\vec{x}-\vec{y}(\sigma_1,\sigma_2))=\frac{\partial[\xi_1,\xi_2,\xi_3]}{\partial[x_1,x_2,x_3]}\times\delta(\xi_1-\sigma_1)\delta(\xi_2-\sigma_2)\delta(\xi_3) \tag{5.4}$$

into (5.3), we obtain

$$G_{0k}^{(\alpha)}(x)=\sum_l M^{\alpha l}\frac{\partial[x_k,x_l]}{\partial[\xi_1,\xi_2]}\frac{\partial[\xi_1,\xi_2,\xi_3]}{\partial[x_1,x_2,x_3]}\delta(\xi_3). \tag{5.5}$$

Let us consider the line integral

$$B^\alpha\equiv\int_C ds_k\,\partial_k u_\alpha(x). \tag{5.6}$$

Path C is a closed path going below the surface ($\xi_3=0_-$) from a point $Q(\xi_1^i,\xi_2^i,0)$ to a point $P(\xi_1^f,\xi_2^f,0)$, and then coming back above the surface ($\xi_3=0_+$) from P to Q. The quantity B^α is the sum of the Burgers vectors contained in the interval PQ. On the other hand, B^α can be expressed in terms of $M^{\alpha l}$ as follows. The Stokes theorem leads to

$$\oint_C ds_k\,\partial_k u_\alpha(x)=\int_{S_C} dS_{ij}G_{ij}^{\dagger(\alpha)}(x)=\int_{S_C} dS_k\, G_{0k}^{(\alpha)}(x), \tag{5.7}$$

where S_C is the area enclosed by the path C, and

$$dS_{ij}=\tfrac{1}{2}dx_i\wedge dx_j, \tag{5.8a}$$

$$dS_k=\epsilon_{kij}\left(\frac{\partial x_i}{\partial\xi_1}\frac{\partial x_j}{\partial\xi_3}d\xi_1\,d\xi_3+\frac{\partial x_i}{\partial\xi_2}\frac{\partial x_j}{\partial\xi_3}d\xi_2\,d\xi_3\right). \tag{5.8b}$$

Using the explicit form of $G_{0k}^{(\alpha)}(x)$ given by (5.5) in (5.7), we arrive at the relation

$$B^\alpha = \sum_l M^{\alpha l} \iint_{S_C} \left(\frac{\partial x_l}{\partial \xi_2} d\xi_2 d\xi_3 + \frac{\partial x_l}{\partial \xi_1} d\xi_1 d\xi_3 \right) \delta(\xi_3)$$
$$= \sum_l M^{\alpha l} \int_Q^P \left(\frac{\partial x_l}{\partial \xi_2} d\xi_2 + \frac{\partial x_l}{\partial \xi_1} d\xi_1 \right)$$
$$= \sum_l M^{\alpha l} V_l \,, \tag{5.9}$$

where $\vec{V}$ is the vector from point Q to point P;

$$V_l = x_l(\xi_1^f, \xi_2^f, 0) - x_l(\xi_1^i, \xi_2^i, 0) \,. \tag{5.10}$$

The matrix $M^{\alpha l}$ determines the misorientation of grains separated by the grain boundary. We suppose that grain A and grain B are rotated by $\vec{\omega}_A = \theta_A \vec{a}^A$ and $\vec{\omega}_B = \theta_B \vec{a}^B$ with respect to the reference crystal, respectively. Here $\vec{a}^i$ $(i = A, B)$ is the unit vector which specifies the axis of rotation, and $\theta_i (i = A, B)$ denotes the angle of the rotation around $\vec{a}^i$ axis. Let us introduce vectors $\vec{V}_+$ and $\vec{V}_-$; $\vec{V}_+$ is the vector from a point Q on the surface to a point P_+ in the grain B and $\vec{V}_-$ is the vector from Q to a point P_- in the grain A. The displacement of the vector $\vec{V}_+$ due to the rotation $\vec{\omega}_B$ in the grain B is given by $\vec{u}^B(\vec{V}_+)$, while the displacement of $\vec{V}_-$ due to the rotation $\vec{\omega}_A$ in the grain A is given by $\vec{u}^A(\vec{V}_-)$. Therefore, in the limit of $\vec{V}_+ = \vec{V}_- \equiv \vec{V}$, we have

$$\vec{u}^A(\vec{V}) = (e^{i\theta_A \vec{a}^A \cdot \vec{J}} - 1)\vec{V} \,,$$
$$\vec{u}^B(\vec{V}) = (e^{i\theta_B \vec{a}^B \cdot \vec{J}} - 1)\vec{V} \,, \tag{5.11}$$

where J_i is the generator of rotation around the x_i axis. On the other hand, the line integral

$$\oint_C ds_k \partial_k u_\alpha(x)$$

gives the difference of the displacements $\vec{u}^B(\vec{V}_+)$ and $\vec{u}^A(\vec{V}_-)$, where path C is a closed path QP_+P_-Q. Then, considering the limit $\vec{V}_+ = \vec{V}_- \equiv \vec{V}$ again, we have

$$\oint_C ds_k \partial_k u_j(x) = u_j^B(\vec{V}) - u_j^A(\vec{V}) \,. \tag{5.12}$$

Using (5.9), (5.11), and (5.12), we obtain

$$M_{ij} = (e^{i\theta_B \vec{a}^B \cdot \vec{J}} - e^{i\theta_A \vec{a}^A \cdot \vec{J}})_{ij} \tag{5.13}$$

and

$$\vec{B} = \vec{a}^B(\vec{V} \cdot \vec{a}^B) - \vec{a}^A(\vec{V} \cdot \vec{a}^A) + [\vec{V} - \vec{a}^B(\vec{V} \cdot \vec{a}^B)] \cos\theta_B$$
$$- [\vec{V} - \vec{a}^A(\vec{V} \cdot \vec{a}^A)] \cos\theta_A + \sin\theta_B (\vec{V} \times \vec{a}^B)$$
$$- \sin\theta_A (\vec{V} \times \vec{a}^A) \,. \tag{5.14}$$

Let us consider the case $\vec{a}^A = -\vec{a}^B \equiv \vec{d}$. In this case, the reference crystal can always be orientated in such a way that $\theta_A = \theta_B = \frac{1}{2}\theta$, and therefore (5.14) reduces to

$$\vec{B} = 2(\vec{V} \times \vec{d}) \sin\tfrac{1}{2}\theta \,. \tag{5.15}$$

This is the Frank's formula[5,9] for a large-angle grain boundary. When $\vec{d}$ is contained in the plane of boundary, the grain boundary is called a tilt boundary. When $\vec{d}$ is perpendicular to the boundary plane, it is called a twist boundary. In general, a boundary is of mixed character, containing both tilt and twist component.

The following comments require special attention. First, the statement that the matrix $M^{\alpha l}$ determines the misorientation of grains (A and B) separated by the grain boundary does not imply that the displacement fields in grains A and B are different only in the orientation. In general, the displacement fields on each side of the boundary contain not only rotation but also expansion (or contraction). Second, in the discussion from (5.11) to (5.15), assumption that there is no expansion (or contraction) *on the boundary surface* was used. Here "on the boundary surface" was emphasized since certain expansion (or contraction) is permitted inside each grain. We shall come back to this point at the end of this section where expression of the displacement field in both grain will be explicitly presented.

