Elastic Green's Function for Anisotropic Cubic Crystals*

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The Green's function describing the elastic displacement due to a unit force in an infinite cubic material is investigated in detail. Only for special cases can an exact solution be given, i.e., for $c_{11}-c_{12}-2c_{44}=0$ (isotropy), for $c_{12}+c_{44}=0$, and for ⟨100⟩ directions. Perturbation theory is applied to the cases where these conditions are only approximately fulfilled. Divergencies or strong maxima of the Greens' function, occurring in nearly unstable materials for $c_{11}-c_{12}\to 0$ or $c_{44}\to 0$, are examined. Analytical approximations for the Green's function are given by fitting the exact known Fourier transform with a suitably chosen ansatz in certain directions. Other simple approximations are derived by variational techniques and give good results for crystals with small and medium anisotropy.

I. INTRODUCTION

THE problem of determining the displacement field in an infinite elastic medium due to a point force, which is normally called the fundamental integral or the elastic Green's function, has a long history. In 1846, Thompson first gave the solution for the case of an isotropic solid.[1] Then, in 1900, Fredholm gave an implicit expression for the more general anisotropic case.[2] Unfortunately, analytical expressions can only be given for hexagonal crystals, which have been evaluated by Lifshitz and Rozentsveig[3] and Kröner.[4]

Therefore, some effort has been made in the past to get approximate solutions of the problem.[3,5,6] For weakly anisotropic cubic crystals, Lifshitz and Rozentsveig[3] and Leibfried[6] applied perturbation theory with respect to the anisotropy, but unfortunately only a few substances such as W, Al, and diamond show a weak anisotropy (see Fig. 2). Recently, the problem has been reconsidered.[7–9] Using Fredholm's formula, Mann *et al.*[8] made a point-by-point computer calculation of the Green's function and gave an expansion in spherical harmonics (for Cu). A similar calculation has been done by Lie and Koehler[9] for Al, Cu, and Li. For better convergence, the results are expanded into Fourier series. Despite these very accurate computer calculations for specific crystals, there is still a need for analytical expressions in terms of the elastic constants. Such expressions would be very useful to obtain a survey for the anisotropy behavior of different crystals, to evaluate displacement fields and interaction energies of point defects, dislocation arrangements, etc. The purpose of this paper is to derive such analytical approximations.

II. GENERAL EQUATIONS FOR ELASTIC GREEN'S FUNCTION

The Green's function[3,4,7,9] $G_{ij}(\mathbf{r},\mathbf{r}')$ of an infinite elastic medium is defined as the displacement at point $\mathbf{r}$ in the direction i due to a unit force $f_k(\mathbf{r})=\delta_{kj}\delta(\mathbf{r}-\mathbf{r}')$ at point $\mathbf{r}'$ in the direction j. It is determined by the elastic equations

$$C_{ijkl}\partial_{r_j}\partial_{r_l}G_{km}(\mathbf{r},\mathbf{r}')+\delta_{im}\delta(\mathbf{r}-\mathbf{r}')=0, \tag{1}$$

and the boundary condition $G_{km}(\mathbf{r}\to\infty)=0$. Here, C_{ijkl} is the tensor of elasticity ($C_{ijkl}=C_{jikl}=C_{klij}$). Because of the translational invariance and the symmetry of C_{ijkl}, the Green's function satisfies the relations

$$G_{ij}(\mathbf{r},\mathbf{r})=G_{ij}(\mathbf{r}-\mathbf{r}')=G_{ji}(\mathbf{r}-\mathbf{r}')=G_{ij}(\mathbf{r}'-\mathbf{r}). \tag{2}$$

The Fourier transform $\tilde{G}_{ij}(\mathbf{k})$ of $G_{ij}(\mathbf{r})$ defined by

$$G_{ij}(\mathbf{r})=\int [d\mathbf{k}/(2\pi)^3]e^{i\mathbf{k}\cdot\mathbf{r}}\tilde{G}_{ij}(\mathbf{k}) \tag{3}$$

is simply obtained from (1):

$$T_{ik}(\mathbf{k})\tilde{G}_{km}(\mathbf{k})=\delta_{im} \quad \text{or} \quad \tilde{G}_{ij}(\mathbf{k})=T^{-1}{}_{ij}(\mathbf{k}), \tag{4}$$

with

$$T_{ik}(\mathbf{k})=C_{ijkl}k_jk_l=T_{ki}(\mathbf{k})=T_{ik}(-\mathbf{k}). \tag{5}$$

Introducing a unit vector $\boldsymbol{\kappa}$ in the direction of $\mathbf{k}=k\boldsymbol{\kappa}$, we can write

$$T_{ik}(\boldsymbol{\kappa})=k^2C_{ijkl}\kappa_j\kappa_l=k^2t_{ik}(\boldsymbol{\kappa})$$

and

$$\tilde{G}_{ij}(\mathbf{k})=k^{-2}\tilde{g}_{ij}(\boldsymbol{\kappa}), \quad \boldsymbol{\kappa}^2=1, \tag{6}$$

where $t_{ik}(\boldsymbol{\kappa})$ and $\tilde{g}_{ij}(\boldsymbol{\kappa})$ depend only on the direction $\boldsymbol{\kappa}$. Instead of (4), we then get

$$t_{ik}(\boldsymbol{\kappa})\tilde{g}_{km}(\boldsymbol{\kappa})=\delta_{im} \quad \text{or} \quad \tilde{g}_{ij}(\boldsymbol{\kappa})=t^{-1}{}_{ij}(\boldsymbol{\kappa})=\Delta_{ij}(\boldsymbol{\kappa})/\Delta(\boldsymbol{\kappa}), \tag{7}$$

where $\Delta(\boldsymbol{\kappa})$ is the determinant $|t_{ij}(\boldsymbol{\kappa})|$, being of 6th order in κ, and $\Delta_{ij}(\boldsymbol{\kappa})$ are the appropriate subdeterminants, being of 4th order in κ.

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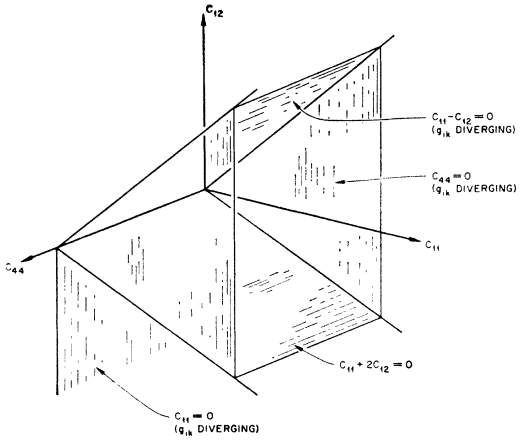

FIG. 1. $\{c_{11},c_{12},c_{44}\}$ coordinate system showing the stable wedge-shaped region.

With the unit vector ϱ in the direction of $\mathbf{r}=r\varrho$, we get from (3),

$$G_{ij}(\mathbf{r})=(4\pi r)^{-1}g_{ij}(\varrho)\,,\quad \varrho^2=1 \tag{8}$$

where $g_{ij}(\varrho)$ is only an angular function. By performing the radial integration in (3) we get a direct angular transformation between the functions $\tilde{g}_{ij}(\kappa)$ and $g_{ij}(\varrho)$:

$$g_{ij}(\varrho)=\int\frac{d\Omega_\kappa}{2\pi}\delta(\varrho\ \kappa)\tilde{g}_{ij}(\kappa)=\int_{\kappa\perp\rho}\frac{d\phi_\kappa}{2\pi}\frac{\Delta_{ij}(\kappa)}{\Delta(\kappa)}. \tag{9}$$

The back transformation (P = principal value) is

$$\tilde{g}_{ij}(\kappa)=\int(d\Omega_\rho/2\pi)\{\tfrac{1}{2}\partial_{(\kappa\cdot\rho)}P(1/\kappa\cdot\varrho)\}g_{ij}(\kappa). \tag{10}$$

