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WORKING PARTY ON
MODELLING THERMOMECHANICAL BEHAVIOUR OF MATERIALS
(29 May - 16 June 1989)

GREEN'S FUNCTION METHOD

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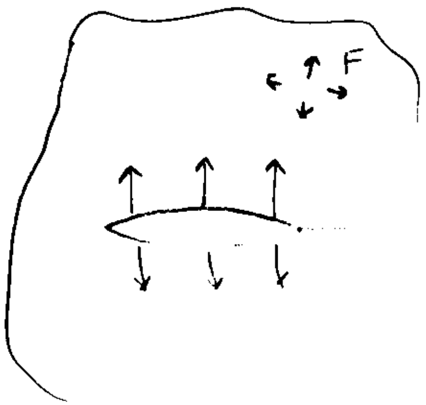
Green's Function Method



Models of a Solid

1. Born von Karman Model
2. Continuum Model

A. General References

1. Born & Huang - Dyn. Theory of Crystal Lattic
2. Eshelby - Solid St. Phys. 3 79 (1956).
3. Maradudin et. al. – Solid St. Phys.; Supp-3 (1

B. Review of Fracture Mechanics

R. Thomson – Solid St. Phys 39 1 (1986)

C. Review of Lattice Statics GF

V.K.T. – Adv. in Phys. 22 757 (1973)

D. Quasi Static GF

E. J. Savino & V.K.T. - J. Phys F 3 1919 (1973)

E. Composites

1. V.K.T., R. Wagoner & J.P. Hirth - J. Mat. Res.
   (a) 4 p 113, (1989)
   (b) 4 p. 124, (1989)

2. V.K.T.; Ed Fuller & Robb Thomson – J. Mat. Res.
   (a) 4, p. 309 (1989)
   (b) 4, p. 320 (1989)

1. Basic Models - Lattice statics GF (B-VK model), Continuum Model, Correspondence between the two models

2. Continuum GF for a crack - Hilbert's eqn & its solution

3. Continuum GF for an interfacial crack in a composite

4. Continuum GF for a composite containing a free surface or a crack normal to the interface

5. Lattice statics GF for a crack.

6. Lattice statics GF for a free surface.

GF - Math. definition

$$\hat{L}(x)\, y(x) = f(x)$$

Subject to Homogeneous Dirichlet, Neumann or Mixed Boundary Cond.

GF is a soln of

$$\hat{L}(x)\, G(x, x') = \delta(x - x')$$

$$y(x) = \int_{sp.} G(x, x')\, f(x')\, dx'$$

In matrix representation

$$L_{ij}\, G_{jk} = \delta_{ik}$$

$$G = [L]^{-1}$$

G - Response Function

$f(x) \rightarrow$ Probe function

Math Prob Zeroes of L are Poles or Singularities of G.

Examples

$$L(x)\,y(x) \equiv \frac{d^2 y}{dx^2} - a^2 y = e^{-x^2}$$

$y=0$ at $x=0$, $\quad y=0$ at $x=\ell$

$$d^2G/dx^2 - a^2 G = \delta(x-x')$$

$$0 \le x, x' \le \ell$$

$$G = \sum_n A_n \sin n\pi x/\ell$$

$$-\sum_n (n^2+a^2)\sin\frac{n\pi x}{\ell} A_n = \delta(x-x')$$

$$A_n = -\frac{\sin n\pi x'/\ell}{n^2+a^2}$$

$$G(x,x') = -\sum_n \frac{1}{n^2+a^2}\cdot \sin\frac{n\pi x}{\ell}\sin\frac{n\pi x'}{\ell}$$

$$y(x) = -\sum_n \frac{1}{n^2+a^2}\sin\frac{n\pi x}{\ell}\int_0^\ell \sin\frac{n\pi x'}{\ell}\, e^{-x'^2}\,dx'$$

satisfies B.C. and the eqn.

2-d example

$(\mathrm{Re}\, p > 0)$

$$\hat{L}(\underline{x})\,y(\underline{x}) = f(x) \qquad x \equiv (x_1, x_2)$$

$$\hat{L} = p^2\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2}$$

Generalised Laplace's eqn / Elliptic eqn.

B.C. $\qquad \nabla y \to 0$ at $|x| \to \infty$

$$p^2\frac{\partial^2 G}{\partial x_1^2} + \frac{\partial^2 G}{\partial x_2^2} = \delta(x-x')$$

$$G(x,x') = \int_{-\infty}^{\infty} dk_1\,dk_2\; G(k)\, e^{i(k_1x_1+k_2x_2)}$$

$$\partial/\partial x_1 = ik_1, \quad \partial/\partial x_2 = ik_2$$

Diff. eqn becomes

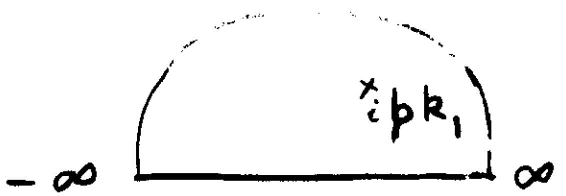
$$-\int_{-\infty}^{\infty} dk_1\,dk_2\,[k_2^2 + p^2k_1^2]\,G(k)\,e^{ik\cdot x} = \delta(x-x')$$

$$k\cdot x = k_1x_1 + k_2x_2$$

$$G(k) = -\frac{e^{-ik\cdot x'}}{k_2^2 + p^2 k_1^2}$$

$$G(x,x') = -\int_{-\infty}^{\infty} dk_1\, dk_2 \frac{e^{ik\cdot(x-x')}}{k_2^2 + p^2 k_1^2}$$

$$G(x) = -\int_{-\infty}^{\infty} dk_1\, e^{ik_1 x_1} \int_{-\infty}^{\infty} \frac{e^{ik_2 x_2}\, dk_2}{(k_2 + ipk_1)(k_2 - ipk_1)}$$



$$G(x) = -\frac{2\pi i}{2ip} \cdot \int_{-\infty}^{\infty} \frac{e^{ik_1 x_1 - p|k_1| x_1}}{|k_1|}\, dk_1$$

$$= -\frac{\pi}{p} \cdot Re \int_0^{\infty} \frac{e^{ik_1 z}}{k_1}\, dk_1$$

$$= -\frac{\pi}{p}\, Re\ I(z)$$

where $I(z) = \int_0^{\infty} \frac{e^{ik_1 z}}{k_1}\, dk_1$

$$I(z) = \int_0^{\infty} \frac{e^{ik_1 z}}{k_1}\, dk_1$$

$$z = x_1 + ipx_2$$

$$\frac{dI}{dz} = i\int_0^{\infty} e^{ik_1 z}\, dk_1$$

$$= i \left| \frac{e^{ik_1 z}}{iz} \right|_0^{\infty}$$

$$= \frac{1}{z} \quad ; \quad I(z) = \int dz/z$$

$$I(z) = Ln\ z$$

$$G(x) = -\frac{\pi}{p}\ Re\ Ln\left[x_1 + ipx_2\right]$$

Continuum Model

$\underline{u}(\underline{x})$ Displacement Field

$$\underline{x} \Rightarrow x_1, x_2, x_3$$

$$\underline{u} \Rightarrow u_1, u_2, u_3$$

Strain Tensor ϵ_{ij} $(i, j = 1, 2, 3,$

$$\epsilon_{11} = \partial u_1/\partial x_1 \quad , \quad \epsilon_{22} = \partial u_2/\partial x_2$$

$$\epsilon_{12} = \frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}$$

Stress Tensor τ_{ij}

$$\tau_{ij} = c_{ijkl} \, \epsilon_{kl}$$

(ij) & (kl) can be interchanged

$\left.\begin{matrix} i & l & j \\ k & \delta & l \end{matrix}\right\}$ can be interchanged

