MULTIWELL PROBLEMS AND RESTRICTIONS ON MICROSTRUCTURE

KEWEI ZHANG

§1. Problems and Background.

Consider a variational problem:

$$\min_{u=u_0 \, on \partial\Omega} \int_\Omega F(Du(x))dx, \tag{1}$$

and suppose the integrand F is continuous and bounded below with reasonable growth at infinity. (1) is wealky lower semicontinuous in $W^{1,p}$ if F is *quasiconvex* (see e.g. Acerbi-Fusco [AF]). By definition this means

$$\int_G F(P + D\phi(x))dx \geq F(P)\,\text{meas}(G),$$

for some domain G and for all $P \in M^{n\times n}$, $\phi \in W_0^{1,\infty}(G; R^N)$.

Integrands F that arise in the study of martenstic phase transitions are not quasiconvex. (1) is not lower semicontinuous and it cannot be solved by the direct method of the calculus of variations. A minimizing sequence can develop spatial oscillations in its gradients Du_k, leading to weak rather than strong convergence. The central idea of the energy minimizing is that these oscillations model the microstructure observed in real materials (Ball-James [BJ1, BJ2]).

The most interested integrands at the moment are those F which have 'multiple well structure', i.e. $F \geq 0$ everywhere and $F = 0$ on a known set K. The connected components of K are 'elastic energy wells'. They represent preferred gradients.

In this talk I will restrict to the situation when K is a finite subset of $M^{n\times N}$, in particular, a finite set of $M^{2\times 2}$ or $M^{3\times 3}$.

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There are two interesting situations:

(a) when the minimum value of (1) is 0 and it is achieved. This occurs if there is a Lipschitz continuous deformation $u(x)$, satisfying the boundary condition, such that $Du(x) \in K$ for a.e. x;

(b) when the minimum value of (1) is 0, but it is not achieved. Then a minimizing sequence u_k has the property that Du_k is approximately in K except on a subset of Ω of arbitrarily small measure as $k \to \infty$ (Young measure). We may think of Du_k as determining a *microstructure*, with length scale gets finer as $k \to \infty$. When k is large, Du_k partitions Ω into regions which are nearly stress free (where Du_k is near K and some 'transition layers' (sets of small measure, where Du_k is not near K).

Lemma (Young measure). *(see e.g. [T], [B]) Suppose* $\{U_k\} \subset L^\infty(\Omega; R^s)$ *is a sequence and for some compact set* $K \subset R^s$, $\text{meas}(\{x \in \Omega : U_k(x) \notin G\}) \to 0$ *as* $k \to 0$ *for every open set* $G \supset K$. *Then there exists a subsequence (still denoted by* U_k*) and an associated family of probability measures* ν_x *on* R^s *such that (i)* ν_x *is supported on* K *for a.e.* $x \in \Omega$*; (ii) for any continuous function* ψ *on* R^s, $\psi(U_k)$ *converges weakly to the function* $x \to \int_{R^s} \psi(\lambda) d\nu_x(\lambda)$.

In (1) the sequence U_k has the form $U_k = Du_k$, where u_k is the minimizing sequence of (1). The corresponding ν_x is called *Young measure limit of gradients.* The Young measure is *trivial* if ν_x is a Dirac measure for a.e. x. In this case there exists a function u such that ν_x is the Dirac measure at $Du(x)$ and in general, the Young measure may be nontrivial. The minimum value of (1) is

$$\lim_{k\to\infty} \int_\Omega F(Du_k)dx = \int_\Omega \int_K F(\lambda) d\nu_x dx.$$

In particular, if $F \geq 0$ with $F(P) = 0$ exactly for $P \in K$, then $\lim_{k\to\infty} \int_\Omega F(Du_k)dx = 0$ if and only if ν_x is supported on K for a.e. $x \in \Omega$.

Question 1. (Existence) Given a set of matrices K, does K support nontrivial Young measures? i.e. does Du_k develop non-trivial microstructure?

Question 2. (Regularity) Are there non-affine deformations $u(x)$ such that $Du(x) \in K$ almost everywhere?