Equation (9) is a line integral along the intersection of the plane $\kappa\cdot\varrho=0$ with the unit sphere $\kappa^2=1$ and ϕ_κ is the azimuth in that plane. Introducing polar coordinates Θ and Φ for $\varrho=(\sin\Theta\cos\Phi,\sin\Theta\sin\Phi,\cos\Theta)$ and counting ϕ_κ from the intersection of the $\rho_1-\rho_2$ plane with the plane $\kappa\cdot\varrho=0$, we have

$$\begin{aligned}\kappa_1&=\cos\phi_\kappa\sin\Phi+\sin\phi_\kappa\cos\Theta\cos\Phi,\\ \kappa_2&=-\cos\phi_\kappa\cos\Phi+\sin\phi_\kappa\cos\Theta\sin\Phi,\\ \kappa_3&=\sin\phi_\kappa\sin\Theta.\end{aligned} \tag{11}$$

By the substitution $Z=\tan\phi_\kappa$, the integral (9) can be transformed into a line integral $-\infty\leq Z\leq\infty$ [3] which can be evaluated. Following Lifshitz and Rozentsveig, we set $\kappa_i=\cos\phi_\kappa\ a_i(Z)$ with $a_1(Z)=\sin\Phi+Z\cos\Theta\cos\Phi$; $a_2(Z)=-\cos\Phi+Z\cos\Theta\cos\Phi$; $a_3(Z)=Z\sin\Theta$; and $\Delta(\kappa)=\cos^6\phi_\kappa\cdot F(Z)$ and $\Delta_{ik}(\kappa)=\cos^4\phi_\kappa\ F_{ik}(Z)$, where $F(Z)=\mathrm{Det}|C_{ijkl}a_j(Z)a_l(Z)|$ and of 6th order in Z. Then we have:

$$g_{ik}(\varrho)=\frac{1}{\pi}\int_{-\infty}^{\infty}dZ\frac{F_{ik}(Z)}{F(Z)}=2i\sum_{\alpha=1}^{3}\frac{F_{ik}(Z_\alpha)}{\partial_{Z_\alpha}F(Z_\alpha)}. \tag{12}$$

Here Z_α are the three roots of the 6th order algebraic equation $F(Z)=0$ which lie in the upper half plane and, for simplicity, are supposed to be simple roots.

The very simple result (12), known as Fredholm's formula,[1] is only of practical use if the roots of $F(Z)=0$ are elementary. This is the case only for hexagonal crystals, where $\Delta(\kappa)=0=F(Z)$ factorizes into three quadratic equations and where the Green's function is therefore elementary.[3,4]

III. GREEN'S FUNCTION FOR CUBIC CRYSTALS

The elasticity tensor for cubic crystals is

$$C_{ijkl}=c_{12}\delta_{ij}\delta_{kl}+c_{44}(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk})+d\delta_{ijkl}\,, \tag{13}$$

with

$$d=c_{11}-c_{12}-2c_{44}\quad\text{and}\quad\delta_{ijkl}=\sum_{s=1}^{3}e_i^{(s)}e_j^{(s)}e_k^{(s)}e_l^{(s)}.$$

Here $\mathbf{e}^{(1)}$, $\mathbf{e}^{(2)}$, $\mathbf{e}^{(3)}$ are the unit vectors of the cubic system. In the following, the coordinate system will always coincide with the cubic system. Then we have $\delta_{ijkl}=1$ if $i=j=k=l$ or $\delta_{ijkl}=0$ otherwise. The values of the elastic constants c_{11}, c_{12}, and c_{44} are restricted by the stability condition, i.e., the energy density

$$\begin{aligned}&\tfrac{1}{2}C_{ijkl}\epsilon_{ij}\epsilon_{kl}>0\quad\text{or}\\ &c_{44}>0,\quad c_{11}-c_{12}>0,\quad c_{11}+2c_{12}>0.\end{aligned} \tag{14}$$

To illustrate this, we have drawn in Fig. 1 a coordinate system with c_{44}, c_{11}, and c_{12} as coordinate axes. The elastic constants of all stable solids lie within the wedge-shaped space which is enclosed by the planes $c_{44}=0$, $c_{11}-c_{12}=0$, and $c_{11}+2c_{12}=0$. To give an example of what combinations of the elastic constants are actually realized in nature, we have plotted c_{12}/c_{44} over c_{11}/c_{44} in Fig. 2 and have marked the values for some cubic crystals with points. All isotropic materials lie on the line $c_{11}-c_{12}-2c_{44}=0$. It is seen that only a few cubic crystals such as W, diamond, and Al are isotropic or nearly isotropic.

From (13) we get for $t_{ik}(\kappa)$:

$$t_{ik}(\kappa)=c_{44}\delta_{ik}+(c_{44}+c_{12})\kappa_i\kappa_k+d\kappa_{(i)}{}^2\delta_{ik}. \tag{15}$$

(The summation convention will not be applied to indices in brackets.) The eigenvalues τ_α of t_{ik} determine the eigenfrequencies ω_α of the elastic waves: $k^2\tau_\alpha=n\omega_\alpha{}^2=nk^2C_\alpha{}^2$ (n = mass density, C_α = velocity of sound). "Dynamical" stability requires $\tau_\alpha(\kappa)>0$:

$$t_{ik}(\kappa)a_ia_k>0\quad\text{or}\quad c_{44}>0,\ c_{11}-c_{12}>0,\ c_{11}>0. \tag{16}$$

These conditions are contained in (14) if there ϵ_{ij} is replaced by $\frac{1}{2}(a_ik_j+a_jk_i)$. Therefore, the conditions (16) or $c_{11}>0$ are less restrictive than (14) or $c_{11}+2c_{12}>0$.

The validity of (16) implies that $\Delta(\kappa)=|t_{ik}(\kappa)|>0$, which guarantees the existence of $\tilde{g}_{ik}(\kappa)=t^{-1}{}_{ik}(\kappa)$. Therefore, the Green's function g_{ik} is always finite for all stable materials which lie within the "wedge" in Fig. 1. On the other hand, g_{ik} is diverging on the plane $c_{11}=0$ and, more importantly, on the two planes $c_{11}-c_{12}=0$

and $c_{44}=0$, which limit the stable region. Thus, the Green's function g_{ik} has very strong maxima for materials with very high anisotropy, which in Fig. 1 lie very near to the planes $c_{11}-c_{12}=0$ or $c_{44}=0$. This will be discussed in more detail later.

From Eq. (15) we get then for $\tilde{g}_{ik}(\boldsymbol{\kappa})$:

$$\tilde{g}_{ik}=(\boldsymbol{\kappa})\frac{\delta_{ik}}{c_{44}+d\kappa_{(i)}^2}-\frac{\kappa_i\kappa_k}{(c_{44}+d\kappa_{(i)}^2)(c_{44}+d\kappa_{(k)}^2)}\times(c_{44}+c_{12})\Big/\left(1+\sum_{j=1}^{3}\frac{c_{44}+c_{12}}{c_{44}+d\kappa_j^2}\kappa_j^2\right). \quad (17)$$

The Green's function $g_{ik}(\boldsymbol{\varrho})$ can be given in elementary form only for two special ratios of the elastic constants. For isotropic materials ($d=c_{11}-c_{12}-2c_{44}=0$, Fig. 2) we have:

$$g_{ik}(\boldsymbol{\varrho})=\frac{1}{2c_{44}}\frac{c_{12}+3c_{44}}{c_{12}+2c_{44}}\delta_{ik}+\frac{1}{2c_{44}}\frac{c_{12}+c_{44}}{c_{12}+2c_{44}}\rho_i\rho_k. \quad (18)$$

For the case $c_{44}+c_{12}=0$ (Fig. 2) the second term in (17) vanishes and $g_{ik}(\boldsymbol{\varrho})$ is diagonal:

$$g_{ik}(\rho)=\frac{1}{c_{44}}\left[1+\frac{d}{c_{44}}(1-\rho_{(i)}^2)\right]^{-\frac{1}{2}}\delta_{ik}. \quad (19)$$

For arbitrary constants, $g_{ik}(\boldsymbol{\varrho})$ is elementary only if $\boldsymbol{\varrho}$ coincides with one of the cubic axes. $\Delta(\boldsymbol{\kappa})$ reduces in this case to a quadratic equation and the poles can be found.[3,7] We get for $\boldsymbol{\varrho}=(1,0,0)$ [$\boldsymbol{\varrho}=(1,0,0)$ or $(0,0,1)$ follows by cyclic permutation]:

$$g_{11}=\frac{1}{c_{44}};\quad g_{12}=0=g_{13}=g_{23},\quad \text{for}\quad \boldsymbol{\varrho}=(1,0,0)$$
$$g_{22}=g_{33}=\frac{c_{11}+c_{44}}{[(c_{11}-c_{12})c_{44}(c_{11}+c_{12}+2c_{44})c_{11}]^{1/2}}. \quad (20)$$

To our knowledge, (18), (19), and (20) represent the only cases for which elementary solutions can be given. Otherwise, we have to make approximations. This is easy if $d=0$, $c_{44}+c_{12}=0$, $\boldsymbol{\varrho}=(1,0,0)$ are only approximately valid. Then we can apply perturbation theory starting from the unperturbed solutions (18)–(20).