Transformation Law

$$c_{ijkl} = S_{ii'} S_{jj'} S_{kk'} S_{ll'} c_{i'j'k'l'}$$

Calculation of displacement field

Equations of elastic equilibrium

$$\hat{L}_{ij}(x) \, u_j(x) = -f_i(x)$$

where

$$\hat{L}_{ij} = c_{ikjl} \frac{\partial^2}{\partial x_k \partial x_l}$$

$$\hat{L}_{ij}(x) \, G_{jk}(x, x') = -\delta_{ik} \, \delta(x - x')$$

Then

$$u_i(x) = \int_{sp.} G_{ij}(x, x') \, f_j(x') \, dx'$$

GF – Displacement for a unit force

$$\tau_{i2}(x) = \int G^{\tau_2}_{ij}(x, x') \, f_j(x') \, dx'$$

Stress Green's function for $\tau_{i1} \sim \tau_{i2}$

Fourier Transform Method

$$u_i(x) = \frac{1}{(2\pi)^3}\int_{-\infty}^{\infty} u_i(q)\, e^{i q\cdot x}$$

Normalization

$$\frac{1}{(2\pi)^3}\int_{-\infty}^{\infty} e^{i q\cdot x}\, d\underline{q} = \delta(\underline{x})$$
$$\equiv \delta(x_1)\,\delta(x_2)\,\delta(x_3)$$

$$\partial/\partial x_i = i q_i$$

$$G_{ij}(x) = \frac{1}{(2\pi)^3}\int_{-\infty}^{\infty} G_{ij}(q)\, e^{i q\cdot x}\, dq$$

$$\hat{L}_{ij}(x)\, G_{jm}(x) =$$
$$\frac{1}{(2\pi)^3}\int_{-\infty}^{\infty} d\underline{q}\; c_{ikjl}\, q_k q_l\, G_{jm}(q)\, e^{i q\cdot x}$$
$$= -\delta_{im}\,\delta(x)$$

$$c_{ikjl}\, q_k q_l\, G_{jm}(q) = \delta_{im}$$

Christoffel's Matrix

$$\Lambda_{ij}(q) = c_{ikjl}\, q_k q_l$$

$$\Lambda_{ij}(q)\, G_{jm}(q) = \delta_{im}$$

$$\Lambda(q)\, G(q) = 1$$

$$G(q) = \left[\Lambda(q)\right]^{-1}$$

Christoffel's matrix is a representation of $\hat{L}$ in q-space / Fourier space

$G(q)$ is inverse of $\Lambda(q)$

$\Lambda(q)$ also(!) determines wave propagation in solids

Eigen values of $\Lambda(q)$ = $\omega^2(q)$

Eigen vectors — Polarisation vectors

q — wave vector of the wave

Christoffel's Matrix for Cubic Solids

$C_{11}\,,\ C_{12}\,,\ C_{44}$

$$\Lambda_{ij} = C_{44}\left(q^2 + \tau q_i^2\right)\delta_{ij} + \left(C_{12}+C_{44}\right) q_i q_j \qquad \left[\begin{array}{l}\text{No sum}\\ \text{over } i\end{array}\right]$$

$$\begin{bmatrix} C_{44}(q^2+\tau q_1^2)+(C_{12}+C_{44})q_1^2 & (C_{12}+C_{44})q_1q_2 & \cdots \\ & C_{44}(q^2+\tau q_2^2)+(C_{12}+C_{44})q_2^2 & \cdots \\ (C_{12}+C_{44})q_3q_1 & \cdots & \cdots \end{bmatrix}$$

$$\tau = \left(C_{11} - C_{12} - 2C_{44}\right)/C_{44}$$

$$q^2 = q_1^2 + q_2^2 + q_3^2$$

Eigen values of $\Lambda(q) = O(q^2)$

$$\omega^2(q) \propto q^2$$

$\omega(q)/q$ or $d\omega/dq \rightarrow$ Indep. of the Magnitude of q

Continuum Model is <u>NON DISPERSIVE</u>

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$$G_{ij}(q) = \frac{1}{C_{44}q^2}\left[K_i\delta_{ij} - \gamma_0 K_i K_j n_i n_j \times \left\{1 + \gamma_0 \sum_{i=1}^{3} K_i n_i^2\right\}^{-1}\right]$$

$$K_i = \frac{1}{1+\tau n_i^2}$$

$$\gamma_0 = (C_{12}+C_{44})/C_{44}$$

$$n_i = q_i/q$$

<u>For $\tau = 0$</u>

$$G_{ij}(x) = \frac{1}{4\pi C_{44}}\left[\frac{\delta_{ij}}{|x|} - \frac{\beta_0}{2}\nabla_i\nabla_j x\right]$$

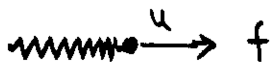
$$\beta_0 = (C_{12}+C_{44})/(C_{12}+2C_{44})$$

Dependence of $G(x)$ on x in the Cont Model

<u>3d</u> $\quad G(x) \propto 1/x$

2d $\quad G(x) \propto \ln x$

Lattice Statics



$$f = ku$$

$$u = \frac{1}{k} f$$

$1/k$ is the Green's function

$$W = -\frac{1}{2} k u^2$$

$$f = -dW/du = ku$$

$$W = W(u_\ell)$$

$$= W_0 + \sum_{i\ell} \Phi_i(\ell)\, u_i(\ell) + \frac{1}{2} \sum_{\ell\ell'} \Phi_{ij}(\ell,\ell')\, u_i(\ell)\, u_j(\ell')$$

$$+ \cdots$$

$$\Phi_i(\ell) = \frac{\partial W}{\partial u_i(\ell)} = -f_i(\ell)$$

$$\Phi_{ij}(\ell,\ell') = \frac{\partial^2 W}{\cdots}$$

For equilibrium

$$\frac{\partial W}{\partial u_i(\ell)} = 0$$

$$\sim \quad -f_i(\ell) + \sum_{j\ell'} \phi_{ij}(\ell,\ell')\, u_j(\ell') = 0$$

$$\sim \quad \sum_{j\ell'} \phi_{ij}(\ell,\ell')\, u_j(\ell') = f_i(\ell)$$

$$\begin{array}{cc} & \begin{array}{ccc} 0 & 1 & 2 \end{array} \\ \begin{array}{c} 0 \\ 1 \\ 2 \end{array} & \left[\begin{array}{ccc} \Phi_0 & \Phi_1 & \cdots \\ \vdots & & \\ & & \end{array}\right] \end{array} \begin{bmatrix} u_1(0) \\ u_2(0) \\ u_3(0) \\ \vdots \end{bmatrix} = \begin{bmatrix} f_1(0) \\ f_2(0) \\ f_3(0) \\ \vdots \end{bmatrix}$$

$$\Phi \cdot u = f$$

$$u = Gf \equiv [\Phi]^{-1} f$$

$$G = [\Phi]^{-1}$$

$$\sum_{j\ell'} G_{ij}(\ell,\ell')\, \Phi_{jk}(\ell',\ell'') = \delta_{ik}\, \delta(\ell,\ell'')$$

Stability Conditions

$$u_j(l) = \epsilon \, \delta_{jk}$$

$$F_i(l) = \sum_{l'} \Phi_{ik}(l,l')\,\epsilon = 0$$

$$\sum_{l'} \Phi_{ik}(l,l') = 0 \quad \text{for all } l, \; i \,\&\, k$$

Total force on a solid $= 0$

$$\sum_{l} f_i(l) = 0$$

Symmetry Considerations

Translation symmetry - All sites alike

$$\Phi(l,l') \equiv \Phi(l'-l)$$

$$f(l) \; - \; \text{Independent of } l$$

$$f(l) = 0 \quad \text{for all } l$$

Rotation Symmetry

S - Matrix of proper or improper rotation

$$\Phi(L,L') = \tilde{S}\,\Phi(l,l')\,S$$

where $L = Sl$

$L' = Sl'$

and

$$f(L) = S\,f(l)$$

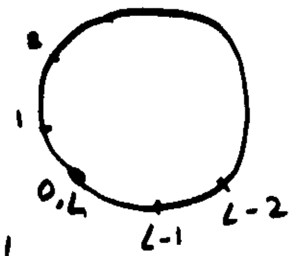
Assumptions

1. Adiabatic Approx.

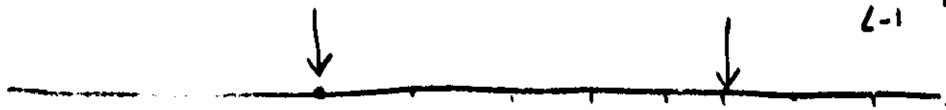
2. Cyclic Boundary Condition

$$u(0) = u(L)$$

$$\Phi(1,0) = \Phi(1,L)$$



Super Cell



$$\Phi u = f$$

&

$$u = G f$$

1. Perfect Crystal – Full Trans. Symm.

$$\Phi(l,l') \equiv \Phi(l-l')$$

$$f(l) = 0$$

or/and

$$= \text{External force}$$

2. Any defect in crystal or any discontinuity

$$\Phi^*(l,l') \text{ depend upon } l \text{ \& } l'$$

$$f(l) \text{ non zero}$$

1. Perfect Latt. GF

$$G = \Phi^{-1}$$

2. Defect GF

$$G^* = [\Phi^*]^{-1}$$

Effect of Defects on a lattice

$f(l)$ become non zero

$\Phi(l,l')$ changes to $\Phi^*(l,l')$

Object is to calculate G^*

$$u = G^*[f + F_{Load}]$$

$$\Phi^* = \Phi - \delta\Phi$$

$$G^* = [\Phi^*]^{-1} = \{\Phi[1-\Phi^{-1}\delta\Phi]\}^{-1}$$

$$= [1-\Phi^{-1}\delta\Phi]^{-1}\cdot\Phi^{-1}$$

$$= [1-G\delta\Phi]^{-1}G$$

$$[1-G\delta\Phi]G^* = G$$

$$\boxed{G^* = G + G\,\delta\Phi\,G^*}$$ Dyson's Equation

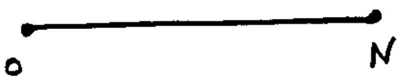
For any additional defect, Take G^* for one defect as the starting GF

Calculation of G

Fourier Transform & Reciprocal Space Formulation.