If $F(Du_j)$ grows like $| Du_j |^p$, then the natural growth hypothesis of the minimizing sequence of (1) would seem to be $u_k \in W^{1,p}$. However, we have

Theorem. *(Zhang [Z2],) If a Young measure limit of gradients has compact support, then it arises from a bounded sequence $u_k \in W^{1,\infty}$.*

§2. Results on finite number of matrices

In this section, Young measure means Young measure limit of gradients.

Definition.. *Two $N \times n$ matrices A and B are compatible if they are 'rank-one connected', i.e. if*

$$\operatorname{rank}(A - B) \leq 1.$$

Otherwise they are called incompatible.

This terminology is from the layer construction: If $\operatorname{rank}(A - B) = 1$, then $A - B = c \otimes n$ for some vectors c and n, and 'mixing A and B in layers orthogonal to n' yields a nontrivial Young measures supported on $\{A, B\}$ (see e. g. [BJ1]).

The following theorem is the simplest case in multiwell problems. The number p corresponds to the Sobolev space $W^{1,p}$ such that the Young measure limit of gradients was generated by a bounded $W^{1,p}$ sequence.

Theorem 2.1. **(Two incompatible matrices)**

(Chipot-Kinderlehrer [CK] ($p = \infty$), Ball-James [BJ1] ($p > 2$,), Zhang [Z1] ($p = 2$,), Šverák [Sv1] ($1 < p < 2$).)

Suppose that A and B are incompatible and ν_x is a Young measure supported on $\{A, B\}$. Then

a) *ν_x is trivial - it is a Dirac measure for a.e. x; and*

b) *ν_x is independent of x.*

Remark. For the quasiconvexification of two-well and multiwell energies, some important work has been done by Kohn [K], Firoozye and Kohn [FK]. In [K], an explicit formular is given for the relaxed enery of the two-well problem.

Theorem 2.2.. Three matrices *Let A, B and C be $N \times n$ matrices which are pairwise incompatible. Assume that ν_x is a Young measure limit of gradients supported on $\{A, B, C\}$. Then*

a) *(Šverák [Sv2]) ν_x is trivial - it is a Dirac measure for a.e. x; and*

b) *(Jodeit-Olver [JO], Zhang [Z4]) ν_x is independent of x.*

Theorem 2.3.. Four matrices

(Tartar [T2], Bhattacharya-Firoozye-James-Kohn [BFJK])

There exist four pairwise incompatible diagonal 2×2 matrices A, B, C and D and a Young measure limit of gradients ν_x supported on $\{A, B, C, D\}$, such that ν_x is nontrivial.

The example is given in Figure 1 below. We call the sets in Fig. *standard patterns.*

Remark. To study a finite set of diagonal 2×2 or 3×3 matrices, we take the projection (e. g. for 2×2 matrices):

$$\begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix} \to (a, b)$$

so that we can draw pictures in R^2 or R^3. The line segments in figures below are rank-one connections.

In order to solve the multiwell problem for finite subsets of diagonal 2×2 matrices, we need the following

Definition 2.4. *A finite set K of diagonal 2×2 matrices without rank-one connections is called* separable *if there exists a diagonal 2×2 matrix C, such that*

$$K - C := \{A - C,\, A \in K\} = K_1 \cup K_2,$$

K_1, K_2 are both non-empty and $K_1 \cap K_2 = \emptyset$, satisfying either

a) *the elements in K_1 are all positive definite, those in K_2 are negative definite; or*

b) *the elements in* JK_1 *are all positive definite, those in* JK_2 *are negative definite, where*

$$JK_i = \{JA,\, A \in K_i\}, \qquad J = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

K *is called completely separable if every subset of* K *with more than one element is separable.*

Lemma 2.5. *([Z3]) If a finite set* K *of diagonal* 2×2 *matrices without rank-one connections is not separable. Then it contains at least one of the standard patterns.*

Theorem 2.6.. several 2×2 **diagonal matrices** *(Zhang [Z3]) Suppose* A_i $(i = 1, \ldots, m)$ *be pairwise incompatible matrices and* ν_x *is a Young measure supported on* $K = \{A_1 \ldots, A_m\}$. *Then* ν_x *is trivial if and only if the set* K *is "separable." Furthermore, if* K *is separable,* ν_x *is independent of* x.

The idea of the proof is to use Theorem 4.6 which is a generalization of a result due to V. Šverák [Sv2] and the induction.