IV. PERTURBATION THEORY FOR G_{ik}

The case of weak anisotropy has been treated by Lifshitz and Rozentsveig[3] [there is a misprint in Eqs. (2.10)–(2.12) of Lifshitz and Rozentsveig's paper. The last term $\kappa_i\kappa_k\sum_j\kappa_j^4$ of Eq. (21) is missing] and Leibfried.[6] For $|d|\ll c_{44}$ we can expand $\tilde{g}_{ik}(\boldsymbol{\kappa})$ into powers of d. Taking only the linear term into account, we get from (17).

$$\tilde{g}_{ik}(\boldsymbol{\kappa})\simeq\tilde{g}_{ik}^{(0)}(\boldsymbol{\kappa})+\tilde{g}_{ik}^{(1)}(\boldsymbol{\kappa})\simeq\frac{1}{c_{44}}[\delta_{ik}-\beta\kappa_i\kappa_k]+\frac{d}{c_{44}^2}[-\kappa_{(i)}^2\delta_{ik}+\beta\kappa_i\kappa_k(\kappa_{(i)}^2+\kappa_{(k)}^2)-\beta^2\kappa_i\kappa_k\sum_j\kappa_j^4], \quad (21)$$

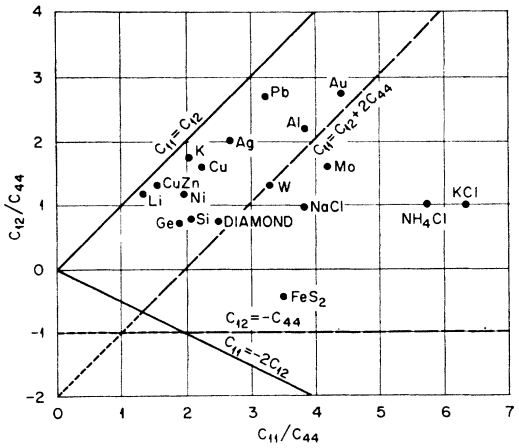

FIG. 2. c_{12}/c_{44} versus c_{11}/c_{44} for various crystals.

with

$$\beta=c_{12}+c_{44}/c_{12}+2c_{44}.$$

The result for $g_{ik}(\boldsymbol{\varrho})=g_{ik}^{(0)}(\boldsymbol{\varrho})+g_{ik}^{(1)}(\boldsymbol{\varrho})$ is

$$g_{ik}(\boldsymbol{\varrho})\simeq\frac{1}{c_{44}}[(1-\tfrac{1}{2}\beta)\delta_{ik}+\tfrac{1}{2}\beta\rho_i\rho_k]+\frac{d}{c_{44}^2}\Big[(-\tfrac{1}{2}+\tfrac{3}{4}\beta-\tfrac{3}{16}\beta^2)\delta_{ik}(1-\rho_{(i)}^2)+(-\tfrac{3}{4}\beta+\tfrac{3}{16}\beta^2)\rho_i\rho_k+(\tfrac{3}{8}\beta-\tfrac{3}{16}\beta^2)\rho_i\rho_k(\rho_{(i)}^2+\rho_{(k)}^2)-\frac{\beta^2}{16}(\delta_{ik}-5\rho_i\rho_k)\sum_j\rho_j^4\Big]. \quad (22)$$

For the integration we have used the convenient formula ($\mathbf{r}=r\boldsymbol{\varrho}$):

$$\int_{\kappa=1}(d\phi_\kappa/2\pi)\kappa_{\alpha_1}\kappa_{\alpha_2}\cdots\kappa_{\alpha_{2n}}=\frac{r}{(2n)!}\partial_{\alpha_1}\partial_{\alpha_2}\cdots\partial_{\alpha_{2n}}r^{2n-1}, \quad (23)$$

which can be derived by transforming $(1/k^2)\kappa_{\alpha_1}\cdots\kappa_{\alpha_{2n}}$ according to Eq. (3). Leibfried[6] used a slightly different approach. He first derived for each anisotropic tensor C_{ijkl} (13) an averaged isotropic tensor $\bar{C}_{ijkl}$ by rotating the cubic axes $\mathbf{e}^{(s)}$ over the whole unit sphere, thus replacing δ_{ijkl} in (13) by $\frac{1}{5}\delta_{ik}+\frac{2}{5}\kappa_i\kappa_k$. The corresponding averaged isotropic constants are

$$\bar{c}_{12}=c_{12}+\tfrac{1}{5}d,\quad \bar{c}_{44}=c_{44}+\tfrac{1}{5}d,\quad \bar{c}_{11}=\bar{c}_{12}+2\bar{c}_{44}. \quad (24)$$

They have been proposed by Voigt[10] as the isotropic constants of polycrystals. If we introduce these constants $\bar{c}_{12}$ and $\bar{c}_{44}$ instead of c_{12} and c_{44} into (17) and expand them linearly in d, we get Leibfried's result, which is

$$g_{ik}(\boldsymbol{\varrho})\simeq g_{ik}^{(0)}(\boldsymbol{\varrho})+g_{ik}^{(1)}(\boldsymbol{\varrho})=\frac{1}{\bar{c}_{44}}[(1-\tfrac{1}{2}\bar{\beta})\delta_{ik}+\tfrac{1}{2}\bar{\beta}\delta_i\delta_k]+\frac{d}{\bar{c}_{44}^2}\Big[\Big(-\frac{1}{10}+\frac{3}{20}\bar{\beta}+\frac{9}{80}\bar{\beta}^2\Big)\delta_{ik}+\Big(-\frac{1}{5}-\frac{3}{30}\bar{\beta}-\frac{9}{80}\bar{\beta}^2\Big)\rho_i\rho_k$$

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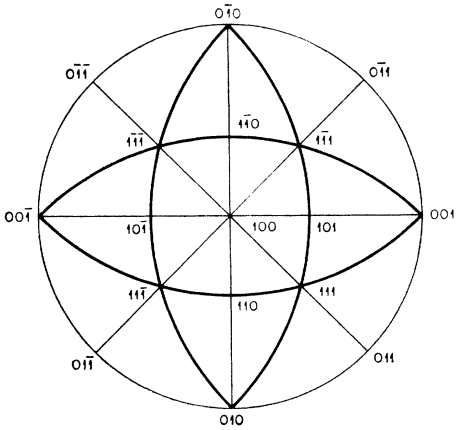

FIG. 3. Divergencies of $g_{11}(\varrho)$ for $c_{11}\to c_{12}$ (full lines).

$$+(\tfrac{1}{2}-\tfrac{3}{4}\bar{\beta}+\tfrac{3}{16}\bar{\beta}^2)\rho_{(i)}{}^2\delta_{ik}+(\tfrac{3}{8}\bar{\beta}-\tfrac{3}{16}\bar{\beta}^2)\rho_i\rho_k(\rho_{(i)}{}^2+\rho_{(k)}{}^2)-\frac{\bar{\beta}^2}{16}(\delta_{ik}-5\rho_i\rho_k)\sum_j\rho_j{}^4\Big],\quad \bar{\beta}=\frac{\bar{c}_{12}+\bar{c}_{44}}{\bar{c}_{12}+2\bar{c}_{44}}. \tag{25}$$

For small anisotropy, i.e., linear in d, this result is the same as (22), but it is better for higher anisotropy. The reason for this is that the zeroth approximation $g_{ik}{}^{(0)}(\varrho)$ of (25) represents for each anisotropic crystal the best isotropic Green's function, as will be shown later by variation (49).