It is possible to derive a continuity relation for grain boundaries in a way similar to the derivation of continuity relation for dislocations. We consider an aggregate of grain boundaries $(a = 1, 2, \ldots, N)$ expressed by

$$G_{\lambda\rho}^{(\alpha)}(x) = \sum_a M_a^{\alpha\mu} \iiint d\tau\, d\sigma_1\, d\sigma_2 \times \frac{\partial[y_\lambda^a, y_\rho^a, y_\mu^a]}{\partial[\tau, \sigma_1, \sigma_2]} \times \delta^{(4)}(x - y^a(\tau, \sigma_1, \sigma_2)) \,. \tag{5.16}$$

When the system is static, (5.2) leads to

$$\partial^k G_{k0}^{(\alpha)}(x) = \sum_a \sum_\beta M_a^{\alpha\beta} \iint d\sigma_1 d\sigma_2 \left(\frac{\partial y_\beta}{\partial \sigma_2} \frac{\partial}{\partial \sigma_1} - \frac{\partial y_\beta}{\partial \sigma_1} \frac{\partial}{\partial \sigma_2} \right) \delta^{(3)}(\vec{x} - \vec{y}^a(\sigma_1, \sigma_2))$$
$$= \sum_a \sum_\beta M_a^{\alpha\beta} \int dS_3 \left(-\frac{\partial y_\beta}{\partial \vec{\sigma}} \times \frac{\partial}{\partial \vec{\sigma}} \right)_3 \delta^{(3)}(\vec{x} - \vec{y}^a(\sigma_1, \sigma_2)) \,, \tag{5.17}$$

where $dS_3 = d\sigma_1 d\sigma_2$. We now construct the three-dimensional σ space by introducing the spurious parameter

σ_3. Then, making use of the Stokes theorem, we can rewrite (5.17) as follows:

$$\begin{aligned}\partial^k G_{k0}^{(\alpha)}(x) &= \sum_a \sum_\beta M_a^{\alpha\beta} \int d\vec{S}\left(-\frac{\partial y_\beta^a}{\partial\vec{\sigma}}\frac{\partial}{\partial\vec{\sigma}}\right)\delta^{(3)}(\vec{x}-\vec{y}^a(\sigma_1,\sigma_2)) \\ &= \sum_a\sum_\beta M_a^{\alpha\beta}\int d\vec{S}\cdot\frac{\partial}{\partial\vec{\sigma}}\times\frac{\partial y_\beta^a}{\partial\vec{\sigma}}\,\delta^{(3)}(\vec{x}-\vec{y}^a(\sigma_1,\sigma_2)) \\ &= \sum_a\sum_\beta M_a^{\alpha\beta}\int_{C_a} d\vec{\sigma}\cdot\frac{\partial y_\beta^a}{\partial\vec{\sigma}}\,\delta^{(3)}(\vec{x}-\vec{y}^a(\sigma_1,\sigma_2)). \end{aligned} \tag{5.18}$$

The path C_a is the boundary of surface $y_i^a(\sigma_1, \sigma_2)$. A joint line of more than two grain boundaries is called a nodal line. Consider a nodal line C parametrized as $\vec{y}(\sigma)$. The boundaries which meet along the line $\vec{y}(\sigma)$ will be denoted by $\vec{y}^b(\sigma)$ ($b = 1, 2, \ldots, M$). Then, the divergenceless relation (3.17) requires that the following condition should hold on the line

$$\sum_b \sum_\beta (\pm) M_b^{\alpha\beta} n_\beta(\sigma) = 0 \quad (\alpha = 1, 2, 3). \tag{5.19}$$

Here $\vec{n}(\sigma) = \partial\vec{y}/\partial\sigma$ is the tangential vector of line C and $\pm$ sign is specified by the direction of path integral in (5.18). The relation (5.19) will be referred as the continuity relation for grain boundaries. Similar to the dislocation network, it is known[9] that grain boundaries make the cellular structure. The continuity relation (5.19) indicates that, in general, three boundaries meet along a nodal line. As a special case, let us consider the case $b = 1$, that is, there is only one grain boundary. We notice that (5.19) is satisfied when only one component of $\vec{n}$ (say, n_3) is nonvanishing and $M_1^{\alpha 3}$ ($\alpha = 1, 2, 3$) are zero. Therefore, a grain boundary can end within the crystal. This is an example of the disinclination (or rotational dislocation).[10]

So far the discussions in this section are far from any approximation. We shall hereafter discuss the properties of a flat grain boundary by employing the low-momentum approximation and isotropic approximation. Let us consider a flat surface singularity given by

$$\begin{aligned} y_1(\sigma_1, \sigma_2) &= \sigma_1, \\ y_2(\sigma_1, \sigma_2) &= \sigma_2, \\ y_3(\sigma_1, \sigma_2) &= 0. \end{aligned} \tag{5.20}$$

From (5.3), (5.20), and (3.16), we find that the nonvanishing components of $G_{\mu\nu}^{(\alpha)}(x)$ and $G_{\mu\nu}^{\dagger(\alpha)}(x)$ are

$$\begin{aligned} G_{01}^{(\alpha)}(x) &= -G_{10}^{(\alpha)}(x) = M^{\alpha 2}\delta(x_3), \\ G_{02}^{(\alpha)}(x) &= -G_{20}^{(\alpha)}(x) = -M^{\alpha 1}\delta(x_3), \end{aligned} \tag{5.21}$$

$$\begin{aligned} G_{23}^{\dagger(\alpha)}(x) &= -G_{32}^{\dagger(\alpha)}(x) = M^{\alpha 2}\delta(x_3), \\ G_{31}^{\dagger(\alpha)}(x) &= -G_{13}^{\dagger(\alpha)}(x) = -M^{\alpha 1}\delta(x_3). \end{aligned} \tag{5.22}$$

In terms of Fourier transforms, (3.14) reads as

$$\frac{\partial u_j(x)}{\partial x_m} = \sum_{k,l}\sum_{a,b} C_{kl}^{ab}(0)\int\frac{d^3p}{(2\pi)^3} ip_a \Delta_{jk}[\vec{p}] \times G_{bm}^{\dagger(l)}[\vec{p}]e^{i\vec{p}\cdot\vec{x}}, \tag{5.23}$$

where $G_{bm}^{\dagger(l)}[\vec{p}]$ is the Fourier transform of $G_{bm}^{\dagger(l)}(\vec{x})$;

$$G_{bm}^{\dagger(l)}[\vec{p}] = \int d^3x\, G_{bm}^{\dagger(l)}(\vec{x})e^{-i\vec{p}\cdot\vec{x}}. \tag{5.24}$$

The nonvanishing components of $G_{bm}^{\dagger(l)}[\vec{p}]$ are

$$\begin{aligned} G_{23}^{\dagger(l)}[\vec{p}] &= -G_{32}^{\dagger(l)}[\vec{p}] = M^{l2}(2\pi)^2\delta(p_1)\delta(p_2), \\ G_{31}^{\dagger(l)}[\vec{p}] &= -G_{13}^{\dagger(l)}[\vec{p}] = -M^{l1}(2\pi)^2\delta(p_1)\delta(p_2). \end{aligned} \tag{5.25}$$