Theorem 2.7.. six matrices in 3D*(Zhang [Z3]) There exists a set* K *of six pairwise incompatible diagonal* 3×3 *matrices* A_i $(i = 1, \ldots, 6)$ *and a Young measure limit of gradients* ν_x *supported on* $K := \{A_1 \ldots, A_6\}$, *such that* ν_x *is nontrivial. However, Young measure limit of gradients* ν_x *supported on any fixed five elements of* K *must be trivial and independent of* x.

The examples are given in figure 2. The proof of the theorem is similar to that in [T2] for separately convex functions. If the claim is not true, the Young measures are trivial. Then there exists a quasiconvex function F such that $F \geq 0$, $F(P) = 0$ if and only if $P \in K$. However, for the special feature of K we can show that $F = 0$ on those line segments in Fig.2. This leads to a contradiction.

Definition 2.8. *A finite set* $K \subset M^{N\times n}$ *is called minimal if it can support nontrivial Young measure limit of gradients, while for any* $A \in K$, $K \setminus \{A\}$ *can only support trivial Young measures.* $K \subset M^{N\times n}$ *is called weakly minimal if it can support nontrivial Young* *measure limit of gradients and there exists at least one element $A_0 \in K$, $K \setminus \{A_0\}$ can only support trivial Young measures.*

The standard patterns in Fig.1 are the only minimal set for 2×2 diagonal matrices. The examples shown in Fig. 2 are the known patterns for 3×3 diagonal matrices. There are some examples of weakly minimal sets which I do not know whether they are minimal.

Example 2.9. The three sets described in Figures 3, 4 and 5 are weakly minimal.

In Fig. 3, the element to be removed is A_7; in Fig. 4, A_8; in Fig. 5, A_4 or A_5.

§3. A stability result for the multiwell problem

The question of stability for the multiwell structure is that suppose the original set K supports only trivial Young measures, what happens if we perturb the set a little bit?

The following is a general stability result due to Ball and James [BJ3].

Theorem 3.1. *Suppose $K = K_1 \cup K_2$, K_1, K_2 are both non-empty and $K_1 \cap K_2 = \emptyset$. Let $\Omega \subset R^n$ be open, bounded and satisfies the cone condition. K_1 and K_2 separate Young measures in the sense that if $\{\nu_x\}_{x\in\Omega}$ is any family of Young measure limit of gradients, such that* $\operatorname{supp}\nu_x \subset K$ a.e. $x \in \Omega$, *then* $\operatorname{supp}\nu_x \subset K_1$ a.e. *or* $\operatorname{supp}\nu_x \subset K_2$ a.e..

Then there exists $\epsilon > 0$ and an ϵ-neighbourhood of K^ϵ of K, $K^\epsilon = \{A \in M^{n\times N}$, $\operatorname{dist}(A; K$ *$\epsilon\}$ such that* $\operatorname{supp}\nu_x \subset K^\epsilon$ a.e. $x \in \Omega$, *implies* $\operatorname{supp}\nu_x \subset K_1^\epsilon$ a.e. $x \in \Omega$ *or* $\operatorname{supp}\nu_x \subset K_2^\epsilon$ a.e. $x \in \Omega$.

The following is a special case of Theorem 3.1. However, in this case the ϵ in the theorem is computable.

Theorem 3.2. *(Zhang [Z5]) Suppose $K \subset M^{2\times 2}$ is finite, diagonal and completely separable. Then, there exists an $\epsilon = \epsilon(d)$,*

$$d = \min_{i\neq j}\{| a_i - a_j |, | b_i - b_j |\}$$

$$A_i, A_j \in K,\ A_i = \begin{pmatrix} a_i & 0 \\ 0 & b_i \end{pmatrix}$$

such that if ν is a homogeneous Young measure limit of gradients ([KP], see Proposition 4.3 below), $\operatorname{supp}\nu \subset \cup_{A\in K}\overline{B(A,r)}$, *then there exists $A_0 \in K$, such that* $\operatorname{supp}\nu \subset \overline{B(A_0,r)}$, *where $\overline{B(A,r)} \subset M^{2\times 2}$ is a closed ball.*

The proof of the theorem relies on the following observations:

(1) Since K is completely separable, we may use the induction argument and assume that $K = K_+ \cup K_-$, $a_i \geq d/2$, $b_i \geq d/2$ for $A_i \in K_+$ and $a_j \leq -d/2$, $b_j \leq -d/2$ for $A_j \in K_-$. We seek to prove that $\operatorname{supp}\nu \subset \cup_{A\in K_+}\overline{B(A,r)}$ or $\operatorname{supp}\nu \subset \cup_{A\in K_+}\overline{B(A,r)}$.