1-d Case

$$u(l) = \frac{1}{N} \sum_q u(q)\, e^{iql}$$



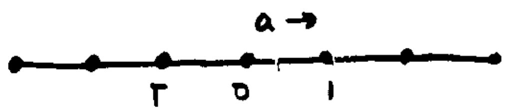
$$u(0) = u(N)$$

$$e^{iqL} = 1 \; ; \quad q = 2n\pi/N$$

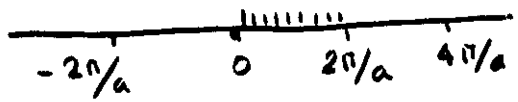
$$n = 0, 1, \dots N$$

q takes N discrete values

Brillouin zone



Reciprocal space →



Half weight for 0 & N — Real Space

0 & 2π — Recip. space

Gen. Case

$$u(l) = \frac{1}{N} \sum_q u(q)\, e^{iq\cdot l}$$

orthogonality

$$\frac{1}{N} \sum_q e^{iq\cdot l} = \delta(l)$$

$$\frac{1}{N} \sum_l e^{iq\cdot l} = \delta(q)$$

$$G(l, l') = G(l-l') = \frac{1}{N} \sum_q G(q)\, e^{iq\cdot(l-l')}$$

$$\phi(l, l') = \frac{1}{N} \sum_q \phi(q)\, e^{iq\cdot(l-l')}$$

$$\sum_{l'} \phi(l, l')\, G(l', l'') = \delta(l - l'')$$

$$\phi(q)\, G(q) = 1$$

$$G(q) = \left[\phi(q)\right]^{-1}$$

$$\phi(q) = \sum_l \phi(0, l)\, e^{iq\cdot l}$$

Statics & Dynamics

$$\sum_{\ell'} \Phi(\ell,\ell')\, u(\ell') = f(\ell)$$

$$\Phi(q)\, u(q) = f(q)$$

For dynamics $u(\ell) \to u(\ell)\, e^{i\omega t}$

$$f(\ell) = M\, \partial^2 u(\ell)/\partial t^2$$

$$= -M\omega^2 u(\ell)$$

$$\Phi(q)\, u(q) = -M\omega^2 u(q)$$

Eigenvalues of $\Phi(q)$ are ω^2

ie $(\text{phonon frequencies})^2$

Eigenvectors of $\Phi(q)$ are the polarisation vectors

$$G(q,\omega^2) = \left[M\omega^2 + \Phi(q)\right]^{-1}$$

Time dependent forces

$$u(q,\omega^2) = G(q,\omega^2)\, f(q)$$

Static GF $= \underset{\omega=0}{Lt}$ Dynamic G.F

No explicit dependence on Mass

$$G(0,\ell) = \frac{1}{N}\sum_q \left[\Phi(q)\right]^{-1} e^{iq\cdot\ell}$$

Correspondence with the continuum

$Lt\ q \to 0$, $\omega^2(q) \to$ same

$$\frac{1}{M}\Phi(q) = \frac{1}{\rho}\Lambda(q)$$

$$\rho = M/(\text{Volm of a unit cell})$$

$$\Phi(q) = a^3 \Lambda(q)$$

Force/Length $\quad L^3 \cdot \frac{F}{L^2} \cdot \frac{1}{L^2}$

$$\underset{q\to 0}{Lt}\ \Phi(q) = \Lambda(q)$$ (units to be accounted for)

(Relates Force Constants to Elastic Constt.)

Dispersive Nature of Discrete Model 5

$$\Phi(q) = \sum_{l} \Phi(l)\, e^{iq\cdot l}$$

$$\omega^2(q) \approx \epsilon(q) \approx 1-\cos ql, \ \sin^2 ql$$

$d\omega/dq$ or ω/q is function of q

Lt $q \to 0$

$$\omega^2(q) \approx q^2 \longrightarrow \text{Continuum Model}$$

$$\sin^2 ql, 1-\cos ql \approx q^2$$

At $q=0$, $\Phi(q)$ & $\Lambda(q) = 0$

Since $\mathop{Lt}_{q\to 0} \Phi(q) = \sum_{l} \Phi(l) = 0$

Limiting form of G F

$$G(l) = \frac{1}{N}\sum_{q} G(q)\, e^{iq\cdot l}$$

$$= \frac{1}{N}\sum_{q} \left[\Lambda(q)\right]^{-1} e^{iq\cdot l}$$

$$G(l) \approx \frac{1}{N}\sum_{q} \frac{1}{\omega^2(q)}\, e^{iq\cdot l}$$

For $l \to \infty$

$$\approx \int_0^\infty \frac{e^{iq\cdot l}}{q^2}\, d\underline{q} \quad \text{(Dubbin's Lemma)}$$

$$\approx \int_0^\infty\int_0^\pi \frac{e^{iql\cos\theta}\, q^2 \sin\theta\, d\theta\, d\phi}{q^2}$$

$$\approx \int_0^\infty \frac{\sin ql}{ql}\, dq \approx 1/l$$

For 2-d

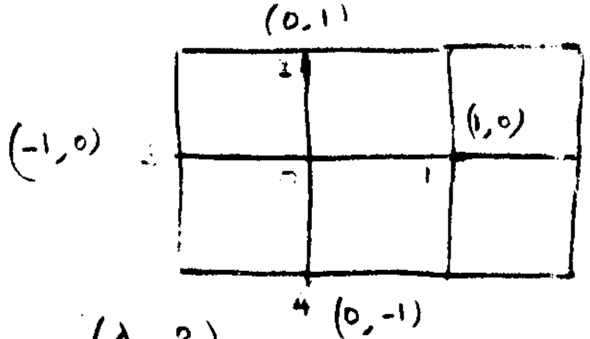
$$\int_0^\infty\int_0^{2\pi} \frac{e^{iql\cos\theta}}{q^2}\, q\, d\theta\, dq$$

$$\approx \int d\theta \int_0^\infty \frac{e^{iql\cos\theta}}{q}\, dq \approx \ln l$$

For large l

Discrete G.F. $\rightarrow$ Continuum G.F

Example



$$\Phi(0,1) = -\begin{pmatrix} \lambda & 0 \\ 0 & \mu \end{pmatrix}$$

$$r(0,2) = S\, r(0,1)$$

$$S_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\Phi(0,2) = \tilde{S}_1 \Phi(0,1) S_1 = -\begin{pmatrix} \mu & 0 \\ 0 & \lambda \end{pmatrix}$$

$$\Phi(0,3) = \tilde{S}_2 \Phi(0,1) S_2 = -\begin{pmatrix} \lambda & 0 \\ 0 & \mu \end{pmatrix}$$

$$S_2 = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\Phi(0,4) = \tilde{S}_2 \Phi(0,2) S_2 = -\begin{pmatrix} \mu & 0 \\ 0 & \lambda \end{pmatrix}$$

Calculation of $\Phi(0,0)$

$$\sum_{l} \Phi(l) = 0$$

$$\Phi(0,0) = -\left[\Phi(0,1) + \Phi(0,2) + \Phi(0,3) + \Phi(0,4)\right]$$

$$\Phi(0,0) = 2(\lambda+\mu)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Calculation of $\Phi(q)$

$$\Phi(q) = \sum_{l} \Phi(l) e^{iq\cdot l} \qquad \Big| \quad q\cdot l = q_1 l_1 + q_2 l_2$$

$$\Phi_{ij} = \Phi_{ij}(0,0) + \Phi_{ij}(0,1) e^{iq_1} + \Phi_{ij}(0,2) e^{iq_2} + \Phi_{ij}(0,3) e^{-iq_1} + \Phi_{ij}(0,4) e^{-iq_2}$$

$$= \begin{bmatrix} 2\lambda(1-\cos q_1) + 2\mu(1-\cos q_2) & 0 \\ 0 & 2\lambda(1-\cos q_2) + 2\mu(1-\cos q_1) \end{bmatrix}$$

$$G(q) = \begin{bmatrix} \dfrac{1}{2\left[\lambda(1-\cos q_1) + \mu(1-\cos q_2)\right]} & 0 \\ 0 & \dfrac{1}{2\left[\lambda(1-\cos q_2) + \mu(1-\cos q_1)\right]} \end{bmatrix}$$

units $\mu = 1$

Low q Limit

$$G(q) = \begin{bmatrix} \dfrac{1}{A^2 q_1^2 + q_2^2} & 0 \\ 0 & \dfrac{1}{A^2 q_2^2 + q_1^2} \end{bmatrix}$$

$$G(\ell) = \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} \frac{e^{i(q_1 \ell_1 + q_2 \ell_2)}}{A^2 q_1^2 + q_2^2}\, dq_1\, dq_2$$

$$\approx \ln(\ell_1 + iA\ell_2)$$

$$\ell_1 + iA\ell_2 \rightarrow \left[\ell_1^2 + A^2 \ell_2^2\right]^{1/2} \exp i \tan^{-1} \frac{A\ell_2}{\ell_1}$$

$$\approx \frac{1}{2} \ln\left[\ell_1^2 + A^2 \ell_2^2\right] + i \tan^{-1} \frac{A\ell_2}{\ell_1}$$

Edge dislocation component

Screw Dislocation Component

Defect Green's function

$$\phi^* = \phi - \delta\Phi$$

$$G^* = G + G\,\delta\Phi\, G^*$$

$$= (1 - G\,\delta\Phi)^{-1} G$$

$$\delta\Phi = \begin{array}{c|c} & \begin{array}{cc} n & N-n \end{array} \\ \begin{array}{c} n \\ N-n \end{array} & \left[\begin{array}{c|c} \delta\varphi & 0 \\ \hline 0 & 0 \end{array}\right] \end{array}$$

Defect Space

$$G = \begin{array}{c|c} & n \\ n & \left[\begin{array}{c|c} g_0 & G_I \\ \hline \tilde{G}_I & G_{II} \end{array}\right] \end{array}$$

$$G^* = \left[\begin{array}{c|c} g^* & G_I^* \\ \hline \tilde{G}_I^* & G_{II}^* \end{array}\right]$$

$$G\,\delta\Phi\, G^* = \left[\begin{array}{c|c} g\,\delta\varphi\, g^* & --- \\ \hline --- & --- \end{array}\right]$$

Dyson's equation in defect space

$$g^{*} = g + g\,\delta\phi\, g^{*}$$

$$= (1 - g\,\delta\phi)^{-1} g$$

g, $\delta\phi$ are matrices of finite dimensions & Inverse can be easily obtained.