Substituting (5.25), (3.30), and (3.26) into (5.23), we obtain

$$\begin{aligned} &\frac{\partial u_j(x)}{\partial x_1} = M^{j1}I_0(x_3), \quad \frac{\partial u_j(x)}{\partial x_2} = M^{j2}I_0(x_3), \\ &\frac{\partial u_j(x)}{\partial x_3} = \left(-M^{31}\delta_{j1} - M^{32}\delta_{j2} - \frac{\lambda}{\lambda+2\mu}(M^{11}+M^{22})\delta_{j3}\right)I_0(x_3), \end{aligned} \tag{5.26}$$

where

$$I_0(x_3) = \frac{1}{2\pi}\int dp_3 \frac{i}{p_3} e^{ip_3x_3}. \tag{5.27}$$

Let us denote the stress tensor by σ_{ij}; σ_{ij} is the jth component of the force per unit area on a plane whose outward normal is parallel to the positive x_i direction. According to Hook's law, we have

$$\sigma_{ij} = \sum_{k,l} C_{ijkl}\frac{\partial u_k}{\partial x_l} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) + \lambda\delta_{ij}(\vec{\nabla}\cdot\vec{u}). \tag{5.28}$$

It is remarkable that the free surface condition, $\sigma_{i3} = 0$ ($i = 1, 2, 3$), is automatically satisfied as can be seen from (5.28) and (5.26). We impose the boundary condition for the integral $I_0(x_3)$ as follows:

$$I_0(x_3) = \lim_{\epsilon\to 0_+}\frac{1}{2\pi}\int dp_3\frac{i}{p_3+i\epsilon}e^{ip_3x_3} = \begin{cases} 0, & x_3 > 0 \\ 1, & x_3 \leq 0 \end{cases}. \tag{5.29}$$

Therefore, the displacement field $u_j(x)$ outside of the singularity at $x_3=0$ is given by

$$\vec{u}(x)=0 \quad \text{for } x_3>0, \tag{5.30a}$$

$$\vec{u}(x)=U\vec{x} \quad \text{for } x_3<0, \tag{5.30b}$$

where the matrix U is

$$U_{ij}=\begin{bmatrix} M^{11} & M^{12} & -M^{31} \\ M^{21} & M^{22} & -M^{32} \\ M^{31} & M^{32} & -\dfrac{\lambda}{\lambda+2\mu}(M^{11}+M^{22}) \end{bmatrix}. \tag{5.31}$$

If the displacement field $u_j(x)$ is expressed by an orthogonal matrix T_R as

$$\vec{u}(x)=0 \quad \text{for } x_3>0, \tag{5.32a}$$

$$\vec{u}(x)=(T_R-I)\vec{x} \quad \text{for } x_3<0, \tag{5.32b}$$

the grain in $x_3<0$ can be brought into the same orientation as the grain in $x_3>0$ by a pure rotation, that is, the grain in $x_3<0$ is the perfect crystal. However, it can be proved that $(I+U)$ is not an orthogonal matrix except for a trivial case $U=0$. Therefore there is always the expansion (or contraction) in addition to the rotation. As an example, consider the rotation around x_3 axis:

$$T_R=\begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{5.33}$$

The requirement (5.32b) at $x_3=0$ leads to $M^{11}=M^{22}=\cos\theta-1$, $M^{12}=-M^{21}=\sin\theta$, and $M^{31}=M^{32}=0$. From (5.30b) and (5.31), we have

$$\vec{u}(x)=(T_R-1)\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}-\frac{2\lambda}{\lambda+2\mu}(\cos\theta-1)\begin{pmatrix} 0 \\ 0 \\ x_3 \end{pmatrix},$$

implying that the expansion (or contraction) along the third axis is associated. There are two exceptional cases. First, when the rotation is infinitesimally small, deviation from the pure rotation is the second order of θ. Therefore, the displacement field can be approximated by pure rotation. Second, on the plane $x_3=ax_1+bx_2$, one can satisfy the relation (5.32b) by suitable choice of matrix M^{ij}. Specially, we can choose matrix M^{ij} such that the displacement near the surface is pure rotation. This is easily seen from the fact that the third column of the matrix U has no contribution at $x_3=0$. Now it is instructive to recall the derivation of Frank's formula (5.15). There, it is implicitly assumed that there is no expansion (or contraction) of the structure near the surface. The above discussion shows that this assumption is not quite general. Even when the assumption is satisfied, the effect of expansion (or contraction) manifests itself for large angle case or in the regions far from the surface. In our formalism for grain boundaries, proper choice of the matrix M^{ij} enables us to prepare a surface both with rotation and expansion (or contraction) components.

VI. POINT DEFECTS

In Sec. III, we have shown that a closed singularity in three-dimensional space is expressed by

$$G^{(\alpha)}_{\mu\nu}(x)=\sum_\beta M^{\alpha\beta}\iiiint d\tau\, d\sigma_1\, d\sigma_2\, d\eta \frac{\partial[y_\mu, y_\nu, y_\beta]}{\partial[\tau,\sigma_1,\sigma_2]}\rho(\eta) \times\delta^{(4)}(x-y(\tau,\sigma_1,\sigma_2,\eta)). \tag{6.1}$$

When $\rho(\eta)$ is of a finite range, the singular domain is confined in a finite domain of three-dimensional space. For example, the closed surface (3.24) is obtained by the choice of $\rho(\eta)=\delta(\eta-R)$, R being some constant. We now consider the static spherical objects;

$$y_\mu(\tau,\sigma_1,\sigma_2,\eta) =(\tau, \eta\sin\sigma_1\cos\sigma_2, \eta\sin\sigma_1\sin\sigma_2, \eta\cos\sigma_1), \quad 0\le\eta<\infty,\ 0\le\sigma_1<\pi,\ 0\le\sigma_2\le 2\pi. \tag{6.2}$$

Then, the nonvanishing components of $G^{(\alpha)}_{\mu\nu}(x)$ are

$$G^{(\alpha)}_{0i}(x)=\sum_\beta M^{\alpha\beta}\epsilon_{ik\beta}\frac{x_k}{r}\rho(r) =\sum_\beta M^{\alpha\beta}\epsilon_{ik\beta}\frac{\partial}{\partial x_k}\sigma(r), \tag{6.3}$$

where r means $|\vec{x}|=(x_1^2+x_2^2+x_3^2)^{1/2}$ and

$$\rho(r)=\frac{\partial}{\partial r}\sigma(r). \tag{6.4}$$

In the following discussions, we assume that $\rho(r)$ and $\sigma(r)$ are of finite range;

$$\rho(r)=\sigma(r)=0 \quad \text{for } r>R. \tag{6.5}$$

From (6.3) and (3.16), we have

$$G^{\dagger(\alpha)}_{lm}(x)=M^{\alpha l}\frac{x_m}{r}\rho(r)-M^{\alpha m}\frac{x_l}{r}\rho(r) =M^{\alpha l}\frac{\partial}{\partial x_m}\sigma(r)-M^{\alpha m}\frac{\partial}{\partial x_l}\sigma(r). \tag{6.6}$$