(2) For small $r > 0$, the set $\cup_{A\in K}\overline{B(A,r)}$ is contained in the class of monotone increasing or decreasing mappings:

$$\mathcal{E}_\epsilon := \{P \in M^{2\times 2}, \det(E(P)) \geq \epsilon\}, \qquad (\epsilon > 0)$$

in the sense that if $P \in \mathcal{E}_\epsilon$, Px is either a monotone increasing mapping from R^2 to R^2 or a monotone decreasing mapping, where $E(P) = \frac{P+P^T}{2}$. Also $\mathcal{E}_\epsilon$ is weakly closed in the sense that if $\operatorname{dist}(Du_j; \mathcal{E}_\epsilon) \to 0$ a.e. and $u_j \to u$ in $W^{1,\infty}(\Omega; R^2)$ weak-$*$, then $Du(x) \in \mathcal{E}_\epsilon$ a.e.. This can be easily seen from the fact that

$$\mathcal{E}_\epsilon = \{P \in M^{2\times 2}, \left(\frac{P_{12} - P_{21}}{2}\right)^2 - \det P \leq -\epsilon\}$$

which is the level set of a polyconvex function.

(3) We may assume that the sequence is bounded in $W^{1,\infty}$ (see [Z2], [KP]). Since we only look at homogeneous Young measures, the weak limit of the sequence Du_j is a constant matrix $P \in \mathcal{E}_\epsilon$. We may assume that Px is monotone decreasing, i.e. $E(P)$ is negative-definite. We try to show that $E(Du_j)$ is 'essentially' semi-negative definite for large j in a fixed ball contained in Ω. Use the change of variable formulars as in [Sv2]:

$$\int_B \phi(u_j(x)) \det Du_j(x)\, dx = \int_{R^2} \phi(y) \deg(u_j, B, y) dy;$$

$$\int_B \phi(u_j(x)) \mid \det Du_j(x) \mid\, dx = \int_{R^2} \phi(y) N(u_j \mid B, y) dy,$$

where B is a unit ball in Ω, $\deg(u_j, B, y)$ is the Brouwer degree of u_j, $N(u_j \mid B, y)$ is the number of solutions of $u_j(x) = y$ in B.

With this topological method, it can be shown that (a): u_j is essentially one-to-one in $B_{1/2}$ and (b):

$$(u_j(x) - u_j(a)) \cdot (x - a) \leq \epsilon_0 \mid x - a \mid^2$$

for $x \in \partial B_{1/2}$ and $a \in B_{1/4}$. We want to claim that essentially $E(Du_j(a))$ is semi-negative definite in $B_{1/4}$. By Rademacher's theorem, u_j is differentiable a.e.. If it is not the case, we may find a set of 'essentially' positive measure such that $E(Du_j(a))$ is positive definite, and $(u_j(x) - u_j(a)) \cdot (x - a) > 0$ whenever $\mid x - a \mid$ is small. However, we can not show that this will lead to contradictions because of the Poincaré-Bendixson theorem, a limit circle may occur. To avoid this we need the following argument:

(4) We may assume that $a = 0$, $u_j(a) = 0$. Since the sequence Du_j converges to a 'thin set', i.e., let $u_j = (u_j^1, u_j^2)$, and $D = \{(a, b) \in R^2, \mid x \mid \leq M, \mid y \mid \leq r\}$, where $M > 0$ and r the radius of the balls. Then $\text{dist}(Du_j^1; D) \to 0$ a.e.. Use the maximal function method as in [Z2], We may find another sequence v_j bounded in $W^{1,\infty}$ such that up to a subsequence, $Du_j - Dv_j \to 0$ a.e. in B, so that Dv_j generates the same Young measure in B and $\mid \partial_y v_j^1(x, y) \mid \leq Cr$ for some constant C independent of j. Similarly, we can have $\mid \partial_x v_j^2(x, y) \mid \leq Cr$. Then consider the new sequence $w_j = v_j + (2Cry, 2Crx)$, we can claim that $\partial_y w_j^1(x, y) \geq Cr$ and $\partial_x w_j^2(x, y) \geq Cr$. If we choose $r > 0$ small, The arguments in previous can go through. Now, if we go back to step (4), and use a simple degree argument, we may find another solution of $u_j(x) = 0$ in the domain