Relaxation Energy of defects

$$\Delta W = W - W_0 = -\sum_{l} f(l)\, u(l) + \frac{1}{2}\sum_{ll'} \Phi^{*}(l,l')\, u(l)\, u(l')$$

$$u(l) = \sum_{l'} G^{*}(l,l')\, f(l')$$

$$= -f G^{*} f + \frac{1}{2} f G^{*} \Phi^{*} G^{*} f$$

$$= -\frac{1}{2} f G^{*} f$$

Cont. GF for a crack $[q_3 = 0]$

$$G_{ij}(q) = [\Lambda(q)]^{-1}_{ij}$$

$$= \Gamma'_{ij}(q) / D(q)$$

Determinant

$$D(q) = \prod_{\alpha=1}^{3} \epsilon_{\alpha}(q)$$

$$\epsilon_{\alpha}(q) = a_{\alpha}(q_2^2 + b_{\alpha} q_2 q_1 + c_{\alpha} q_1^2)$$

$$= a_{\alpha}(q_2 - p_{\alpha} q_1)(q_2 - p_{\alpha}^{*} q_1)$$

$$\mathrm{Im}\; p_{\alpha} > 0$$

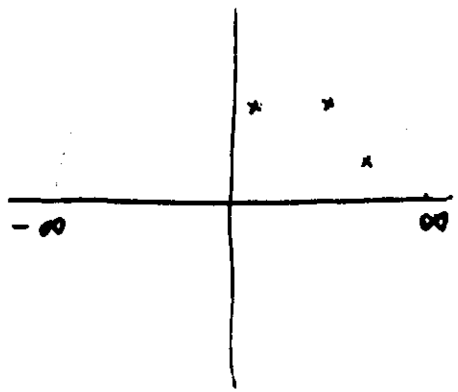
$$D(q) = a \prod (q_2 - p_{\alpha} q_1)(q_2 - p_{\alpha}^{*} q_1)$$

$$G_{ij}(x) = \frac{1}{4\pi^2}\int_{-\infty}^{\infty} G_{ij}(q)\, e^{i(q_1 x_1 + q_2 x_2)}\, dq$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} dq_1\, e^{i q_1 x_1}\, g_{ij}(q_1, x_2)$$

$$g_{ij}(q_1, x_2) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dq_2\, G_{ij}(q)\, e^{i q_2 x_2}$$

$$g_{ij}(q_1, x_2) = \frac{1}{2\pi a}\int_{-\infty}^{\infty} \frac{\Gamma_{ij}(q)\, e^{i q_2 x_2}\, dq_2}{\prod_\alpha (q_2 - p_\alpha q_1)(q_2 - p_\alpha^* q_1)}$$



Poles at $q_2 = p_\alpha q_1$

$$g_{ij}(q_1, x_2) = \frac{2\pi i}{2\pi a}\sum_\alpha \frac{\Gamma_{ij}(q_2 = p_\alpha q_1)\, e^{i p_\alpha q_1 x_2}}{q_1^5 (p_\alpha - p_\alpha^*) \prod_{\beta\neq\alpha}(p_\alpha - p_\beta)(p_\alpha - p_\beta^*)}$$

$$= \frac{1}{q_1}\sum_\alpha l_{ij}(p_\alpha)\, e^{i q_1 p_\alpha x_2}$$

$$l_{ij}(p_\alpha) = \frac{i}{a q_1^4}\, \frac{\Gamma_{ij}(q_2 = p_\alpha q_1)}{\left[\prod_{\beta\neq\alpha}(p_\alpha - p_\beta)(p_\alpha - p_\beta^*)\right]}\, \frac{1}{(p_\alpha - p_\alpha^*)}$$

Independent of q_1

$$\int_{-\infty}^{\infty} \frac{e^{i q_1 [x_1 + p_\alpha x_2]}}{q_1}\, dq_1$$

$$= -2\,\mathrm{Re}\,\ln z_\alpha$$

$$z_\alpha = x_1 + p_\alpha x_2$$

$\boxed{\text{Disp. GF}}$

$$\boxed{G_{ij}(x) = -\frac{1}{\pi}\,\mathrm{Re}\sum_\alpha l_{ij}(p_\alpha)\ln z_\alpha}$$

Stress-2 GF

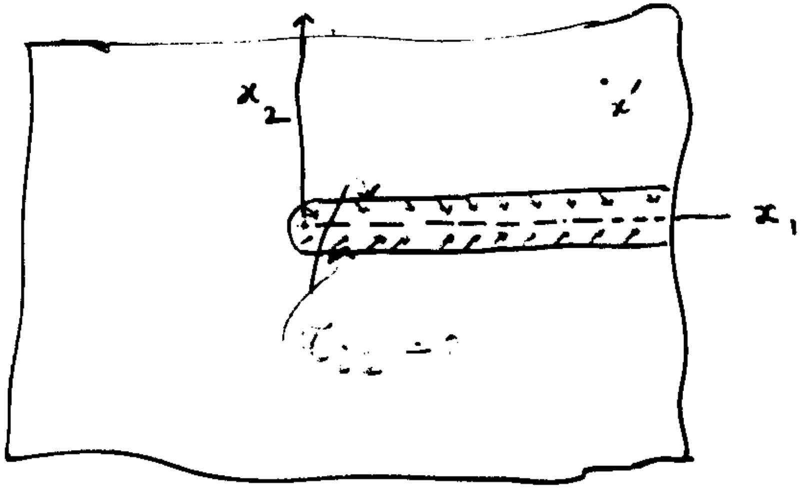
$$\tau_{i2} = C_{i2jk}\left[\partial u_j/\partial x_k + \partial u_k/\partial x_j\right]$$

$$\frac{\partial}{\partial x_1} = \frac{\partial}{\partial z_\alpha}\frac{\partial z_\alpha}{\partial x_1} = \frac{d}{dz_\alpha}$$

$$\frac{\partial}{\partial x_2} = \frac{\partial}{\partial z_\alpha}\frac{\partial z_\alpha}{\partial x_2} = p_\alpha \frac{\partial}{\partial z_\alpha}$$

$$\boxed{G^{\tau_2}_{ij}(x) = -\frac{1}{\pi}\,\mathrm{Re}\sum_\alpha \sigma_{ij}(p_\alpha)\,\frac{1}{z_\alpha}}$$

$$\sigma_{ij}(p_\alpha) = (C_{i2k1} + C_{i2k2}\, p_\alpha)\, l_{kj}(p_\alpha)$$



$$\hat{L} u \equiv c_{ikjl} \frac{\partial^2 u_j}{\partial x_k \partial x_l} = -f_i(x) \equiv f_i \delta(x-x')$$

(except over the crack region)

$$u = \int G(x, x') F(x') \, dx'$$

$$\hat{L} u = F(x)$$

For $F(x)$ outside the solution space

u_0 is a solution of the homogeneous eqn

$$\hat{L} u_0 = 0$$

$$u = u_p + u_0 \quad \text{where } \hat{L} u_p = -f$$

$$u(x) = -\frac{1}{\pi} \operatorname{Re} \sum_{\alpha=1}^{3} \gamma(p_\alpha) \ln(z_\alpha - s_\alpha) f_1$$

upp. surf

$$\operatorname{Re} -\frac{1}{\pi} \left\{ \sum_{\alpha=1} \gamma(p_\alpha) \int_0^\infty \ln(z_\alpha - t_+) \right\} F_1(t) \, dt$$

$$\left[\begin{aligned} z'_\alpha &= t + p_\alpha y = t_+ \quad \text{for } y = 0^+ \\ &\equiv t + i\epsilon \quad (\text{for } \epsilon = 0^+) \end{aligned} \right]$$

Lower surf.