The case $|c_{44}+c_{12}|\ll c_{44}$ or d can also be treated by perturbation theory. From (17) we obtain

$$\tilde{g}_{ik}(\kappa)\simeq\frac{\delta_{ik}}{c_{44}+d\kappa_{(i)}{}^2}-\frac{(c_{44}+c_{12})\kappa_i\kappa_k}{(c_{44}+d\kappa_{(i)}{}^2)(c_{44}+d\kappa_{(k)}{}^2)}. \tag{26}$$

By complex integration, we get from this for the diagonal element $g_{11}(\varrho)$ (g_{22} and g_{33} follow by cyclic permutation):

$$g_{11}(\varrho)\simeq(c_{44})^{-1/2}[c_{44}+d(1-\rho_1{}^2)]^{-1/2}-\frac{(c_{44}+c_{12})(1-\rho_1{}^2)}{2(c_{44})^{1/2}[c_{44}+d(1-\rho_1{}^2)]^{3/2}}. \tag{27}$$

The nondiagonal elements are also elementary but somewhat more complicated:

$$g_{12}(\varrho)\simeq-\frac{c_{44}+c_{12}}{c_{44}{}^2}\frac{\alpha_1\alpha_2(1-\rho_3{}^2)}{y_1y_2[(x_1+x_2)^2+(y_1+y_2)^2]}\times\{\rho_1\rho_2[(y_1+y_2)(\rho_3{}^2y_1y_2-1)+y_1x_2{}^2+y_2x_1{}^2]+\rho_3(\rho_2{}^2-\rho_1{}^2)(x_2y_1-x_1y_2)\}, \tag{28}$$

with

$$y_{1,2}=\alpha_{1,2}(1-\rho_3{}^2)\Big[1+\frac{d}{c_{44}}(1-\rho_{1,2}{}^2)\Big]^{1/2},$$

$$x_{1,2}=\alpha_{1,2}\frac{d}{c_{44}}\rho_1\rho_2\rho_3;\quad \alpha_{1,2}=1\Big/1-\rho_3{}^2+\frac{d}{c_{44}}\rho_3{}^2\rho_{1,2}{}^2.$$

Finally, we can apply perturbation theory to $g_{ik}(\varrho)$ in the vicinity of [100]. According to (9) κ has to be perpendicular to ϱ and κ has to lie nearly in the (100) plane for $\varrho\simeq$[100]. Therefore, we can expand $\tilde{g}_{ik}(\kappa)$ into powers of κ_1 ($\kappa_1{}^2\ll1$) taking only the lowest term into account. The integrals are elementary. For instance for $\rho_2{}^2$, $\rho_3{}^2\ll1$ we get

$$g_{11}(\rho)\simeq\frac{1}{c_{44}}[1-C_1(\rho_2{}^2+\rho_3{}^2)],\quad g_{12}(\varrho)\simeq\frac{1}{c_{44}}C_2\rho_2, \tag{29}$$

with

$$C_1=\frac{1}{2}\frac{d}{c_{44}}+\frac{c_{12}+c_{44}}{d+c_{12}+2c_{44}}\times\Big[-\frac{1}{2}\frac{(1-\eta)^2}{2-a}+\frac{2(1+\eta)^2-(1+\eta)^2a+\eta a^2}{(2-a)^2(2+a)^{1/2}}\Big],$$

$$C_2=\frac{c_{12}+c_{44}}{d+c_{12}+2c_{44}}\Big[\frac{1-\eta}{2-a}+\frac{2\eta-a}{(2-a)(2+a)^{1/2}}\Big], \tag{30}$$

and

$$\eta=\frac{c_{44}+d}{c_{44}},\quad a=\frac{(c_{11}-c_{12})(c_{11}+c_{12})-2c_{12}c_{44}}{c_{44}c_{11}}.$$

The corresponding constants describing the behavior of g_{22}, g_{33}, and g_{23} near $\varrho\simeq$(100) are even more complicated than C_1 and C_2 and will not be given here.

V. BEHAVIOR OF g_{ik} FOR NEARLY UNSTABLE MATERIALS

In Sec. III, we have seen that the elastic constants of all stable solids lie in that wedge-shaped region of Fig. 1 which is bounded by the planes $c_{44}=0$, $c_{11}-c_{12}=0$, and $c_{11}+2c_{12}=0$ [Eq. (14)]. Moreover, the Green's function has divergencies on the three planes $c_{44}=0$, $c_{11}-c_{12}=0$, and $c_{11}=0$ [Eq. (16)]. Therefore, materials for which the elastic constants lie very near to the planes $c_{11}-c_{12}=0$ or $c_{44}=0$ must have near divergencies or very pronounced maxima. What occurs near the plane $c_{11}=0$ is irrelevant because this plane is outside the stability region.

In the first case $c_{11}\to c_{12}+0$ which is nearly realized for such highly anisotropic materials as alkali metals and Cu-Zn (Fig. 2), the determinant $\Delta(\kappa)=|t_{ik}(\kappa)|$ goes to zero only if κ coincides with a ⟨110⟩ direction. We have

$$\Delta(110)\equiv n^3c_l{}^2(110)c_{t_1}{}^2(110)c_{t_2}{}^2(110)=\tfrac{1}{2}(c_{11}+c_{12}+2c_{44})c_{44}\tfrac{1}{2}(c_{11}-c_{12}). \tag{31}$$

Here $c_l(110)$ and $c_t(110)$ are the longitudinal and transverse velocities of sound in a ⟨110⟩ direction. For $c_{11}\to c_{12}$, the transverse velocity with the polarization vector in [$\bar{1}$10] vanishes. For this kind of highly anisotropic material, $\tilde{g}_{ik}(\kappa)$ has, in general, strong maxima in a ⟨110⟩ direction. This means for the Green's function that $g_{ik}(\varrho)$ has strong maxima whenever the integration

path $\kappa \perp \varrho$ [Eq. (9)] includes a ⟨110⟩ direction. To get the position and form of these maxima, we expand both the denominator $\Delta(\kappa)$ and the numerator $\Delta_{ik}(\kappa)$ in the vicinity of the ⟨110⟩ direction, taking only the leading terms into account. The integration can then be performed. For example, $g_{11}(\varrho)$ has such maxima if ϱ lies in a $\{\bar{1}10\}$ plane. Writing

$$\varrho=[1/\sqrt{2}(1-\xi_3)\sin\Theta_3,\ 1/\sqrt{2}(1+\xi_3)\sin\Theta_3,\ \cos\Theta_3], \qquad \xi_3^2 \ll 1 \quad (32)$$

we get

$$g_{11}(\varrho)=\frac{c_{11}+c_{44}}{2c_{44}} \Big/ \Big\{ 4c_{11}(c_{11}+c_{44})\sin^2\Theta_3\xi_3^2 + \frac{c_{11}-c_{12}}{2c_{44}}[4c_{11}(c_{11}+c_{44})\cos^2\Theta_3+(c_{11}+c_{44})^2\sin^2\Theta_3] \Big\}^{1/2}. \quad (33)$$

One sees that in the $(1\bar{1}0)$ plane $g_{11}(\varrho)$ is proportional to $[(2c_{44})/(c_{11}-c_{12})]^{1/2}$ and diverges for $c_{11} \to c_{12}$.

Because of the cubic symmetry, we get the same maxima if ϱ lies in or nearly in a $\{1\bar{1}0\}$, $\{\bar{1}01\}$, or $\{10\bar{1}\}$ plane, but no such maxima for $\{001\}$ or $\{0\bar{1}1\}$ planes because Δ_{11} vanishes in the limit $c_{11} \to c_{12}$ for ⟨110⟩ directions which are perpendicular to [100]. These maxima planes for $g_{11}(\varrho)$ are shown in Fig. 3. At the intersection of two such planes, the contributions from the different planes add to each other and give rise to an extra strong maximum. Therefore, Eq. (33) gives only half the value of g_{11} for $\varrho=[111]$ or $\varrho=[010]$, etc. For $g_{12}(\varrho)$ we get maxima on the planes (110) and $(1\bar{1}0)$ (Fig. 4). Moreover, near these planes we have

$$\begin{aligned} g_{12}(\varrho) &= +g_{11}(\varrho), \quad \text{for} \quad \rho_1\rho_2>0 \\ &= -g_{11}(\varrho), \quad \text{for} \quad \rho_1\rho_2<0, \end{aligned} \quad (34)$$

where $g_{11}(\varrho)$ on the $(1\bar{1}0)$ plane is given by (33). Because of the weak divergence $\sim[(2c_{44})/(c_{11}-c_{12})]^{1/2}$, the maxima are—even for such a highly anisotropic material as Li for which $2c_{44}/(c_{11}-c_{12})=9.4$—not very pronounced. Nevertheless, the maxima can clearly be seen in the computer calculations of Lie and Koehler for Li[9] (Fig. 8; arrows indicate the positions of the maxima for $c_{11} \to c_{12}$).