We regard a point defect as the macroscopic object (extended object) which has certain closed singularity in space. When use is made of the low-momentum approximation, the displacement fields around the point defect in an isotropic media are evaluated as follows. Substituting (6.6) into (3.24), we have

$$\frac{\partial u_j(x)}{\partial x_m} = -M^{jm}\sigma(r) + \frac{2(\lambda+\mu)}{\lambda+2\mu}\sum_l M^{lm}\frac{\partial}{\partial x_l}\frac{\partial}{\partial x_m}I(x) - \frac{\lambda+\mu}{\lambda+2\mu}\sum_{l,b} M^{lm}\frac{\partial}{\partial x_l}\frac{\partial^2}{\partial x_b^2}J_j(x)$$
$$-\frac{\partial}{\partial x_m}\left[\sum_b M^{jb}\frac{\partial}{\partial x_b}I(x) + \sum_l M^{lj}\frac{\partial}{\partial x_l}I(x) + \frac{\lambda}{\lambda+2\mu}\left(\sum_l M^{ll}\right)\frac{\partial}{\partial x_j}I(x) - \frac{\lambda+\mu}{\lambda+2\mu}\sum_{l,b}M^{lb}\frac{\partial}{\partial x_l}\frac{\partial}{\partial x_b}J_j(x)\right], \tag{6.7}$$

where

$$I(x) = \int \frac{d^3x'}{4\pi}\frac{1}{|\vec{x}-\vec{x}'|}\sigma(r'), \tag{6.8a}$$

$$J_j(x) = \int \frac{d^3x'}{4\pi}\frac{x_j - x_j'}{|\vec{x}-\vec{x}'|}\sigma(r'). \tag{6.8b}$$

In deriving (6.7), we used the relations

$$\frac{3(x_j-x_j')(x_l-x_l')(x_b-x_b')}{|\vec{x}-\vec{x}'|^5} = \frac{\partial}{\partial x_l}\frac{\partial}{\partial x_b}\frac{x_j-x_j'}{|\vec{x}-\vec{x}'|} + \frac{x_l-x_l'}{|\vec{x}-\vec{x}'|^3}\delta_{jb} + \frac{x_b-x_b'}{|\vec{x}-\vec{x}'|^3}\delta_{jl} + \frac{x_j-x_j'}{|\vec{x}-\vec{x}'|^3}\delta_{lb},$$

$$\sum_b \frac{\partial}{\partial x_b'}\left(\frac{x_b-x_b'}{|\vec{x}-\vec{x}'|^3}\right) = \sum_b \frac{\partial^2}{\partial^2 x_b'}\left(\frac{1}{|\vec{x}-\vec{x}'|}\right) = -4\pi\delta^{(3)}(\vec{x}-\vec{x}').$$

Hereafter we consider the case where singularity is on the sphere with radius R;

$$\sigma(r) = -\Theta(R-r), \quad \rho(r) = \delta(r-R). \tag{6.9}$$

When the formulas

$$\int d\Omega' \frac{1}{|\vec{x}-\vec{x}'|} = \begin{cases} 4\pi/r', & r'>r \\ 4\pi/r, & r'<r \end{cases}, \tag{6.10a}$$

$$\int d\Omega' \frac{x_j'}{|\vec{x}-\vec{x}'|} = \begin{cases} \frac{4}{3}\pi(x_j/r'), & r'>r \\ \frac{4}{3}\pi(x_j/r^3)r'^2, & r'<r \end{cases} \tag{6.10b}$$

are used, the integrals in (6.8) are found to be

$$I(x) = \begin{cases} -\frac{1}{3}R^3\frac{1}{r}, & r>R \\ -\frac{1}{2}R^2 + \frac{1}{6}r^2, & 0<r<R, \end{cases} \tag{6.11a}$$

$$J_j(x) = \begin{cases} -\frac{1}{3}(x_j/r)R^3 + \frac{1}{15}(x_j/r^3)R^5, & r>R \\ -\frac{1}{3}x_jR^2 + \frac{1}{15}x_jr^2, & 0<r<R. \end{cases} \tag{6.11b}$$

Substituting (6.11) into (6.7), we obtain

$$\frac{\partial u_j(x)}{\partial x_m} = M^{jm} - \frac{\partial}{\partial x_m}\left[\frac{3\lambda+8\mu}{15(\lambda+2\mu)}\left(\sum_l M^{lj}x_l + \sum_b M^{jb}x_b\right) + \frac{3\lambda-2\mu}{15(\lambda+2\mu)}\left(\sum_l M^{ll}\right)x_j\right] \quad \text{for } 0<r<R \tag{6.12a}$$

$$\frac{\partial u_j(x)}{\partial x_m} = -\frac{\partial}{\partial x_m}\left\{\frac{R^3}{3r^3}\left[\frac{\mu}{\lambda+2\mu}\left(\sum_l M^{lj}x_l + \sum_b M^{jb}x_b - x_j\sum_l M^{ll}\right)\right] + \frac{R^5}{5r^5}\left[\frac{\lambda+\mu}{\lambda+2\mu}\left(\sum_l M^{lj}x_l + \sum_b M^{jb}x_b + x_j\sum_l M^{ll}\right)\right]\right.$$
$$\left. - \frac{\lambda+\mu}{\lambda+2\mu}\left(-\frac{R^3}{r^5}+\frac{R^5}{r^7}\right)x_j\sum_{l,b}M^{lb}x_lx_b\right\} \quad \text{for } r>R. \tag{6.12b}$$

These results lead to the following expression for the displacement fields around the point defect;

$$u_j(x) = \frac{2}{15}\frac{6\lambda+11\mu}{\lambda+2\mu}\sum_b M^{jb}x_b - \frac{1}{15}\frac{3\lambda+8\mu}{\lambda+2\mu}\sum_l M^{lj}x_l - \frac{1}{15}\frac{3\lambda-2\mu}{\lambda+2\mu}\left(\sum_l M^{ll}\right)x_j, \quad 0<r<R, \tag{6.13a}$$

$$u_j(x) = -\frac{R^3}{3r^3}\frac{\mu}{\lambda+2\mu}\left(\sum_l M^{lj}x_l + \sum_b M^{jb}x_b - x_j\sum_l M^{ll}\right) - \frac{R^5}{5r^5}\frac{\lambda+\mu}{\lambda+2\mu}\left(\sum_l M^{lj}x_l + \sum_b M^{jb}x_b + x_j\sum_l M^{ll}\right)$$
$$-\frac{\lambda+\mu}{\lambda+2\mu}\left(\frac{R^3}{r^5}-\frac{R^5}{r^7}\right)x_j\sum_{l,b}M^{lb}x_lx_b, \quad r>R. \tag{6.13b}$$

The volume expansion (or contraction) evaluated on the sphere due to the point defect is given by

$$\Delta V = \int_{r>R} d\vec{S}\cdot\vec{u}(x). \tag{6.14}$$

Substituting (6.13b) into (6.14), we have

$$\Delta V = -\frac{4\pi}{9} R^3 \frac{3\lambda+2\mu}{\lambda+2\mu}\sum_l M^{ll}. \tag{6.15}$$

This constant does not depend on the radius of integral sphere as far as $r>R$.