$$\underline{\operatorname{Re}} -\frac{1}{\pi} \left\{ \sum_\alpha \gamma(p_\alpha) \int_{-\infty}^0 \ln(z_\alpha - t_-) \right\} F_2(t) \, dt$$

$$\tau_{i2} = -\frac{1}{\pi} \operatorname{Re} \sum_\alpha \sigma(p_\alpha) \cdot \frac{1}{z_\alpha - s_\alpha}$$

$$-\frac{1}{2\pi} \sum_\alpha \int_0^\infty \left[\frac{\sigma(p_\alpha)}{z_\alpha - t_+} + \frac{\sigma^*(p_\alpha)}{z^*_\alpha - t_-} \right] F_1(t) \, dt$$

$$-\frac{1}{2\pi} \sum_\alpha \int_\infty^0 \left[\frac{\sigma(p_\alpha)}{z_\alpha - t_-} + \frac{\sigma^*(p_\alpha)}{z^*_\alpha - t_+} \right] F_2(t) \, dt$$

$$F_2(t) = -F_1(t)$$

$\tau_{i2} = 0$ at $x_2 = 0$

i.e. at $z_\alpha = x_1 + p_\alpha x_2 = x_1$

$$(\sigma_s + \sigma_s^*)\left[\int_0^\infty \frac{F(t)}{t_+ - x_1} + \int_0^\infty \frac{F(t)}{t_- - x_1}\right] dt$$

$$= 2\,\mathrm{Re} \sum_\alpha \sigma(p_\alpha) \cdot \frac{1}{x_1 - \rho_\alpha}$$

$$P\int_0^\infty \frac{F(t)\,dt}{t - x_1} = 2\left[\sigma_s + \sigma_s^*\right]^{-1} \sum_\alpha \sigma(p_\alpha) \cdot \frac{1}{x_1 - \rho_\alpha}$$

Hilbert's equation

Muskhelishvili – Singular Integ. Eqns

Sinclair & Hirth – J. Phys. F $\underline{5}$ 236 (1975)

Solution of Hilbert's equation

$$\boxed{T(q, t) = t^{iq - 1/2}}$$

$0 \le t \le \infty$

$-\infty \le q \le \infty$

$$I = \int_0^\infty t^{iq - \frac{1}{2}} \cdot t^{-iq' - 1/2}\,dt$$

$$= \int_0^\infty \frac{t^{i(q-q')}}{t}\,dt$$

$$I = \int_0^\infty \frac{e^{i(q-q')\ln t}}{t}\,dt$$

Let $\ln t = \eta$, $\frac{dt}{t} = d\eta$

$$I = \int_{-\infty}^\infty e^{i(q-q')\eta}\,d\eta = 2\pi\,\delta(q-q')$$

Orthogonality over t

$$\int_{-\infty}^{\infty} t_1^{\,iq-1/2}\, t_2^{\,-iq-1/2}\, dq$$

$$= \int_{-\infty}^{\infty} (t_1/t_2)^{iq} \cdot \frac{1}{\sqrt{t_1 t_2}}\, dq$$

$$= \int_{-\infty}^{\infty} e^{iq \ln(t_1/t_2)} \cdot \frac{1}{\sqrt{t_1 t_2}}\, dq$$

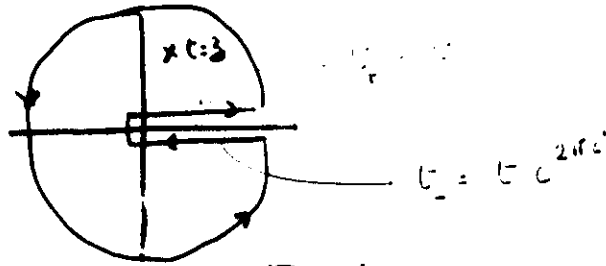
$$= 2\pi\, \frac{\delta\left[\ln t_1/t_2\right]}{\sqrt{t_1 t_2}} \qquad \{t_1 = t_2\}$$

$$= 2\pi\, \delta(t_1 - t_2)$$

$$F(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} A(q)\, t^{\,iq-1/2}\, dq$$

$$H(z) = \int_0^{\infty} \frac{F(t)}{t-z}\, dt$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} A(q)\, dq \int_0^{\infty} \frac{t^{\,iq-1/2}}{t-z}\, dt$$



Consider the contour integral

$$\oint \frac{T^{\,iq-1/2}}{T-z} = 2\pi i\, z^{\,iq-1/2}$$

$$= \int_0^{\infty} \frac{t^{\,iq-1/2}}{t-z} + \int_{\infty}^{0} \frac{\left(e^{2\pi i}\right)^{iq-1/2} t^{\,iq-1/2}}{t-z}$$

$$= \left[1 + e^{-2\pi q}\right] \int_0^{\infty} \frac{t^{\,iq-1/2}}{t-z}\, dt = 2\pi i\, z^{\,iq-1/2}$$

$$\int_0^\infty \frac{t^{iq-1/2}\,dt}{t-z} = \frac{2\pi i}{1+e^{-2\pi q}}\, z^{iq-1/2}$$

$$H(z) = i\int_{-\infty}^{\infty} \frac{A(q)\,dq}{1+e^{-2\pi q}}\, z^{iq-1/2}$$

Principal Values on the real axis

$$H(x_{1+}) = i\int_{-\infty}^{\infty} \frac{A(q)\, x_1^{iq-1/2}}{1+e^{-2\pi q}}$$

$(x_{1+} = x_1)$

$$H(x_{1-}) = -i\int_{-\infty}^{\infty} \frac{e^{-2\pi q}}{1+e^{-2\pi q}}\, A(q)\, x_1^{iq-1/2}$$

Hilbert's eqn

$$i\int_{-\infty}^{\infty} A(q)\, \frac{1-e^{-2\pi q}}{1+e^{-2\pi q}}\cdot x_1^{iq-1/2} = \sum_\alpha C(\alpha)\frac{1}{x_1-\rho_\alpha}$$

Multiply both sides by $x_1^{-iq-1/2}$ & integrate over x_1 from 0 to ∞

$$A(q) = \sum_\alpha \frac{C(\alpha)\,(\rho_\alpha)^{-iq-1/2}}{[e^{2\pi q}-1]}$$

Calculation of $H(z)$

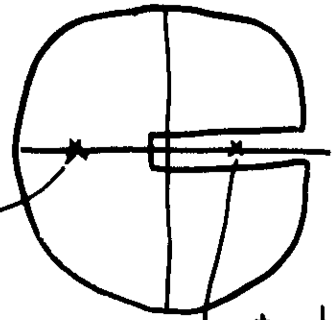
$$H(z) = i\sum_\alpha \frac{C(\alpha)}{\sqrt{z\rho_\alpha}}\int_{-\infty}^{\infty} \frac{(z/\rho_\alpha)^{iq}}{(e^{2\pi q}-1)(e^{-2\pi q}+1)}\,dq$$

$$e^{2\pi q} = t, \qquad dq = \frac{1}{2\pi}\frac{dt}{t}$$

$$I = \frac{1}{2\pi}\int_0^\infty \frac{dt}{t(t-1)(1/t+1)}\, t^{i\xi}$$

where $\xi = \frac{1}{2\pi}\ln z/\rho_\alpha$

$$I = \frac{1}{2\pi}\int_0^\infty \frac{t^{i\xi}\,dt}{(t^2-1)}$$



$T = -1 = e^{\pi i}$

$t = 1_+$

$T = 1_- = e^{2\pi i}$

$$\oint \frac{T^{i\xi}\,dT}{T^2-1} = 2\pi i\left[\frac{e^{-\pi\xi}}{-2} + \frac{1}{2\cdot 2}\left\{1+e^{-2\pi\xi}\right\}\right]$$

$$= \left[1-e^{-2\pi\xi}\right]\int_0^\infty \frac{t^{i\xi}}{t^2-1}\,dt$$

$$\int_0^\infty \frac{t^{i\epsilon}}{(t^2-1)}\,dt = \frac{\pi i}{2}\,\frac{\left[-2e^{-\pi\epsilon}+1+e^{-2\pi\epsilon}\right]}{1-e^{-2\pi\epsilon}}$$

$$= \frac{\pi i}{2}\,\frac{\left[1-e^{-\pi\epsilon}\right]^2}{1-e^{-2\pi\epsilon}}$$

$$= \frac{\pi i}{2}\,\frac{1-e^{-\pi\epsilon}}{1+e^{-\pi\epsilon}}$$

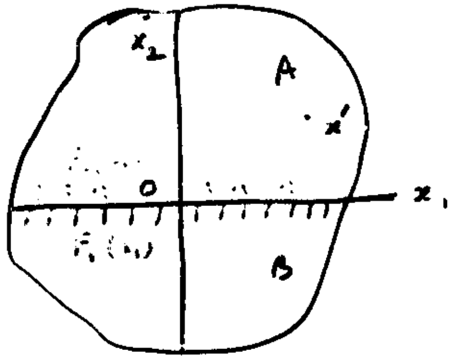
$$e^{-\pi\epsilon} = \exp -\tfrac{1}{2}\ln z/\zeta_\alpha = \sqrt{\zeta_\alpha}/\sqrt{z}$$

$$I = \frac{\pi i}{2}\,\frac{\sqrt{z}-\sqrt{\zeta_\alpha}}{\sqrt{z}+\sqrt{\zeta_\alpha}}$$

$$H(z) = -\frac{1}{4}\sum_\alpha C(\alpha)\,\frac{\sqrt{z}-\sqrt{\zeta_\alpha}}{\sqrt{z}+\sqrt{\zeta_\alpha}}\cdot\frac{1}{\sqrt{z}\,\zeta_\alpha}$$

The Familiar $1/\sqrt{z}$ singularity!