$$V = \{(x, y) \in B_{1/2};\ \delta < \sqrt{x^2 + y^2} < 1/2,\ x > 0,\ y > 0.\}$$

This contradicts to the uniqueness of the solution $u_j(x) = 0$ in $B_{1/2}$.

§4. Some restrictions of microstructure

The following are some of the tools used to study Young measure limit of gradients.

Lemma 4.1. *Let $F : M^{N\times n} \to R$ be quasiconvex, and ν_x be a Young measure defined for $x \in \Omega$ and supported on K. Then*

$$F\left(\int_K \lambda d\nu_x(\lambda)\right) \le \int_K F(\lambda) d\nu_x(\lambda), \text{ for a.e. } x \in \Omega.$$

Corollary 4.2. (**minors relations**)

Let $J : M^{N\times n} \to R$ be a minors, and ν_x be a Young measure defined for $x \in \Omega$ and supported on K. Then

$$J\left(\int_K \lambda d\nu_x(\lambda)\right) = \int_K J(\lambda) d\nu_x(\lambda), \text{ for a.e. } x \in \Omega.$$

If ν_x is independent of x, it is called a *homogeneous Young measure.*

Proposition 4.3. (**Homogeneous Young measure** *(Kinderlehrer-Pedregal)) Let ν_x be a Young measure limit of gradients. Then for a.e. $a \in \Omega$, the parameterized measure $\tilde{\nu}_x = \nu_a$ is a Young measure limit of gradients.*

Theorem 4.4. *(BFJK) Let ν be a nontrivial, homogeneous Young measure limit of gradients. Assume as normalization $\int \lambda d\nu(\lambda) = 0$ The the linear span of the support of ν must contain a rank-one matrix.*

Theorem 4.5. *(Šverák [Sv2]) Let K be a bounded subset of*

$$\{A : A \text{ is symmetric } 2 \times 2 \text{ matrix and } \det A = 1\}.$$

Then Young measure limits of gradients supported on K must be trivial.

Theorem 4.6. *(Separation Lemma [Z3]) Assume $\Omega \subset R^2$, $p > 2$. Let*

$$K_0 = \{A \in M^{2\times 2}, A \text{ is symmetric and } \det A \ge 0\}$$

and we denote by K_0^+, K_0^- and G_0 the subsets of K_0 as

$$K_0^+ = \{A \in K_0, A \text{ is semi-positive definite }\}$$

$$K_0^- = \{A \in K_0, A \text{ is semi-negative definite }\}$$

$$G_0 = \{A \in K_0, \det A = 0\}$$

respectively and we assume that $u_k \to u$ *weakly in* $W^{1,p}(\Omega)$ *and*

$$\operatorname{dist}(D^2 u_k; K_0) \to 0 \qquad \text{in } L^1(\Omega).$$

Then

(i) *for almost every* $x \in \Omega$ *such that* $D^2u(x)$ *is positive (negative) definite, there exists* $\delta_x > 0$ *such that the Young measures corresponding to* D^2u_k *satisfy* $\operatorname{supp} \nu_y \subset K_0^+ \cup G_0$ *(respectively* $K_0^- \cup G_0$ *) for a.e.* $y \in B_{x,\delta_x}$. *Moreover,* $D^2u(y) \in K_0^+ \cup G_0$ *(respectively* $K_0^- \cup G_0$*) for a.e.* $y \in B_{x,\delta_x}$. *If moreover, all the elements in* K_0 *are diagonal matrices,* $D^2u(y)$ *is nonnegative definite (respectively nonpositive definite) a.e. in* $D \subset B_{x,\delta_x}$, *where* D *is any square centred at* x.

(ii) *for almost every* $x \in \Omega$ *such that* $D^2u(x) \in G_0$, $\operatorname{supp} \nu_x \subset G_0$.