According to (5.28) and (6.12), the stress tensor σ_{ij} is given by

$$\sigma_{ij} = \mu\left(\frac{9\lambda+14\mu}{15(\lambda+2\mu)}(M^{ij}+M^{ji}) + \frac{14\lambda+4\mu}{15(\lambda+2\mu)}\delta_{ij}\sum_l M^{ll}\right), \quad 0<r<R, \tag{6.16a}$$

$$\begin{aligned}\sigma_{ij} = {}&\mu\left(-\frac{\lambda}{\lambda+2\mu}\frac{R^3}{r^5} + 2\frac{\lambda+\mu}{\lambda+2\mu}\frac{R^5}{r^7}\right)\left[x_i\left(\sum_l M^{lj}x_l + \sum_b M^{jb}x_b\right) + x_j\left(\sum_l M^{li}x_l + \sum_b M^{ib}x_b\right)\right]\\ &+\mu\left(-\frac{\mu}{\lambda+2\mu}\frac{R^3}{r^5} + \frac{\lambda+\mu}{\lambda+2\mu}\frac{R^5}{r^7}\right)2x_ix_j\sum_l M^{ll} - \mu\left(\frac{\mu}{\lambda+2\mu}\frac{R^3}{3r^3} + \frac{\lambda+\mu}{\lambda+2\mu}\frac{R^5}{5r^5}\right)2(M^{ij}+M^{ji})\\ &+\mu\left(\frac{\mu-\lambda}{\lambda+2\mu}\frac{R^3}{3r^3} - \frac{\lambda+\mu}{\lambda+2\mu}\frac{R^5}{5r^5}\right)2\delta_{ij}\sum_l M^{ll} + \mu\frac{\lambda+\mu}{\lambda+2\mu}\left(\frac{5R^3}{r^7} - \frac{7R^5}{r^9}\right)2x_ix_j\sum_{l,b}M^{lb}x_lx_b\\ &+\mu\left(-\frac{\mu}{\lambda+2\mu}\frac{R^3}{r^5} + \frac{\lambda+\mu}{\lambda+2\mu}\frac{R^5}{r^7}\right)2\delta_{ij}\sum_{l,b}M^{lb}x_lx_b, \quad r>R.\end{aligned} \tag{6.16b}$$

The stress tensor σ_{ij} tends to zero as $r\to\infty$, which implies that no external pressure is needed to keep this point defect in crystal. We define σ_{rr} by

$$\sigma_{rr} = \sum_{i,j}\frac{x_i}{r}\sigma_{ij}\frac{x_j}{r}. \tag{6.17}$$

Since (6.16) and (6.17) lead to

$$\sigma_{rr} = \begin{cases} \mu\left(\frac{2}{15}\frac{9\lambda+14\mu}{\lambda+2\mu}\sum_{i,j}M^{ij}\frac{x_ix_j}{r^2} + \frac{2}{15}\frac{7\lambda+2\mu}{\lambda+2\mu}\sum_l M^{ll}\right), & 0<r<R, \quad (6.18a)\\ \mu\left(\frac{2}{3}\frac{9\lambda+10\mu}{\lambda+2\mu}\frac{R^3}{r^3} - \frac{24}{5}\frac{\lambda+\mu}{\lambda+2\mu}\frac{R^5}{r^5}\right)\sum_{i,j}M^{ij}\frac{x_ix_j}{r^2} + \mu\left(-\frac{2}{3}\frac{R^3}{r^3} + \frac{8}{5}\frac{\lambda+\mu}{\lambda+2\mu}\frac{R^5}{r^5}\right)\sum_l M^{ll}, & r>R \quad (6.18b)\end{cases}$$

we find that σ_{rr} changes continuously through the singular surface $r=R$. Unless the choice of M^{ij} is restricted, the stress σ_{rr} has certain angular dependence. When the angular dependence is averaged out, we obtain a simple relation between the volume expansion (or contraction) and the averaged stress:

$$\langle\sigma_{rr}\rangle_{r>R} \equiv \frac{1}{4\pi}\int_{r>R} d\Omega\,\sigma_{rr} = \frac{4\mu(3\lambda+2\mu)}{9(\lambda+2\mu)}\frac{R^3}{r^3}\sum_l M^{ll} = -\frac{\mu}{\pi r^3}\Delta V. \tag{6.19}$$

To simplify our discussion, let us choose diagonal M^{ij}:

$$M^{ij} = M\delta_{ij}. \tag{6.20}$$

Then, the displacement field $u_j(x)$, the volume expansion (or contraction) ΔV and stress tensors σ_{ij} and σ_{rr} have simple expressions as follows.

$$u_j(x) = \begin{cases} \frac{4}{3}\frac{\mu}{\lambda+2\mu}Mx_j, & 0<r<R \quad (6.21a)\\ -\frac{2\mu+3\lambda}{3(\lambda+2\mu)}M\frac{R^3}{r^3}x_j, & r>R, \quad (6.21b)\end{cases}$$

$$\Delta V = -\frac{2\mu+3\lambda}{\lambda+2\mu}M\frac{4\pi}{3}R^3, \tag{6.22}$$

$$\sigma_{ij} = \begin{cases} \frac{4}{3}\frac{\mu(2\mu+3\lambda)}{\lambda+2\mu}M\delta_{ij}, & 0<r<R \quad (6.23a)\\ 2\frac{\mu(2\mu+3\lambda)}{\lambda+2\mu}M\frac{R^3}{r^5}x_ix_j - \frac{2}{3}\frac{\mu(2\mu+3\lambda)}{\lambda+2\mu}M\frac{R^3}{r^3}\delta_{ij}, & r>R \quad (6.23b)\end{cases}$$

$$\sigma_{rr}=\begin{cases}\frac{4}{3}\frac{\mu(2\mu+3\lambda)}{\lambda+2\mu}M, & 0<r<R \quad (6.24a)\\ \frac{4}{3}\frac{\mu(2\mu+3\lambda)}{\lambda+2\mu}\frac{R^3}{r^3}, & r>R. \quad (6.24b)\end{cases}$$

In this case, $\vec{\nabla}\cdot\vec{u}(x)=0$ for $r>R$. Therefore, ΔV does not depend on the choice of integral surface as far as integral surface does not cross the singularity at $r=R$. In other words, ΔV is a topological constant.[4] The strain energy density w is

$$w=\frac{1}{2}\sum_{i,j,k,l}C_{ijkl}\frac{\partial u_i}{\partial x_j}\frac{\partial u_k}{\partial x_l}=\frac{1}{2}\sum_{i,j}\sigma_{ij}\frac{\partial u_i}{\partial x_j}. \qquad (6.25)$$

Making use of (6.21) and (6.23) in (6.25), we get

$$w=\begin{cases}\frac{8}{3}\frac{\mu^2(2\mu+3\lambda)}{(\lambda+2\mu)^2}M^2, & 0<r<R \quad (6.26a)\\ \frac{2}{3}\frac{\mu(2\mu+3\lambda)^2}{(\lambda+2\mu)^2}M^2\frac{R^6}{r^6}, & r>R. \quad (6.26b)\end{cases}$$

Therefore, the total strain energy W is

$$W=\int w(x)\,d^3x=2\mu\frac{2\mu+3\lambda}{\lambda+2\mu}M^2\frac{4\pi}{3}R^3. \qquad (6.27)$$

It is reasonable to expect that the volume expansion (or contraction) due to the point defect is the order of the unit cell volume per atom. Therefore when we roughly take $R\approx a$ (a; lattice constant) we find from (6.22) that M is of the order of 1. Typical values of λ and μ are known to be order of 10^{12} dyn/cm^2. Then, the total strain energy is roughly 1 eV, which agrees qualitatively with the energy for the formation of a lattice vacancy.[11]

VII. SURFACE WAVES

In Sec. V we have presented a new theory of grain boundaries, where grain boundary is treated as an extended object with surface singularity created by the boson condensation of phonons. In this section, we shall apply the theory to the problem of surface waves. In particular, we shall show explicitly that the dispersion relations of surface waves in isotropic media is obtained by considering the oscillating surface singularity with free surface condition.