Also in the second case ($c_{44} \to +0$), which is approximately realized for example for the alkali halides ($c_{44} \approx c_{12} \ll c_{11}$, Fig. 2), we get such "near divergencies." In the simple isotropic case ($d=0$), $g_{ik}(\kappa)$ is directly proportional to $1/c_{44}$ [Eq. (17)]. But for $d \neq 0$, the behavior is more complicated. For $c_{44} \to 0$, $\Delta(\kappa)$ goes to zero ($\sim c_{44}$) only if κ lies in a $\{100\}$ plane. If κ coincides with a ⟨100⟩ direction, then $\Delta(\kappa)$ is even proportional to c_{44}^2:

$$\Delta(\kappa=(\kappa_1,\kappa_2,0))=c_{44}[\kappa_1^2\kappa_2^2 d(c_{11}+c_{12})+c_{44}c_{11}]. \quad (35)$$

To evaluate $g_{ik}(\varrho)$, we expand again $\Delta(\kappa)$ and $\Delta_{ik}(\kappa)$ around the maxima planes of $\tilde{g}_{ik}(\kappa)$ taking only the most diverging terms for $c_{44} \to 0$ into account. Then for

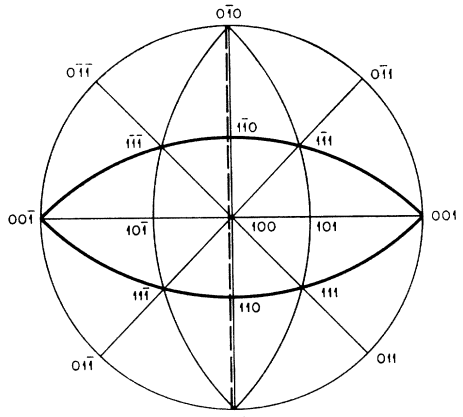

FIG. 4. Divergencies of $g_{12}(\varrho)$ for $c_{11} \to c_{12}$ (full lines) and for $c_{44} \to 0$ (dashed line).

$g_{11}(\varrho)$ we obtain

$$g_{11}(\rho)=1 \Big/ c_{44}\left[1+\frac{d}{c_{44}}\frac{c_{11}+2c_{12}}{c_{11}+c_{12}}(1-\rho_1^2)\right]^{1/2}. \quad (36)$$

We see that in the limit $c_{44} \to 0$, $g_{11}(\varrho)$ diverges proportionally to $(c_{44})^{-1/2}$ with the exception of the point [100], where g_{11} goes as $1/c_{44}$, in agreement with (20). Equation (36) is not valid if ϱ lies in or near the (010) and (001) planes, with the exception of the region near [100]. On these two planes, g_{11} is also proportional to $(c_{44})^{-1/2}$, but the ϱ dependence is somewhat more difficult. In the limit $c_{12} \to 0$, Eq. (36) gives g_{11} on the whole unit sphere in agreement with (19).

The nondiagonal element $g_{12}(\varrho)$ diverges for $c_{44} \to 0$ proportional to $(c_{44})^{-1/2}$ if ϱ lies in the (001) plane (Fig. 4; dashed line). In this case we obtain:

$$g_{12}(\varrho)=-\frac{\sqrt{2}c_{12}}{(c_{44}d)^{1/2}(c_{11}+2c_{12})} \times \frac{1}{[b+(b^2-c^2)^{1/2}]^{1/2}+[b-(b^2-c^2)^{1/2}]^{1/2}} \quad (37)$$

for $\rho_1\rho_2>0$, with $b=(c_{11}+c_{12})/(c_{11}+2c_{12})$ and $c^2=4\rho_1^2\rho_2^2(c_{11}/(c_{11}+2c_{12}))$.

VI. A FITTING APPROXIMATION FOR $g_{ik}(\varrho)$

The solutions obtained in Secs. IV and V by perturbation theory give us information only about the Green's function for the very special cases $c_{11}-c_{12}-2c_{44} \simeq 0$, $c_{12}+c_{44} \simeq 0$, $c_{11}-c_{12} \to 0$, $c_{44} \to 0$, or $\varrho \simeq$ ⟨100⟩. Moreover, the expressions are rather complicated, preventing us from applying second-order perturbation theory which would lead to elementary, but even more complicated, results.

In the following, therefore, we will try to get some sort of an over-all approximation which gives us a reasonable solution for all allowed values of the elastic

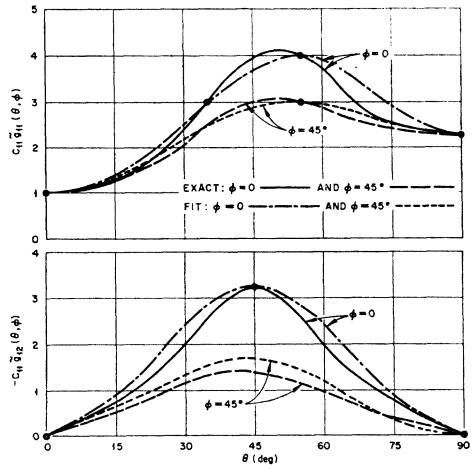

FIG. 5. Fourier transforms $\tilde{g}_{11}(\kappa)$ and $\tilde{g}_{12}(\kappa)$ for Cu: exact: $\phi=0$ —— and $\phi=45°$ — — fitted: $\phi=0$ —·— and $\phi=45°$ - - - (fitting points are marked by ●).

constants, but which cannot, of course, be a very accurate approximation in each case. In order to do this, we make the following ansatz for the Fourier transform $\tilde{g}_{ik}(\kappa)$ with the undetermined constants $\tilde{c}_1,\cdots,\tilde{c}_{10}$:

$$\begin{aligned}\tilde{g}_{ik}(\kappa)=&\tilde{c}_1\delta_{ik}+\tilde{c}_2\kappa_i\kappa_k+\tilde{c}_3\kappa_{(i)}{}^2\delta_{ik}+\tilde{c}_4\tfrac{1}{2}\kappa_i\kappa_k(\kappa_{(i)}{}^2+\kappa_{(k)}{}^2)\\&+\tilde{c}_5\kappa_{(i)}{}^4\delta_{ik}+\tilde{c}_9\sum_j\kappa_j{}^4\delta_{ik}+\tilde{c}_6\kappa_i\kappa_k\sum_j\kappa_j{}^4\\&+\tilde{c}_7\tfrac{1}{2}\kappa_i\kappa_k(\kappa_{(i)}{}^4+\kappa_{(k)}{}^4)+\tilde{c}_8\kappa_{(i)}{}^6\delta_{ik}\\&+\tilde{c}_{10}\sum_j\kappa_j{}^6\delta_{ik}.\end{aligned}\quad(38)$$

This expression contains all linear independent power expressions up to the sixth order in κ which have the same cubic symmetry as the tensor function $\tilde{g}_{ik}(\kappa)$. This is equivalent to using all cubic harmonics[4,11] up to the sixth order which have the appropriate symmetry. Cubic harmonics are only orthogonalized combinations of the linear independent expressions of (35).

The first term in the exact Eq. (17), being proportional to δ_{ik}, depends only on $\kappa_{(i)}{}^2$. Therefore, we can restrict our ansatz (38) and set $\tilde{c}_9\equiv 0\equiv\tilde{c}_{10}$. Comparing (35) with the exact formula (17) and with (21), we see that this ansatz can give us the exact solution only in the case of isotropy (c_1, $c_2\neq 0$) or weak anisotropy (c_1, $c_2\neq 0$; c_3,c_4,c_6 small). Because of the divergence of $\tilde{g}_{ik}$ for $c_{11}-c_{12}\to 0$ and $c_{44}\to 0$, it is clear than an ansatz like (38) cannot be good for very high anisotropy, because any expansion into regular functions diverges in these limits. We have, of course, chosen the ansatz for $\tilde{g}_{ik}(\kappa)$ so that the corresponding ansatz for the Green's function $g_{ik}(\varrho)$ is elementary. The transformation can be performed easily using formula (23).