Interface Green Function



$C^A_{ijkl}\ ;\ p^A_\alpha$

$C^B_{ijkl}\ ;\ p^B_\alpha$

I Line force in UHP

UHP $\quad C^A_{ikjl}\dfrac{\partial^2 u^A_j}{\partial x_k \partial x_l} = \delta(x-x')$

LHP $\quad C^B_{ikjl}\dfrac{\partial^2 u^B_j}{\partial x_k \partial x_l} = 0$

Soln in UHP $\quad x_2 \geq 0$

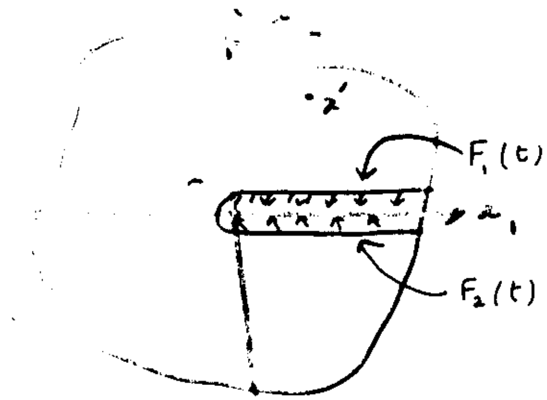
$$u^A(x) = -\frac{1}{\pi}\sum_\alpha v^A(p^A_\alpha) f \ln\left(z^A_\alpha - z'^A_\alpha\right)$$

$$-\frac{1}{\pi}\sum_\alpha v^A(p^A_\alpha)\int_{-\infty}^{\infty}\ln\left(z^A_\alpha - t_-\right)F_1(t)\,dt$$

$$u^B(x) = -\frac{1}{\pi}\sum_\alpha v^B(p^B_\alpha)\int_{-\infty}^{\infty}\ln\left(z^B_\alpha - t_+\right)F_2(t)\,dt$$

Boundary Conditions

$$\left.\begin{aligned} u^{A}(x_1, 0^{+}) &= u^{B}(x_1, 0^{-}) \\ \tau_{i2}(x_1, 0^{+}) &= \tau_{i2}(x_1, 0^{-}) \end{aligned}\right\} -\infty \le x_1 \le \infty$$



Green's Functions

UHP

$$G_i^{cA}(x, x') = -\frac{1}{\pi}\sum_{\alpha=1}^{3} v^{A}(p_\alpha^{A}) \, Ln(z_\alpha^{A} - z_\alpha'^{A})$$
$$-\frac{1}{\pi}\sum_{\alpha\beta=1}^{3} v^{A}(p_\alpha^{A}) \, \theta_\beta^{I} \, Ln(z_\alpha^{A} - z_\beta'^{A*})$$

LHP

$$G^{cB}(x, x') = -\frac{1}{\pi}\sum_{\alpha\beta=1}^{3} v^{*B}(p_\alpha^{B}) \, \theta_\beta^{II} \, Ln(z_\alpha^{B*} - z_\beta'^{A*})$$

$$\theta_\beta^{I} = M\left[\sigma^{*A}(p_\beta^{A}) - \sigma_s^{*B} \, v_s^{*B^{-1}} \, v^{*A}(p_\beta^{A})\right]$$

$$M = v_s^{A-1}\left[\sigma_s^{*B} \, v_s^{*B^{-1}} - \sigma_s^{A} \, v_s^{A-1}\right]^{-1}$$

$$u^{A}(x) = -\frac{1}{\pi}\sum_{\alpha=1}^{3} v^{A}(p_\alpha^{A}) \, f \, Ln(z_\alpha^{A} - z_\alpha'^{A})$$
$$-\frac{1}{\pi}\sum_{\alpha\beta=1}^{3} v^{A}(p_\alpha^{A}) \, \theta_\beta^{I} \, f \, Ln(z_\alpha^{A} - z_\beta'^{A*})$$
$$-\frac{1}{\pi}\sum_{\alpha=1}^{3} v^{A}(p_\alpha^{A}) \int_0^\infty Ln(z_\alpha^{A} - t_+) \, F_1(t) \, dt$$
$$-\frac{1}{\pi}\sum_{\alpha}^{3} v^{A}(p_\alpha^{A}) \, Q_s^{I} \int_0^\infty Ln(z_\alpha^{A} - t_-) \, F_1(t) \, dt$$
$$+\frac{1}{\pi}\sum_{\alpha=1}^{3} v^{A}(p_\alpha^{A}) \, Q_s^{III} \int_0^\infty Ln(z_\alpha^{A} - t_-) \, F_2(t) \, dt$$

Similar expression for u^{B}

Details in

V.K.T., R. Wagoner & J.P. Hirth

(i) J. Mater. Res. 4 p 113 (1989)

(ii) " " " 4 p 124 (1989)

Boundary condition

$$\tau_{c2}(x_1, 0^+) = 0$$
$$\tau_{c2}(x_1, 0^-) = 0$$

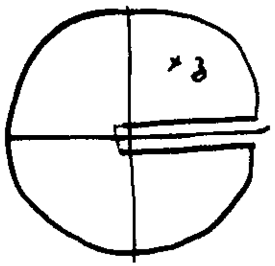
$$T_U H(x_1 +) + T_U^* H(x_1 -) = \sum_\alpha \frac{\sigma_S^{*B} a_\alpha^{*\Pi}}{x_1 - \xi_\alpha^{A*}}$$

$$H(z) = \int_0^\infty \frac{f(t)\,dt}{t - z} \qquad z - \text{a complex variable}$$

$$T_U = 1 + \sigma_S^A a_S^I (\sigma_S^{*A})^{-1}$$

$$f(t) = \frac{1}{2\pi}\int_{-\infty}^\infty A(q)\, t^{iq - 1/2}\, dq$$

$$\int_0^\infty \frac{t^{iq-1/2}}{t - z}\,dt = \frac{2\pi i}{1 + e^{-2\pi q}} z^{iq - 1/2}$$



$$H(z) = i\sum_\alpha \frac{C(\alpha)}{\sqrt{z\,\xi_\alpha^{A*}}} \int_{-\infty}^\infty \frac{(z/\xi_\alpha^{A*})^{iq}\, dq}{[e^{-2\pi q} + 1][T_U e^{2\pi q} - T_U^*]}$$

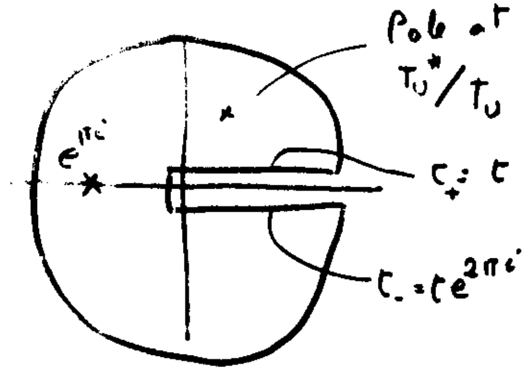
Substitution

$$e^{2\pi q} = t \quad , \quad dq = \frac{1}{2\pi} dt/t$$

$$I = \frac{1}{2\pi}\int_0^\infty \frac{dt \quad t^{i\zeta}\, dt}{(t+1)[T_U t - T_U^*]}$$

$$\zeta = \frac{1}{2\pi}\ln(z/\xi_\alpha)$$

$$\oint \frac{T^{i\zeta}\, dT}{(T+1)(T_U T - T_U^*)}$$



$$= \frac{2\pi i}{T_U}\left[-\frac{e^{-\pi\zeta}}{T_U + T_U^*} + \frac{(T_U^*/T_U)^{i\zeta}}{T_U + T_U^*}\right]$$

$$I = \frac{i}{T_U}\cdot\frac{1}{1 - e^{-2\pi\zeta}}\left[-e^{-\pi\zeta} + (T_U^*/T_U)^{i\zeta}\right]\frac{1}{T_U + T_U^*}$$

$$H(z) = \left(T_\cdot^* / T_\cdot\right)^{i\varepsilon}$$

$$\varepsilon = \frac{1}{2\pi} \ln\left(z/\rho_\alpha\right)$$

$$H(z) = e^{i\varepsilon\lambda 2\pi} \quad ; \quad \lambda = \frac{1}{2\pi} \ln\left(T_U^* / T_U\right)$$

$$= \exp i\lambda . \ln(z/\rho_\alpha)$$

$$\boxed{H(z) = \cos\left[\lambda \ln \frac{z}{\rho_\alpha}\right] + i \sin\left[\lambda \ln z/\rho_\alpha\right]}$$

$$z = x + p_\alpha y$$

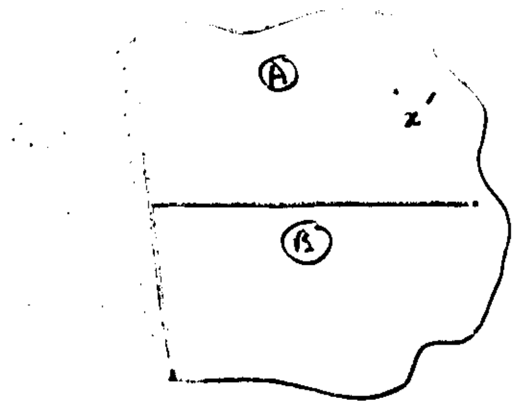
$$T_U = 1 + \sigma_S^A \theta_S^I \left(\sigma_S^{*A}\right)^{-1}$$

Solid A - Solid B Same

$T_U = T_U^*$; $\lambda = 0 \rightarrow$ No oscillations

Displacement field also oscillates out of phase over crack faces.