In terms of Fourier transforms, the displacement field $u_j(x)$ with topological singularity is expressed as

$$\partial_\nu u_j(x)=\sum_{k,l}\sum_{\lambda,\rho}\int\frac{d^4p}{(2\pi)^4}\Delta_{jk}[p]C_{kl}^{\lambda\rho}(p)ip_\lambda G_{\rho\nu}^{\dagger(l)}[p]e^{ipx}. \qquad (7.1)$$

Here $px=-p_0t+\vec{p}\cdot\vec{x}$, and $\Delta_{jk}[p]$ and $G_{\rho\nu}^{\dagger(l)}[p]$ are the Fourier transforms of the Green's function $\Delta_{jk}(x)$ and $G_{\rho\nu}^{\dagger(l)}(x)$, respectively. In order to compare our theory with the conventional one,[12] we shall employ the low-momentum approximation and isotropic approximation. Thus, we shall use (3.27) and (3.29) for $C_{kl}^{\lambda\rho}(p)$ and $\Delta_{jk}[p]$.

Let us consider an oscillating plane surface singularity given by

$$G_{\lambda\rho}^{(\alpha)}(x)=M^{\alpha\mu}\iiint d\tau\,d\sigma_1\,d\sigma_2\frac{\partial[y_\lambda,y_\rho,y_\mu]}{\partial[\tau,\sigma_1,\sigma_2]}\times\delta^{(4)}(x-y(\tau,\sigma_1,\sigma_2)), \qquad (7.2)$$

with

$$y_0(\tau,\sigma_1,\sigma_2)=\tau,\quad y_1(\tau,\sigma_1,\sigma_2)=\sigma_1,$$
$$y_2(\tau,\sigma_1,\sigma_2)=\sigma_2,\quad y_3(\tau,\sigma_1,\sigma_2)=A\,\mathrm{Re}(e^{i\xi}), \qquad (7.3)$$

where Re means the real part of the quantity and $\xi=q\sigma_1-\omega\tau$. Then, we have

$$G_{\mu\nu}^{(\alpha)}(x)=\epsilon_{\mu\nu\rho\lambda}M^{\alpha\rho}\frac{\partial}{\partial x_\lambda}\Theta(x_3-A\cos\eta), \qquad (7.4)$$

$$G_{\mu\nu}^{\dagger(\alpha)}(x)=M_\mu^\alpha\frac{\partial}{\partial x^\nu}\Theta(x_3-A\cos\eta)-M_\nu^\alpha\frac{\partial}{\partial x^\mu}\Theta(x_3-A\cos\eta), \qquad (7.5)$$

where $\eta=qx_1-\omega t$. For the subsequent discussions, we expand $G_{\mu\nu}^{\dagger(\alpha)}$ in power series of A;

$$G_{\mu\nu}^{\dagger(\alpha)}(x)=H_{\mu\nu}^{(\alpha)}(x)+A\,K_{\mu\nu}^{(\alpha)}(x)+\cdots, \qquad (7.6)$$

$$H_{\mu\nu}^{(\alpha)}(x)=(M_\mu^\alpha\delta_{\nu3}-M_\nu^\alpha\delta_{\mu3})\delta(x_3), \qquad (7.7)$$

$$K_{\mu\nu}^{(\alpha)}(x)=-\left(M_\mu^\alpha\frac{\partial}{\partial x^\nu}-M_\nu^\alpha\frac{\partial}{\partial x^\mu}\right)\mathrm{Re}(e^{i\eta})\delta(x_3). \qquad (7.8)$$

First let us consider only the zeroth order with respect to A. The static condition $\dot{u}(x)=0$ for $A=0$, leads to $M^{\alpha0}=0$. Then, (7.7) is the same as (5.22). In Sec. V, we already evaluated the displacement field, (5.26) with (5.27), and the stress tensor, (5.28). There we have observed that the free-surface conditions, $\sigma_{i3}=0$ $(i=1,2,3)$, are satisfied. In order to study the surface wave only, we require that $u_j(x)=0$ for $A=0$. We therefore take M^{12}, M^{21}, M^{31}, M^{32}, M^{11}, and M^{22} are zero, hereafter.

Let us now turn our attention to the first order terms of A. The nonvanishing components of $K_{\mu\nu}^{(l)}[p]$, the Fourier transform of $K_{\mu\nu}^{(l)}(x)$, are

$$K_{03}^{(l)}[p]=-K_{30}^{(l)}[p]=i(2\pi)^3M^{\alpha3}\omega\,\delta(p_0-\omega)\delta(p_1-q)\delta(p_2), \qquad (7.9a)$$

$$K_{13}^{(l)}[p]=-K_{31}^{(l)}[p]=i(2\pi)^3M^{\alpha3}q\,\delta(p_0-\omega)\delta(p_1-q)\delta(p_2). \qquad (7.9b)$$

Substituting (7.9a) and (7.9b) into (7.1) and using (3.28), we obtain

$$\frac{\partial u_j}{\partial x_1}=\mathrm{Re}\Big(-iA\sum_{k,l}\sum_{a}C^{a3}_{kl}M^{l3}\frac{q}{\rho_0}\frac{\partial}{\partial x_a}\times[I_1(x)\delta_{jk}+J_{jk}(x)]\Big), \tag{7.10a}$$

$$\frac{\partial u_j}{\partial x_2}=0, \tag{7.10b}$$

$$\frac{\partial u_j}{\partial x_3}=\mathrm{Re}\Big(A\sum_{l}\omega^2M^{l3}[I_1(x)\delta_{jl}+J_{jl}(x)]+iA\sum_{k,l}\sum_{a}C^{a1}_{kl}M^{l3}\frac{q}{\rho_0}\times\frac{\partial}{\partial x_a}[I_1(x)\delta_{jk}+J_{jk}]\Big), \tag{7.10c}$$

$$\frac{\partial u_j}{\partial x_0}=-\frac{\partial u_j(x)}{\partial t}=-\frac{\omega}{q}\frac{\partial u_j}{\partial x_1}, \tag{7.10d}$$

where

$$I_1(x)\equiv\int\frac{d^4p}{2\pi}\frac{1}{p_0^2-v_t^2|\vec{p}|^2}\delta(p_0-\omega)\delta(p_1-q)\delta(p_2)e^{ipx}=-\frac{1}{2K_tv_t^2}e^{K_tx_3}e^{i\eta}, \tag{7.11a}$$

$$J_{jk}(x)\equiv(v_l^2-v_t^2)\int\frac{d^4p}{2\pi}\frac{p_jp_k\delta(p_0-\omega)\delta(p_1-q)\delta(p_2)}{(p_0^2-v_t^2|\vec{p}|^2)(p_0^2-v_l^2|\vec{p}|^2)}e^{ipx}=\frac{1}{2\omega^2}\Big(\frac{1}{K_t}(q\delta_{j1}-iK_t\delta_{j3})(q\delta_{k1}-iK_t\delta_{k3})e^{K_tx_3}-\frac{1}{K_l}(q\delta_{j1}-iK_l\delta_{j3})(q\delta_{k1}-iK_l\delta_{k3})e^{K_lx_3}\Big)e^{i\eta}. \tag{7.11b}$$