To determine the constants $\tilde{c}_1\cdots\tilde{c}_8$, we will go back to a method used by Houston to evaluate angular integrals of functions with cubic symmetry.[12,13] We postulate that the ansatz (38) coincides with the exact expression (17) at certain points on the unit sphere. The exact location of these points is rather arbitrary, but will be chosen in such a way that the points are more or less equally spaced from each other. To fit $\tilde{g}_{11}(\kappa)$ we choose the points (1,0,0), $(1/\sqrt{3})(\sqrt{2},1,0)$, $(1/\sqrt{3})(1,\sqrt{2},0)$, $(1/\sqrt{3})(1,1,1)$, and (0,0,1). [The last point guarantees that we get the exact value for $g_{11}(100)$, because according to (17), $\tilde{g}_{11}(\kappa)=1/c_{44}$ in the whole plane (100)]. To fit $\tilde{g}_{12}(\kappa)$ with the exact expression, we choose the points $1/\sqrt{2}(1,1,0)$, $\frac{1}{2}(1,1,\sqrt{2})$, and (1,0,0). The latter points are both inclined at 45° to $1/\sqrt{2}(1,1,0)$. Because $\tilde{g}_{12}(100)=0$, we fit the slope of $\tilde{g}_{12}(\kappa)$ at this particular point. Using Eq. (23), we then perform the integration and get

$$\begin{aligned}g_{11}(\varrho)=&a_1+a_2\rho_1{}^2+a_3\rho_1{}^4+a_4\rho_1{}^6+a_5(1-5\rho_1{}^2)\sum_j\rho_j{}^4,\\g_{12}(\varrho)=&\rho_1\rho_2[b_1+b_2\rho_3{}^2+b_3\tfrac{1}{2}(\rho_1{}^4+\rho_2{}^4)+b_4\rho_3{}^4],\end{aligned}\quad(39)$$

with

$$\begin{aligned}a_1&=(1/32)(7A+9B-18C+27D+7E);\\b_1&=(1/24)(7F-20G-27H)-(9/32)(C-D);\\a_2&=(1/32)(47A-225B-144C+405D-83E);\\b_2&=(1/16)(-10F-16G+54H)+(27/8)(C-D);\\a_3&=(1/32)(81A-189B-135C+270D-27E);\\b_3&=(5/4)(-F+G);\\a_4&=(1/32)(-45A+135B+135C-270D+45E);\\b_4&=-5a_5=(135/32)(-C+D);\\a_5&=(1/32)(27C-27D).\end{aligned}\quad(40)$$

For the constants $A,\cdots,H$ we get from (17):

$$\begin{aligned}A&=\tilde{g}_{11}(100)=1/c_{11},\quad E=\tilde{g}_{11}(001)=1/c_{44},\\B&=\tilde{g}_{11}(\sqrt{2}10)\\&=\frac{4c_{44}+c_{12}+d}{2(c_{44}+\frac{1}{3}d)(c_{44}+c_{12})+(c_{44}+\frac{2}{3}d)(4c_{44}+c_{12}+d)}\\C&=\tilde{g}_{11}(1\sqrt{2}0)\\&=\frac{5c_{44}+2c_{12}+2d}{(c_{44}+\frac{2}{3}d)(c_{44}+c_{12})+(c_{44}+\frac{1}{3}d)(5c_{44}+c_{12}+d)}\\D&=\tilde{g}_{11}(111)\\&=\frac{5c_{44}+2c_{12}+d}{(c_{44}+\frac{1}{3}d)(6c_{44}+3c_{12}+d)}\\F&=\left.\frac{\tilde{g}_{12}(1\epsilon 0)}{\epsilon}\right|_{\epsilon\to 0}=-(c_{44}+c_{12})/c_{44}\cdot c_{11}\\G&=\tilde{g}_{12}(110)=-\frac{c_{44}+c_{12}}{(2c_{44}+d)(2c_{44}+c_{12}+\frac{1}{2}d)}\\H&=\tilde{g}_{12}(11/\sqrt{2})=-\frac{c_{44}+c_{12}}{4(c_{44}+\frac{1}{4}d)^2}\\&\quad\times\left\{1+\tfrac{1}{2}\frac{c_{44}+c_{12}}{c_{44}+\tfrac{1}{2}d}+\frac{c_{44}+c_{12}}{c_{44}+\tfrac{1}{4}d}\right\}^{-1}.\end{aligned}\quad(41)$$

[11] F. C. v. d. Lage and H. A. Bethe, Phys. Rev. **71**, 612 (1947).
[12] W. V. Houston, Rev. Mod. Phys. **20**, 161 (1948).
[13] D. D. Betts, A. B. Bhatia, and M. Wyman, Phys. Rev. **104**, 37 (1956).

To check the accuracy of this approximation, we have plotted in Fig. 5 for Cu the fitted expression for the Fourier transforms $\tilde{g}_{11}(\kappa)$ and $\tilde{g}_{12}(\kappa)$ and compared with the exact ones (17). Here θ is the polar angle to the 1 axis and ϕ the azimuth in the (100) plane. The elastic constants used here are (Ref. 14; room temperature):

$$c_{11}=16.84,\ c_{12}=12.14,\ c_{44}=7.54$$
(in units of 10^{11} dyne/cm^2).

Figure 6 shows the so-determined Green's function $g_{11}(\varrho)$ and $g_{12}(\varrho)$ and compares it with the computed values of Ref. 10 for Cu. The agreement is fairly good.

To get better approximations than the given one, we can do essentially two things: First, we can make a better ansatz than (17) and include, e.g., in the next step, all linear independent expressions of 8th order in κ and use some more fitting points to determine the constants. This is, of course, straightforward and can be done easily. Or, we can try to get some better criteria to determine the constants of our ansatz than the simple fitting procedure. This will be done by variational techniques in Sec. VII.

VII. VARIATIONAL PROCEDURE

The energy E of a displacement field $s_i(\mathbf{r})$ due to a force $f_i(\mathbf{r})$ is given by:

$$E=\int d\mathbf{r}\left[\tfrac{1}{2}C_{ijkl}\frac{\partial s_i}{\partial r_j}\frac{\partial s_k}{\partial r_l}-f_i(\mathbf{r})s_i(\mathbf{r})\right]. \tag{42}$$

Introducing the Fourier transforms $\tilde{s}_i(\mathbf{k})$ and $\tilde{f}_i(\mathbf{k})$ by Eq. (3), this can be written

$$E=\int\frac{d\mathbf{k}}{(2\pi)^3}\left[\tfrac{1}{2}T_{ik}(\mathbf{k})\tilde{s}_k(\mathbf{k})\tilde{s}_i(-\mathbf{k})-\tilde{f}_i(\mathbf{k})\tilde{s}_i(-\mathbf{k})\right]. \tag{43}$$

As a functional of $s_i(\mathbf{r})$ or $\tilde{s}_i(\mathbf{k})$, E is minimal for the exact displacement field $s_i(\mathbf{r})$ or $\tilde{s}_i(\mathbf{k})$, respectively.

One sees directly from (42) that for a point force $f_i(\mathbf{r})=\delta_{im}\delta(\mathbf{r})$, the displacement force of which is just the Green's function $G_{im}(\mathbf{r})$, the energy is infinite. To prevent this divergency, we consider an extended force $f_i(\mathbf{r})=\delta_{im}f(r)$, where $f(r)$ depends only on the absolute value r. In this case, the transform $\tilde{s}_i(\mathbf{k})$ is given by $\tilde{s}_i(\mathbf{k})=\tilde{G}_{im}(\mathbf{k})\tilde{f}(k)=(\tilde{f}(k)/k^2)\tilde{g}_{im}(\kappa)$. The energy as a functional of the angular function $\tilde{g}_{im}(\kappa)$ is then

$$E=\epsilon_0\int\frac{d\Omega_\kappa}{4\pi}\left[\tfrac{1}{2}l_{ik}(\kappa)\tilde{g}_{k(m)}(\kappa)\tilde{g}_{i(m)}(-\kappa)-\delta_{i(m)}\tilde{g}_{i(m)}(-\kappa)\right], \tag{44}$$

with

$$\epsilon_0=\int_0^\infty\frac{dk}{2\pi^2}\tilde{f}^2(k).$$

Miminizing E with respect to $\tilde{g}_{im}(\kappa)$, we always get, independently of ϵ_0 and the special form of $f(r)$, the exact Eq. (7) which determines $\tilde{g}_{im}(\kappa)$. This result remains valid also in the limit $\epsilon_0\to\infty$ which corresponds to a point force $f(r)=\delta(\mathbf{r})$ or $\tilde{f}(k)=1$. Therefore, we can use (44) to determine $\tilde{g}_{im}(\kappa)$ or $g_{im}(\varrho)$ by variation.