Free Surface in a Composite



G.F. Calculation

$$u^A(x) = G^A(x, x') f + \int_0^\infty G^A(x, x_2') F_1(x_2') dx_2' + \int_{-\infty}^0 G^B(x, x_2') F_2(x_2') dx_2'$$

Boundary conditions

$$\left.\begin{aligned} \tau_{i1}^A &= 0 \\ \tau_{i1}^B &= 0 \end{aligned}\right\} \text{ for } x_1 = 0$$

$$G \approx \ln(z - x_-)$$

$$\tau^A_{c1} \approx \frac{1}{z - x_2}$$

$$H^A(z) = \int_0^\infty \frac{F_1(t)}{t - z}\,dt$$

$$H^B(z) = \int_{-\infty}^{0} \frac{F_2(t)}{t - z}\,dt$$

<u>UHP</u> $$\int_0^\infty \frac{F_1(t)}{t - x_{2+}}\,dt + \int_0^\infty \frac{F_1(t)\,dt}{t - x_{2-}}$$

$$+ \; C_{AA}\int_0^\infty \frac{F_1(t)}{t - a x_2} + C_{AB}\int_{-\infty}^{0} \frac{F_2(t)}{t - b x_2} = f^A(x_2$$

Similar eqn for LHP

Generalised Vector Inhomogeneous Hilbert's eqn.

$$F_1(t) = \frac{1}{2\pi}\int_{-i\infty}^{i\infty} M^A(q)\, t^{iq - 1/2}\,dq$$

$$F_2(t) = \frac{1}{2\pi}\int_{-i\infty}^{i\infty} M^B(q)\, t^{iq - 1/2}\,dq$$

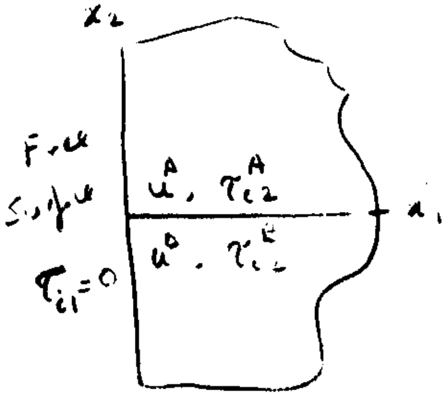
$$\int_{-i\infty}^{i\infty} dq \left[D_{AA}(q)\, M^A(q) + D_{AB}(q)\, M^B(q) \right] x_2^{iq - 1/2} = f^A(x_2)$$

$$\int_{-i\infty}^{i\infty} dq \left[D_{BA}(q)\, M^A(q) + D_{BB}(q)\, M^B(q) \right] x_2^{iq - 1/2} = f^B(x_2)$$

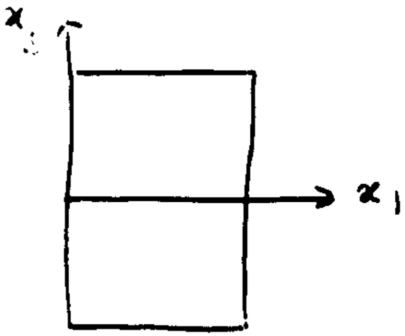
$$\begin{pmatrix} M^A(q) \\ M^B(q) \end{pmatrix} = \begin{pmatrix} D_{AA} & D_{AB} \\ D_{BA} & D_{BB} \end{pmatrix}^{-1} \begin{pmatrix} f^A \\ f^B \end{pmatrix}$$

$$H(z) \propto z^{-\frac{1}{2} + \epsilon} \quad \text{near } z \to 0$$

Generalized Plane Strain



Loading in z direction



$$\frac{\partial u_3}{\partial x_3} = \epsilon_3 \rightarrow \text{constant}$$

Applied Disp.

$$u_i = \delta_{i3}\, x_3\, \epsilon_3 + \text{Induced displacements}$$

$$u_i^A = \delta_{i3}\, x_3\, \epsilon_3 + T_i^A\, x_2 + F^A(x_1, x_2)$$

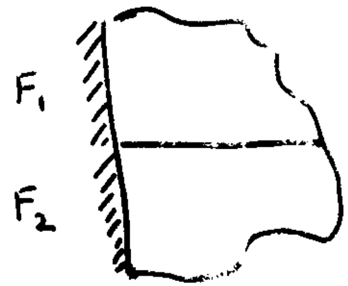
$$u_i^B = \delta_{i3}\, x_3\, \epsilon_3 + T_i^B\, x_2 + F^B(x_1, x_2)$$

$$u_i^A(x_1, 0^+) = u_i^B(x_1, 0^-)$$

$$\tau_{i2}^A(x_1, 0^+) = \tau_{i2}^B(x_1, 0^-) \longrightarrow \text{Determines } T_i^A \ \&\ T_i^B$$

$$u_i^A = \delta_{i3}\, x_3\, \epsilon_3 + T_i^A\, x_2 + \int_0^{\infty} G^{cA}(x, x_2')\, F_1(x_2')\, dx_2'$$

$$u_i^B = \delta_{i3}\, x_3\, \epsilon_3 + T_i^B\, x_2 + \int_{-\infty}^{0} G^{cB}(x, x_2')\, F_2(x_2')\, dx_2'$$



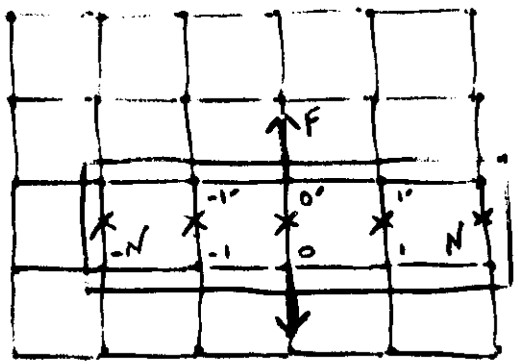
Determine F_1 & F_2

By imposing the condition

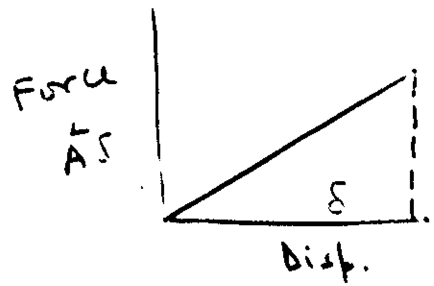
$$\tau_{i1} = 0 \quad \text{at} \quad x_1 = 0$$

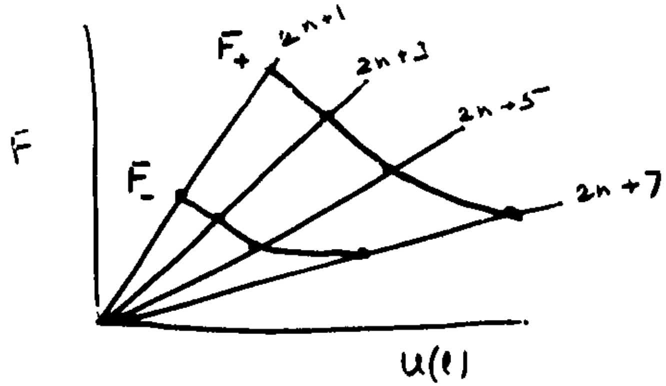
$$H(z) = z^{-\frac{1}{2}+\epsilon} \ ; \quad \ln z \quad \text{at } z \to 0$$

Hsieh & Thomson — J. Appl. Phys. 44 p 2051, (197–)



Atomic Interaction

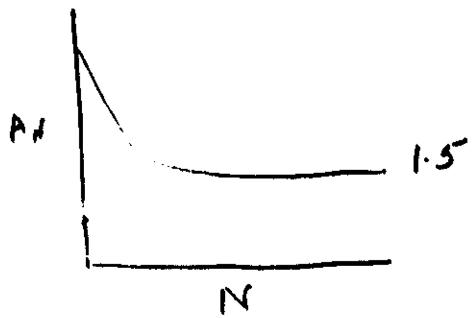




$$\delta\phi \quad \begin{array}{c|c} & 0 \quad 0' \quad 1 \quad 1' \quad -1 \quad -1' \\ \hline \begin{array}{c} 0 \\ 0' \\ 1 \\ 1' \\ \vdots \end{array} & \left[\begin{array}{c} (2N+1) \times (2N+1) \\ N = 1 - 50 \end{array} \right] \end{array}$$

$$u_N = G^*(0, N)\, F$$

$$A_N = \frac{F_+ - F_-}{F_-} \quad \text{— Lattice Trapping Parameter}$$



Composite Materials

1. Bimaterial Interface (Plane)

   Grain boundaries

   Phase boundaries

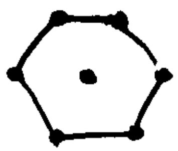
2. Fiber Composites

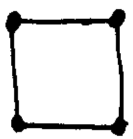
   Fibers reinforced Matrix

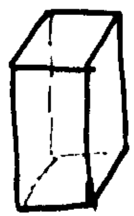
   a. Hexagonal Symmetry

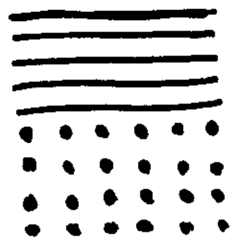
   b. Tetragonal Symmetry

   c. Cubic Symmetry ?