Theorem 4.6 is a generalization of Theorem 4.5 obtained by V. Šverák. The idea of the proof is to use Hodge decomposition and theory of Monge-Ampère equation.

Remark. For 2×2 diagonal matrices, We can obtain a complete picture of whether a finite set supports a nontrivial Young measure by the Separation Lemma. However, for 2×2 symmetric matrices, we can not classify the Young measures by this lemma.

Example 4.7. There exists a set of 2×2 symmetric matrices $K = \{A_1, A_2, B_1, B_2\}$ such that $B_i - A - j$ is positive definite for $i, j = 1, 2$. However, there is no 2×2 symmetric matrix C separating $\{A_1, A_2\}$ and $\{B_1, B_2\}$ in the sense that $B_i - C$, $C - A_j$ are positive definite for $i, j = 1, 2$.

Fig. 6 provides such an example. We may assume that all the matrices are positive definite. Consider the level curve

$$K_{A_j} = \{x \in R^2,\ x^T A_j x \leq 1\}, \qquad K_{B_i} = \{x \in R^2,\ x^T B_i x \leq 1\},\ i, j = 1, 2.$$

If C exists, then $K_{B_1} \cup K_{B_2} \subset K_C \subset K_{A_1} \cap K_{A_2}$. This is not always possible for a quadratic form $x^T C x$.

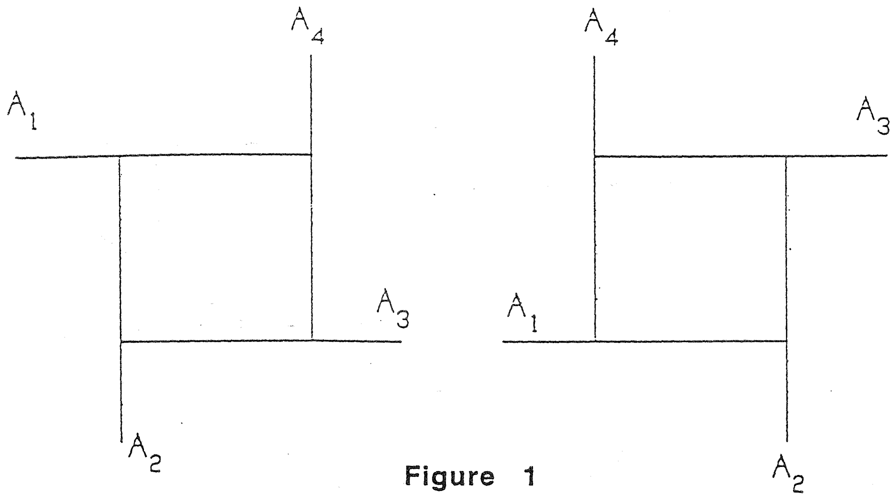
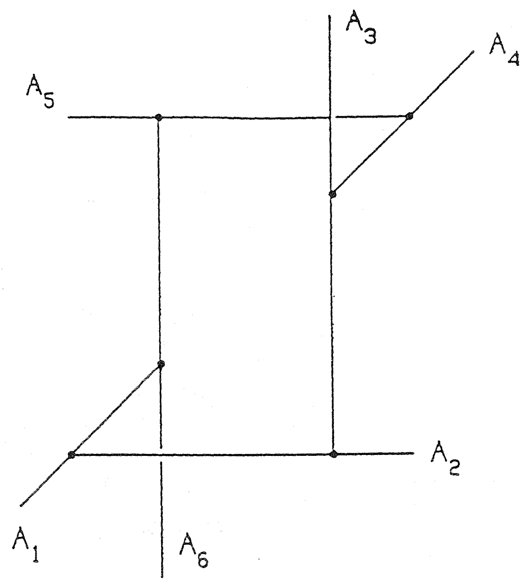