In order to do this we make an ansatz for $\tilde{g}_{im}(\kappa)$ with N linearly independent functions $\tilde{g}_{im}{}^{(\lambda)}(\kappa)$ $(\lambda=1, 2,\cdots, N)$

$$\tilde{g}_{im}(\kappa)=\sum_{\lambda=1}^{N}\tilde{c}_\lambda\tilde{g}_{im}{}^{(\lambda)}(\kappa). \tag{45}$$

Introducing this in (44), we have

$$3E_0/\epsilon_0=\sum_{\lambda,\lambda'=1}^{N}\tfrac{1}{2}T_{\lambda\lambda'}\tilde{c}_\lambda\tilde{c}_{\lambda'}-\sum_{\lambda=1}^{N}D_\lambda\tilde{c}_\lambda, \tag{46}$$

with

$$T_{\lambda\lambda'}=\int\frac{d\Omega_\kappa}{4\pi}l_{ik}(\kappa)\tilde{g}_{km}{}^{(\lambda)}(\kappa)\tilde{g}_{im}{}^{(\lambda')}(-\kappa),$$

$$D_\lambda=\int\frac{d\Omega_\kappa}{4\pi}\tilde{g}_{mm}{}^{(\lambda)}(\kappa).$$

The best set of the constants $\tilde{c}_\lambda$ is then determined by minimizing E, giving the equations

$$\sum_{\lambda'=1}^{N}T_{\lambda\lambda'}\tilde{c}_{\lambda'}=D_\lambda,\quad \lambda=1,\cdots,N. \tag{47}$$

As an instructive example, we make an isotropic ansatz for $\tilde{g}_{im}(\kappa)$ of the form of Eq. (17) for $d=0$ with two constants $\tilde{c}_1$ and $\tilde{c}_2$, which can also be expressed by some effective isotropic constants $c_{12}{}^0$, $c_{44}{}^0$, and $c_{11}{}^0=c_{12}{}^0+2c_{44}{}^0$:

$$\tilde{g}_{im}(\kappa)=\tilde{c}_1\delta_{im}+\tilde{c}_2\kappa_i\kappa_m,$$

with

$$\tilde{c}_1=\frac{1}{c_{44}{}^0},\quad \tilde{c}_2=-\frac{c_{12}{}^0+c_{44}{}^0}{c_{44}{}^0(c_{12}{}^0+2c_{44}{}^0)}. \tag{48}$$

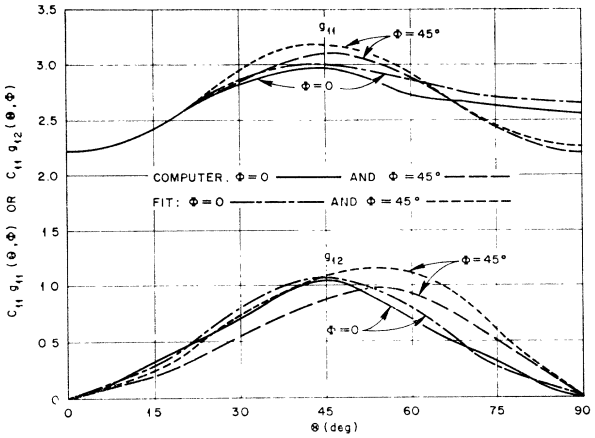

FIG. 6. Green's functions $g_{11}(\varrho)$ and $g_{12}(\varrho)$ for Cu: computer: $\Phi=0$ —— and $\Phi=45°$ — — fitted: $\Phi=0$ —·— and $\Phi=45°$ - - - (Θ polar angle to 1-axis, Φ azimuth in (100) plane).

[14] H. B. Huntington, Solid State Phys. (London) 7, 213 (1958).

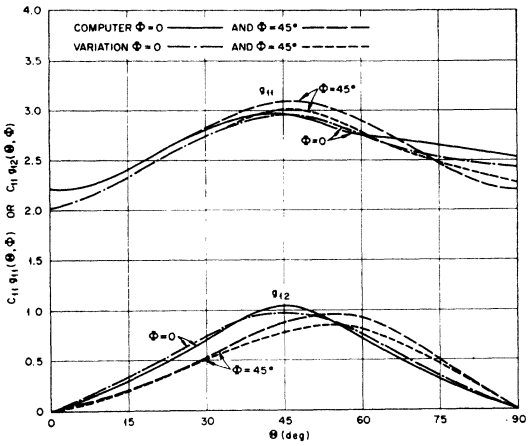

FIG. 7. Green's function $g_{11}(\varrho)$ and $g_{12}(\varrho)$ for Cu: computer: $\Phi=0$ —— and $\Phi=45°$ — — variation (50): $\Phi=0$ —·— $\Phi=45°$ – – –.

The "best" isotropic constants c_{ij}^0 are then determined by variation and are identical with Voigt's averages $\bar{c}_{ij}$ (24),[10]

$$c_{12}^0=\bar{c}_{12}=c_{12}+\tfrac{1}{5}d\,,\quad c_{44}^0=\bar{c}_{44}=c_{44}+\tfrac{1}{5}d\,. \tag{49}$$

To get better approximations, we make an *Ansatz* which has the form of Leibfried's perturbation theory (25) for weak anisotropy,

$$g_{im}(\varrho)=\tilde{c}_0 g_{im}^{(0)}(\varrho)+\tilde{c}_1 g_{im}^{(1)}(\varrho)\,. \tag{50}$$

Here $g_{im}^{(0)}(\varrho)$, given by the first term in Eq. (25), represents according to (48) and (49) the best isotropic approximation, and $g_{im}^{(1)}(\varrho)$, given by the second term in (25), is the correction due to anisotropy. The parameters $\tilde{c}_0$ and $\tilde{c}_1$ are introduced to improve the perturbation theory in a simple way. [For weak anisotropy, i.e., as long as (25) is strictly valid, we have $\tilde{c}_0=\tilde{c}_1=1$.] By variation we get for $\tilde{c}_0$ and $\tilde{c}_1$:

$$\tilde{c}_0=\left\{1-\left(\frac{d}{\bar{c}_{44}}\right)^2\frac{K_0^2}{(3-\bar{\beta})[K_0+(d/\bar{c}_{44})K_1]}\right\}^{-1},$$
$$\tilde{c}_1=\frac{1}{1+(d/\bar{c}_{44})(K_1/K_0)}\tilde{c}_0, \tag{51}$$

with

$$K_0=\frac{4}{25}-\frac{36}{175}\bar{\beta}+\frac{68}{525}\bar{\beta}^2-\frac{16}{525}\bar{\beta}^3,\quad \bar{\beta}=\frac{\bar{c}_{12}+\bar{c}_{44}}{\bar{c}_{12}+2\bar{c}_{44}}$$
$$K_1=\frac{16}{875}-\frac{32}{875}\bar{\beta}+\frac{328}{9{,}625}\bar{\beta}^2-\frac{2{,}016}{125{,}125}\bar{\beta}^3+\frac{384}{125{,}215}\bar{\beta}^4. \tag{52}$$

In Fig. 7, we have plotted this approximation for $g_{im}(\varrho)$ and compared it with the computed results for Cu.[9] The agreement is fairly good and (50) represents a considerable improvement of the perturbation expression (25).

Other approximations can be obtained by using the more general ansatz (38) and determining the constants $\tilde{c}_1, \tilde{c}_2, \cdots, \tilde{c}_8$ by variation. All the integrals $T_{\lambda\lambda'}$ and D_λ needed to solve the linear equations (47) are elementary. In a first step, we have used only five constants ($\tilde{c}_1$, $\tilde{c}_2$, $\tilde{c}_3$, $\tilde{c}_4$, and $\tilde{c}_6$), which are the only important ones for weak anisotropy (22, 25). This ansatz has the same functional ϱ and κ dependences as the ansatz (50), with the difference that now all five constants are varied independently instead of only two. Unfortunately, the result shows no considerable improvement, e.g., for Cu we get, within the drawing limits, the same curves as for the approximation (50) in Fig. 7. The improvement is also not much better if we use all eight constants $\tilde{c}_1\cdots\tilde{c}_8$ of ansatz (38). As an example for this, we have plotted in Fig. 8 this approximation for $g_{11}(\varrho)$ and $g_{12}(\varrho)$ and compared it with the computed results for Li. Li is extremely anisotropic (see Fig. 2) and the elastic constants are (Ref. 14; 78°K):

$$c_{11}=1.48\,,\quad c_{12}=1.25\,,\quad c_{44}=1.08\ [10^{11}\ \text{dyne/cm}^2].$$

The agreement is not very good. In particular, the maxima which are due to the divergencies of $\tilde{g}_{im}(\kappa)$ for $c_{12}\to c_{11}$ ($\mathcal{S}IV$) and which are marked in Fig. 8 by arrows are only poorly reflected in the approximation.