Average Elastic Constants

Rule of Mixtures

Total elastic energy

$$V_c \sigma_c \eta_c = V_1 \sigma_1 \eta_1 + V_2 \sigma_2 \eta_2$$

1. Voigt Estimate

$$\eta_c = \eta_1 = \eta_2$$

$$\sigma_c = K_c \eta_c \ , \ \sigma_1 = K_1 \eta_1 \ , \ \sigma_2 = K_2 \eta_2$$

$$V_c K_c \eta_c^2 = V_1 K_1 \eta_1^2 + V_2 K_2 \eta_2^2$$

$$K_c = \frac{V_1}{V_c} K_1 + \frac{V_2}{V_c} K_2$$

2. Reuss Estimate

$$V_c \sigma_c^2 / K_c = V_1 \sigma_1^2 / K_1 + V_2 \sigma_2^2 / K_2$$

$$\sigma_c = \sigma_1 = \sigma_2$$

$$\frac{1}{K_c} = \frac{V_1}{V_c} \cdot \frac{1}{K_1} + \frac{V_2}{V_c} \cdot \frac{1}{K_2}$$

Actual

$$K_{c\text{-Reuss}} \le K_c \le K_{c\text{-voigt}}$$

Other Methods of Averaging

1. Wave Propagation

ii. Composites Green function compared with that of a homogeneous solid → Stress Distribution

Models

1. Pure Continuum Model

2. Semi discrete Model

Pure Discrete on xy plane

Pure Continuum in z direction

Combined response in a general direction

Adv Accounts for Fiber-Fiber Interaction

Disadv Not valid for high fiber concentrations.

Cubic Symmetry

(x, y, z)	(y, x, z) (x, z, y), (z, y, x)
	(y, z, x), (z, x, y)
$(\bar{x}, y, z)$	
$(x, \bar{y}, z)$	
$(x, y, \bar{z})$	
$(x, \bar{y}, \bar{z})$	
$(\bar{x}, y, \bar{z})$	
$(\bar{x}, \bar{y}, z)$	
$(\bar{x}, \bar{y}, \bar{z})$	

Matrix Representations (Examples)

$$(x, y, z) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$(\bar{x}\ y\ z) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$(y, x, z) \rightarrow \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Tetragonal Symmetry

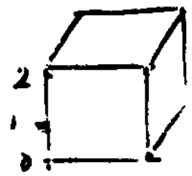
16 operations → 8 sq. type with z to $\bar{z}$

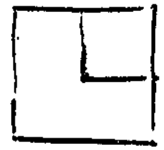
Hexagonal 24 operations

Example $\frac{1}{2}\begin{pmatrix} -1 & \sqrt{3} & 0 \\ \sqrt{3} & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$

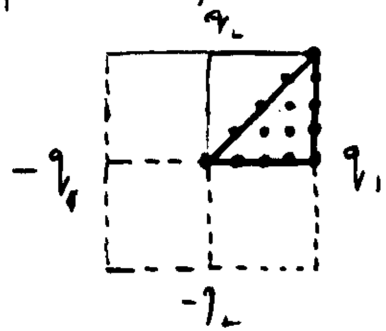
Summation / Integration over q

Cubic symmetry





1. Square symmetry



$q_1 \to 0$ to I

$q_2 \to 0$ to q_1

$NX = 4$

wt for a general point $\to 8$

$q_3 \to 0, 1, 2$

$q_2 \to 0$ to q_3

$q_1 \to 0$ to q_1

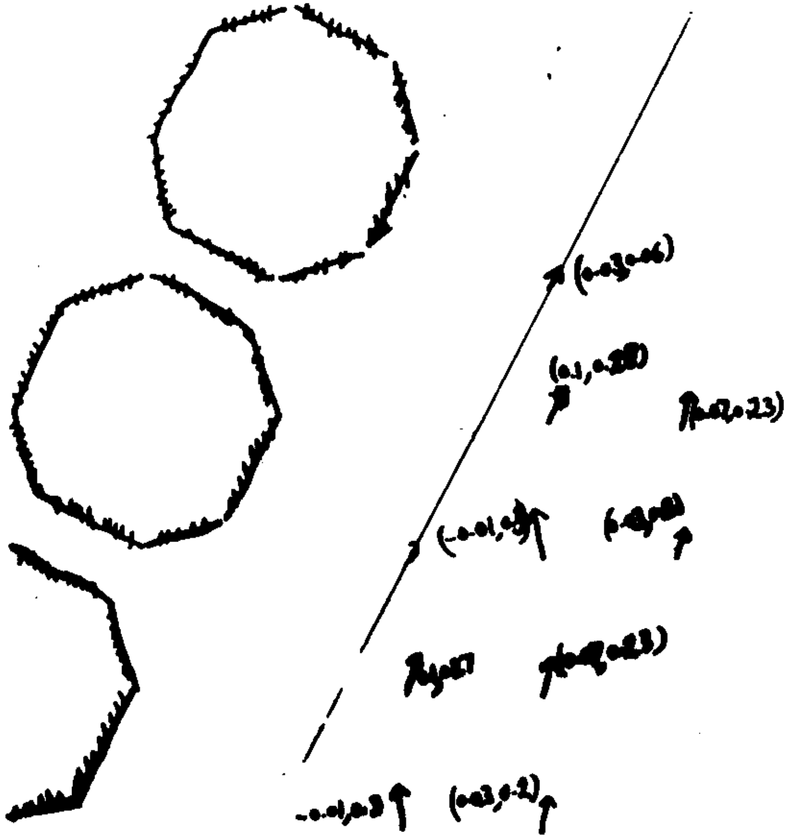
		wt
0, 0, 0	48	1
0, 0, 1	8	6
0, 1, 1	4	12
1, 1, 1	6	8
0, 0, 2	16	3
0, 1, 2	4	12
1, 1, 2	4	12
0, 2, 2	16	3
1, 2, 2	8	6
2, 2, 2	48	1

$64 = 4^3$

q - Values Taken

	Eqvt Pts	wt
(0, 0)	8	1
(1, 0)	2	4
(2, 0)	2	4
(3, 0)	2	4
(4, 0)	4	2
(1, 1)	2	4
(2, 1)	1	8
(2, 2)	2	4
(3, 1)	1	8
(3, 2)	1	8
(3, 3)	2	4
(4, 1)	2	4
(4, 2)	2	4
(4, 3)	2	4
(4, 4)	8	1

Total $= 64$



W_0 (En. of Ref. State) = 1.25×10^4 Ergs/cm^2

E_T (Rel. En) = 5.5 eV ~ -4.47×10^3 Ergs/cm^2

E_-/W_0 ~ 35 %

```
Subroutine WTCUL(I, J, K, N, NW)
(C[illegible], d[illegible] s[illegible]) (I ≤ J ≤ K)

KW = 1
IF (K.EQ.0) KW = 2 * KW
Ib (I.EQ.0. OR. J.EQ.0) KW = 2 * KW
Ib (I.EQ.0. And. J.EQ.0) KW = 2 * KW
Ib (I.EQ.J. AND. K.NE.I) KW = 2 * KW
Ib (J.EQ.K. AND. J.NE.I) KW = 2 * KW
Ib (I.EQ.J. AND. J.EQ.K) KW = KW * 6
Ib (K.EQ.N) KW = KW * 2
Ib (J.EQ.N) KW = KW * 2
Ib (I.EQ.N) KW = KW * 2
NW = 48/KW
Return
End
```

Symmetry operations

Square Symmetry

$$(x, y) \rightarrow \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$(\bar{x}, y) \rightarrow \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$(x, \bar{y}) \rightarrow \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$(\bar{x}, \bar{y}) \rightarrow \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$(y, x) \rightarrow \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$(\bar{y}, x) \rightarrow \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

$$(y, \bar{x}) \rightarrow \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

$$(\bar{y}, \bar{x}) \rightarrow \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$$