The calculations of $I_1(x)$ and $J_{jk}(x)$ are conditioned by the requirements $I_1(x)\to 0$ and $J_{jk}(x)\to 0$ as $x_3=-\infty$, and we used the notations

$$K_t^2=q^2-\omega^2/v_t^2, \tag{7.12a}$$

$$K_l^2=q^2-\omega^2/v_l^2. \tag{7.12b}$$

We require that the surface given by $x_3=0$ is a free surface. The free-surface conditions, $\sigma_{i3}=0$ ($i=1,2,3$) at $x_3=0$, with (7.10a)–(7.10d) yield

$$\begin{pmatrix}(q^2+K_t^2)^2-4K_tK_lq^2 & 0 & 0\\ 0 & v_t^2K_t^2 & 0\\ 0 & 0 & (q^2+K_t^2)^2-4K_tK_lq^2\end{pmatrix}\begin{pmatrix}M^{13}\\ M^{23}\\ M^{33}\end{pmatrix}=0. \tag{7.13}$$

The first, second, and third rows in (7.13) correspond to the conditions $\sigma_{13}=0$, $\sigma_{23}=0$, and $\sigma_{33}=0$. The conditions for a nontrivial solution are

$$(q^2+K_t^2)^2=4K_tK_lq^2, \tag{7.14a}$$

$$M^{23}=0. \tag{7.14b}$$

When these conditions are satisfied, a surface wave exists. Eliminating K_t and K_l from (7.14a), we find that the dispersion relation for the surface wave is

$$\omega=qv_t\alpha. \tag{7.15}$$

Here α is given by

$$\alpha^6-8\alpha^4+8\alpha^2\Big[3-2\Big(\frac{v_t}{v_l}\Big)^2\Big]-16\Big[1-\Big(\frac{v_t}{v_l}\Big)^2\Big]=0. \tag{7.16}$$

Formula (7.15) with (7.16) is the well-known result for surface wave first investigated by Lord Rayleigh.[13]

In the derivation of the dispersion relation (7.15), the condition $0<\alpha^2<1$ was assumed [see (7.12)]. We can show that (7.16) has always a pair of real solutions α and $-\alpha$ satisfying $0<\alpha^2<1$. To prove this, let us first set

$$f(y)=y^3-8y^2+8y\Big[3-2\Big(\frac{v_t}{v_l}\Big)^2\Big]-16\Big[1-\Big(\frac{v_t}{v_l}\Big)^2\Big]. \tag{7.17}$$

Here $y\equiv\alpha^2$. Since $(v_t/v_l)^2=\mu/(\lambda+2\mu)$, the quantity $(v_t/v_l)^2$ takes the value between 0 and $\frac{1}{2}$,

$$0<(v_t/v_l)^2<\tfrac{1}{2}. \tag{7.18}$$

It is readily seen that

$$f(0)=-16[1-(v_t/v_l)^2]<1, \tag{7.19a}$$

$$f(1)=1>0, \tag{7.19b}$$

and, for $0<y<1$,

$$f'(y)=3y^2+16(1-y)+8[1-2(v_t/v_l)^2]>0. \tag{7.20}$$

The relations (7.20) and (7.21) imply that $f(y)=0$ for certain y ($0<y<1$). Therefore, we conclude that there exists a surface wave whose phase velocity is always slower than transverse and longitudinal bulk sound waves.

It is instructive to summarize the differences between our method of derivation of the surface wave with the conventional one.

(i) In our method, while $\partial_\nu u_j(x)$ is single valued, $u_j(x)$ is not single valued. Therefore, $u_j(x)$ cannot be expressed in the form of Fourier transformation. However, in the conventional method, the single valuedness of $u_j(x)$ is assumed and $u_j(x)$ is the sum of a plane wave.

(ii) In the conventional method, the transverse and longitudinal components are superposed to satisfy the free-surface condition. The relations obtained from the free-surface condition are expressed in terms of the transverse and longitudinal components, and diagonalization process is necessary in the derivation of the dispersion relation. On the other hand, in our method, the free surface conditions $\sigma_{13}=0$ and $\sigma_{23}=0$ independently lead to the dispersion relation as can be seen from (7.13).

Although we have considered only a linear surface wave, the nonlinear properties of surface waves can be easily taken into account. When the complete form of (7.5) is used in the evaluation of (7.1) and the free-surface condition on the oscillating surface $x_3=A\cos(qx-\omega t)$ is imposed, certain self-consistent relations among ω, q, and A are obtained. These relations lead to a nonlinear dispersion relation for the surface wave.

We remark that our theory of surface wave can be applied to other physical systems, such as surface magnons, surface properties of superconductor, and surface excitations of "bag" in relativistic field theory.

VIII. CONCLUDING REMARKS

In this paper we have presented a general theory of extended objects in crystals. As examples, dislocations, grain boundaries, point defects, and surface waves were studied in detail. Besides the general discussions, we have employed the low-momentum approximation and the isotropic approximation to evaluate the physical quantities associated with the extended objects. The motivation for using these approximations is to compare our results with those obtained by the conventional method. In the following we briefly show how we can improve the existing phenomenological theory which is essentially based on the classical theory of elasticity.

For this purpose, we expand P_i^u, T_{ij}^u, and n^u in powers of $\vec{u}$;

$$P_i^u(x)=P_i^{(1)}+P_i^{(2)}+\cdots, \tag{8.1a}$$

$$T_{ij}^u(x)=T_{ij}^{(1)}+T_{ij}^{(2)}+\cdots, \tag{8.1b}$$

$$n^u(x)=v(\vec{x})+n^{(1)}(x)+n^{(2)}(x)+\cdots. \tag{8.1c}$$

We then obtain from (2.53), (2.54), and (2.55)

$$P_i^{(1)}(x)=-\sum_j \rho_{ij}(-i\vec{\nabla})\dot{u}_j(x) +\sum_{\lambda\neq-1}\sum_{j,k}\varphi_\lambda(\vec{x})\gamma_{i\lambda k}(-i\vec{\nabla})\eta_{kj}(-i\vec{\nabla})\dot{u}_j(x), \tag{8.2a}$$

$$T_{ij}^{(1)}(x)=\sum_{k,l}C_{jl}^{ik}(-i\vec{\nabla})\nabla_k u_l(x) +\sum_{\lambda\neq-1}\sum_{k,l}\varphi_\lambda(\vec{x})\Gamma_{ij\lambda}^k(-i\vec{\nabla})\eta_{kl}(-i\vec{\nabla})u_l(x), \tag{8.2b}$$

$$n^{(1)}(x)=\frac{1}{M}\sum_{i,j}\nabla_i\rho_{ij}(-i\vec{\nabla})\dot{u}_j(x) +\sum_{\lambda\neq-1}\sum_{i,j}\varphi_\lambda(\vec{x})\gamma_{\lambda i}(-i\vec{\nabla})\eta_{ij}(-i\vec{\nabla})u_j(x). \tag{8.2c}$$

These quantities are called the linear momentum, stress, and density, respectively, while the quantities with superscript (2) are called the bilinear momentum, stress, and density, respectively.