This example shows that our approximations are restricted to materials with weak and medium anisotropy. To get satisfactory approximations for higher anisotropy, we would have either to take many more terms in an expansion like (38) into account or to use such trial functions $\tilde{g}_{im}^{(\lambda)}(\kappa)$ which already have strong maxima or near divergencies in appropriate κ directions. But such functions are not easy to handle and we have made no progress in this direction.

The characteristic advantage of the Green's function $G_{im}(\mathbf{r})$ is that we can obtain the displacement field due to an arbitrary force $f_m(\mathbf{r})$ by superposition:

$$s_i(\mathbf{r})=\int d\mathbf{r}' G_{im}(\mathbf{r}-\mathbf{r}')f_m(\mathbf{r}')\,. \tag{53}$$

In this section, we have made an ansatz for G_{im} and optimized the coefficients by minimizing the *energy for the unit force*. Now the question arises whether the displacement field $s_i(\mathbf{r})$, calculated according to (53) with the optimal Green's function, is also optimal, i.e., is this displacement identical with the displacement field $s_i(\mathbf{r})$ obtained by putting the ansatz for G_{im} into Eq. (53) and then optimizing $s_i(\mathbf{r})$ by minimizing *the energy for the $f_m(\mathbf{r})$ force*? In general, this is not the case, and the optical displacement field $s_i(\mathbf{r})$ and the field calculated by (53) with the optimal $G_{im}(\mathbf{r})$ are normally different. The difference is, of course, the smaller the better the approximations are and vanishes if the *Ansätze* for $G_{im}(\mathbf{r})$ and $s_i(\mathbf{r})$ give the exact results. In the future we want to apply the variational procedure to the calculation of point defect displacement fields and their interactions and certain dislocation arrangements.

Analogously to the variational principle (42) for the displacement field $s_i(\mathbf{r})$, one can also derive a variation principle for the strain field $\sigma_{ij}(\mathbf{r})$:

$$E=\int d\mathbf{r}\{-\tfrac{1}{2}S_{ijkl}\sigma_{kl}(\mathbf{r})\sigma_{ij}(\mathbf{r}) -[\partial_{r_j}\sigma_{ij}(\mathbf{r})+f_i(\mathbf{r})]s_i(\mathbf{r})\}. \quad (54)$$

Here S_{ijkl} is the inverse of C_{ijkl}. For cubic symmetry, it has the same structure (13) as C_{ijkl} with constants s_{12}, s_{44}, and $r=s_{11}-s_{12}-2s_{44}$, which are connected with the c_{ij}'s by

$$s_{11}-s_{12}=\frac{1}{c_{11}-c_{12}}, \quad 2s_{44}=\frac{1}{2c_{44}},$$

and

$$s_{11}+2s_{12}=\frac{1}{c_{11}+2c_{12}}. \quad (55)$$

The displacement field $s_i(\mathbf{r})$ enters as a Lagrange parameter to guarantee the subsidiary condition $\partial_{r_j}\sigma_{ij}+f_i=0$, whereas variation with respect to $\sigma_{ij}(\mathbf{r})$ gives Hooke's law. By Fourier transformation from (54) we get

$$E=\int \frac{d\mathbf{k}}{(2\pi)^3}\{-\tfrac{1}{2}S_{ijkl}\tilde{\sigma}_{kl}(\mathbf{k})\tilde{\sigma}_{ij}^*(\mathbf{k}) -[ik_j\tilde{\sigma}_{ij}(\mathbf{k})+\tilde{f}_i(\mathbf{k})]\tilde{s}_i^*(\mathbf{k})\}. \quad (56)$$

For an extended force $f_i(\mathbf{r})=\delta_{im}f(r)$, we have $\tilde{s}_i(\mathbf{k})=(1/k^2)\tilde{g}_{im}(\boldsymbol{\kappa})$, and analogously, $\tilde{\sigma}_{ij}(\mathbf{k})=(1/k)\tilde{\eta}_{ij;m}(\boldsymbol{\kappa})$. Then we have

$$E=\epsilon_0\int \frac{d\Omega_\kappa}{4\pi}\{\tfrac{1}{2}S_{ijkl}\tilde{\eta}_{kl;(m)}(\boldsymbol{\kappa})\tilde{\eta}_{ij;(m)}^*(\boldsymbol{\kappa}) +[\tilde{\eta}_{ij;(m)}(\boldsymbol{\kappa})\kappa_j-\delta_{i(m)}]\tilde{g}_{i(m)}^*(\boldsymbol{\kappa})\}. \quad (57)$$

As an example we try, analogous to (54), an isotropic ansatz with arbitrary but isotropic constants $\hat{c}_{12}$, $\hat{c}_{44}$, and $\hat{c}_{11}=\hat{c}_{12}+2\hat{c}_{44}$,

$$\tilde{\eta}_{ij;m}(\boldsymbol{\kappa})=i[\kappa_j\delta_{im}+\kappa_i\delta_{jm}+(\hat{c}_{12}/\hat{c}_{12}+2\hat{c}_{44})\kappa_m\delta_{ij} -2(\hat{c}_{12}+\hat{c}_{44}/\hat{c}_{12}+2\hat{c}_{44})\kappa_i\kappa_j\kappa_m]. \quad (58)$$

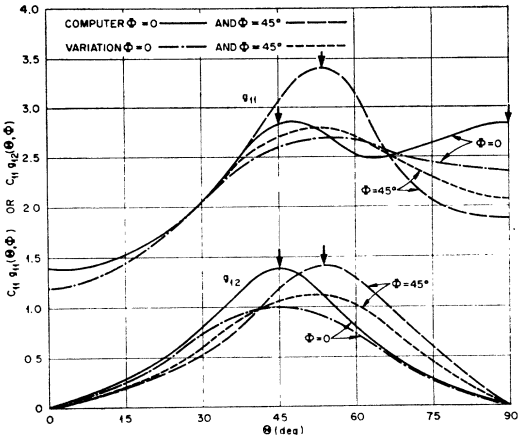

FIG. 8. Green's functions $g_{11}(\boldsymbol{\varrho})$ and $g_{12}(\boldsymbol{\varrho})$ for Li: computer: $\Phi=0$ —— and $\Phi=45°$ —— variation (38): $\Phi=0$ —·— and $\Phi=45°$ - - -. Positions of maxima for $c_{11}\to c_{12}$: ↓.

By variation, we determine the $\hat{c}_{ij}$'s such that the strain field $\tilde{\eta}_{ij;m}$ (58) is optimal. The result is

$$\hat{c}_{12}=c_{12}+\tfrac{1}{5}d\frac{c_{44}+\frac{1}{2}d}{c_{44}+\frac{3}{10}d}, \quad \hat{c}_{44}=c_{44}+\tfrac{1}{5}d\frac{c_{44}}{c_{44}+\frac{3}{10}d},$$

$$\hat{c}_{11}=\hat{c}_{12}+2\hat{c}_{44}. \quad (59)$$

The corresponding isotropic inverse constants $\hat{s}_{ij}$ are

$$\hat{s}_{12}=s_{12}+r/5, \quad \hat{s}_{44}=s_{44}+r/5, \quad \text{and} \quad \hat{s}_{11}=\hat{s}_{12}+2\hat{s}_{44}. \quad (60)$$

Similarly to (24, 49), they can be obtained by averaging the anisotropic S_{ijkl} over all directions of the cubic axes and are identical to the ones used by Reuss[14] for polycrystals. Therefore, whereas the isotropic constants which give the optimal isotropic displacement field $G_{im}(\mathbf{r})$ can be obtained by averaging C_{ijkl}, the best isotropic constants with respect to the strain field $\sigma_{ij}(\mathbf{r})$ are obtained by averaging S_{ijkl}. Both constants (55) and (49) differ only by quadratic and higher terms in the anisotropy d.