Figure 1



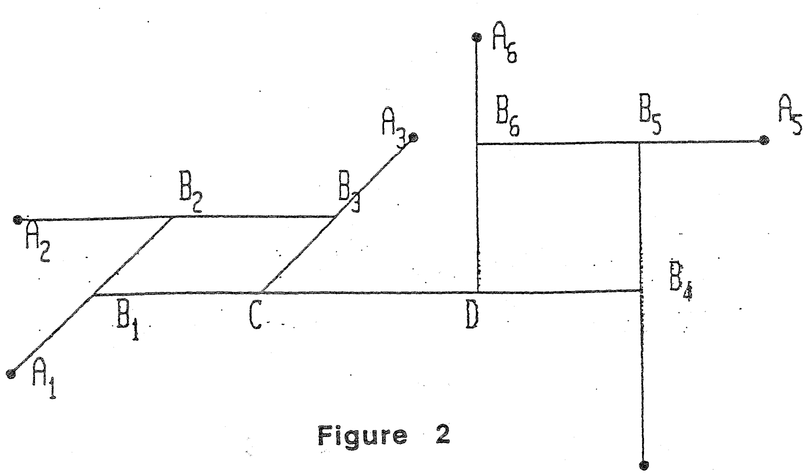


Figure 2

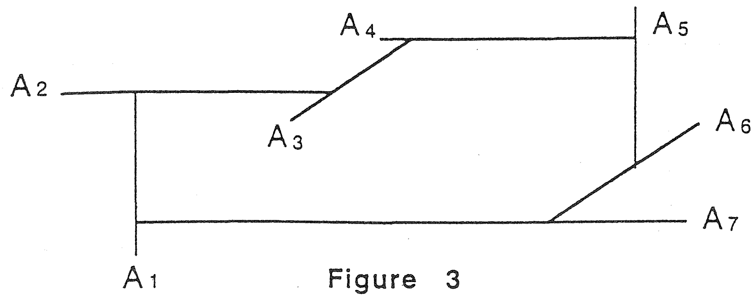


Figure 3

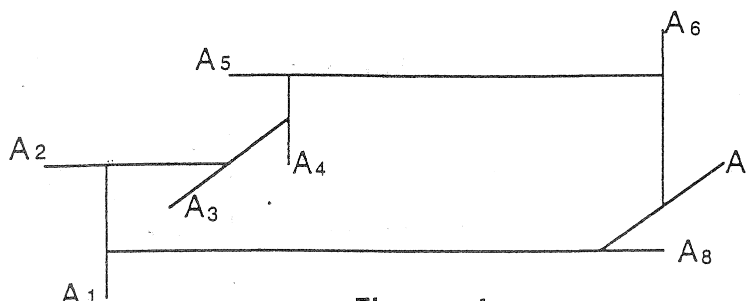


Figure 4

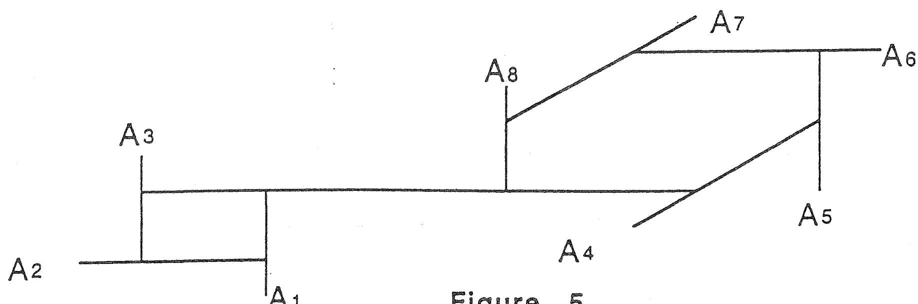


Figure 5

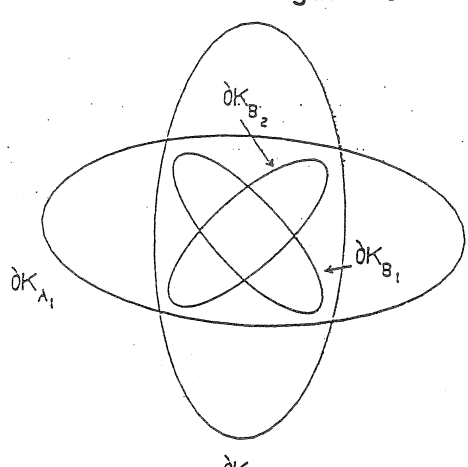


Figure 6

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School of Math., Phys., Macquarie University, NSW 2109, AUSTRALIA
E-mail address: kewei@macadam.mpce.mq.edu.au