The continuity equations (2.35) and (2.37) now hold among quantities with the same powers of $\vec{u}$:

$$\frac{\partial}{\partial t}n^{(i)}(x)+\frac{1}{M}\vec{\nabla}\cdot\vec{P}^{(i)}(x)=0, \tag{8.3a}$$

$$\frac{\partial}{\partial t}P_i^{(i)}(x)+\sum_j\nabla_j T_{ji}^{(i)}(x)=0, \tag{8.3b}$$

for $i=1,2,\ldots$. The relations (8.3) with (8.2) give

$$\gamma_{\lambda k}(-i\vec{\nabla})=-\frac{1}{M}\sum_i\left(\nabla_i\gamma_{i\lambda k}(-i\vec{\nabla}) +\sum_{\lambda'\neq-1}a_{\lambda\lambda'}^i\gamma_{i\lambda' k}(-i\vec{\nabla})\right), \tag{8.4a}$$

$$\gamma_{i\lambda k}(-i\vec{\nabla})=\sum_{j,l}\left(\nabla_j\Gamma_{ji\lambda}^l(-i\vec{\nabla}) +\sum_{\lambda'\neq-1}a_{\lambda\lambda'}^j\Gamma_{ji\lambda'}^l(-i\vec{\nabla})\right)\omega_{lk}^{-2}(-i\vec{\nabla}), \tag{8.4b}$$

where $\Omega a_{\lambda\lambda'}^i=\int_\Omega d^3x\,\varphi_\lambda(\vec{x})\nabla_i\varphi_{\lambda'}(\vec{x})$. The above relations indicate that $\gamma_{k\lambda}$ and $\gamma_{i\lambda k}$ are determined by $\Gamma_{ji\lambda}^l$.

The body force per unit volume is denoted by $\vec{F}$ which is equal to the time change of the linear momentum

$$\vec{F}(x)=-\frac{\partial}{\partial t}\vec{P}^{(1)}(x). \tag{8.5}$$

Hence, (8.3b) gives

$$F_i(x)=+\sum_j\nabla_j T_{ji}^{(1)}(x). \tag{8.6}$$

The usual phenomenological theory of elasticity can be reproduced in our method under the following assumptions.

(a) All the higher terms indicated by dots in (8.1) are neglected.

(b) Terms containing the periodic functions in $\vec{P}^{(1)}$, $T_{ij}^{(1)}$, and $n^{(1)}$ in (8.2) are disregarded.

(c) The bilinear momentum and stress are approximated by the energy-momentum tensor of the free field.

(d) The momentum dependences of the effective density $\rho_{ij}(\vec{k})$ and the elastic constants $C_{il}^{jm}(\vec{k})$ are neglected.

Under the assumptions (a), (b), and (c), we have

$$P_i^{(1)}(x) = -\sum_j \rho_{ij}(-i\vec{\nabla})\dot{u}_j(x), \tag{8.7a}$$

$$T_{ij}^{(1)}(x) = \sum_{l,m} C_{jl}^{im}(-i\vec{\nabla})\nabla_m u_l(x), \tag{8.7b}$$

$$n^{(1)}(x) = \frac{1}{M}\sum_{i,j}\rho_{ij}(-i\vec{\nabla})\nabla_i u_j(x), \tag{8.7c}$$

and

$$P_i^{(2)}(x) = -\sum_{k,l}\rho_{kl}(-i\vec{\nabla})\dot{u}_l(x)\partial_i u_k(x), \tag{8.8a}$$

$$T_{ij}^{(2)}(x) = \left(w(x) - \frac{1}{2}\sum_{k,l}\dot{u}_k(x)\rho_{kl}(-i\vec{\nabla})\dot{u}_l(x)\right)\delta_{ij} + \sum_l T_{jl}^{(1)}(x)\nabla_i u_l(x), \tag{8.8b}$$

$$T_{0i}^{(2)}(x) = \sum_j T_{ij}^{(1)}(x)\dot{u}_j(x), \tag{8.8c}$$

$$\epsilon(x) \equiv T_{00}^{(2)}(x) = \frac{1}{2}\sum_{i,j}\dot{u}_i(x)\rho_{ij}(-i\vec{\nabla})\dot{u}_j(x) + w(x), \tag{8.8d}$$

where

$$w(x) = \frac{1}{2}\sum_{i,j}\sum_{l,m}\epsilon_{il}(x)C_{ij}^{lm}(-i\vec{\nabla})\epsilon_{mj}(x). \tag{8.9}$$

Equations (8.8) are derived from the energy-momentum tensor of the free field with the Lagrangian

$$\mathcal{L}_u(x) = \frac{1}{2}\sum_{i,j}\dot{u}_i(x)\rho_{ij}(-i\vec{\nabla})\dot{u}_j(x) - w(x). \tag{8.10}$$

Note that continuity relations are satisfied:

$$\frac{\partial}{\partial t}n^{(1)}(x) + \frac{1}{M}\vec{\nabla}\cdot\vec{P}^{(1)}(x) = 0, \tag{8.11a}$$

$$\frac{\partial}{\partial t}P_i^{(1)}(x) + \sum_j \nabla_j T_{ji}^{(1)}(x) = 0, \tag{8.11b}$$

$$\frac{\partial}{\partial t}P_i^{(2)}(x) + \sum_j \nabla_j T_{ji}^{(2)}(x) = 0, \tag{8.11c}$$

$$\frac{\partial}{\partial t}\epsilon(x) + \sum_{i,j}\nabla_i[T_{ij}^{(1)}(x)\dot{u}_j(x)] = 0. \tag{8.11d}$$

We point out that the energy density (8.8d) agrees with (2.51). The body force per unit volume, $\vec{F}(x)$, can be calculated by means of (8.6) and (8.7b) as

$$F_i(x) = \sum_j\sum_{l,m} C_{il}^{jm}(-i\vec{\nabla})\nabla_j\nabla_m u_l(x). \tag{8.12}$$

Thus, all the equations agree with the usual macroscopic theory of a material (theory of elasticity) provided that we further adopt the low-momentum approximation (d) in which the effective density $\rho_{ij}(-i\vec{\nabla})$ and the elastic constants $C_{il}^{jm}(-i\vec{\nabla})$ are replaced by $\rho_{ij}(0)$ and $C_{il}^{jm}(0)$, respectively. Obviously, at the low-momentum approximation, the relation (8.7b) gives Hooke's law.

Our argument suggests how the phenomenological theory can be improved. When the Lagrangian is specified, quantities such as $\eta_{ij}(\vec{k})$, $\rho_{ij}(\vec{k})$, $C_{ij}^{lm}(\vec{k})$, and $\Gamma_{ji\lambda}^{l}(\vec{k})$ can be calculated, for instance, by means of the Bethe-Salpeter equation. The calculation of the higher-order terms in (8.1) can be performed by means of the Feynman-diagram method. Furthermore, the effects of the crystal structure are taken into account through the expansion in terms of the orthonormal set $\{\varphi_\lambda(x)\}$, as it is seen in (8.2). These improvements in our theory will determine the detailed structure of extended objects in crystals, for example, the so-called core structure of the dislocation.

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