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## INVARIANT GEOMETRY OF SPIN GLASS STATES

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### ABSTRACT

We study how the geometry of spin glass states changes under redefinitions of the metric. We show that in mean field theory the property of ultrametricity is robust. We present numerical evidence suggesting that in the more realistic  $D = 2$  and  $D = 3$  spin glass models a stronger result may hold, namely that the choice of metric is to a large extent unique.

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Much of the recent progress in understanding the nature of the spin-glass phase has focused on the geometry of the space of thermodynamic equilibrium states. A striking feature of this space in mean-field-theory is its ultrametric structure,<sup>1</sup> implying a hierarchical organization of states in clusters. This feature leads, in particular, to analytically tractable models of dynamical relaxation.<sup>2</sup> Whether it is a generic property of more realistic spin glasses,<sup>3</sup> and other complex frustrated systems<sup>4</sup> is an open and very interesting question with possible ramifications in such diverse fields as combinatorial optimization and brain modelling.<sup>5,6</sup>

One facet of the universality of ultrametricity, that can be explicitly verified, would be its robustness under redefinitions of the metric in the space of states. The distance between two spin-glass states  $a$  and  $b$  has so far been taken to be a measure of the variation in local magnetization<sup>7</sup>

$$d_{ab}^2 = \sum_{\text{site } i=1}^N \frac{1}{N} (m_i^a - m_i^b)^2 \equiv 2(q_{EA} - q_{ab}) \quad (1)$$

where  $q_{ab}$  is their overlap, and the self-overlap  $q_{EA}$  is state-independent. Though natural, this definition is not unique. Indeed, by analogy with (1) we could define

$$\left[ d_{ab}^{(O)} \right]^2 = \sum_i \frac{1}{N} (O_i^a - O_i^b)^2 \equiv 2 \left( q_{EA}^{(O)} - q_{ab}^{(O)} \right) \quad (2)$$

for any observable density  $O_i$ , such as the local molecular field, a coarse grained magnetization, the energy density *etc.*, which can be considered as new coordinates of the infinite dimensional space of states. In this letter we study how the geometry of states is affected by such coordinate changes. This is interesting because invariant features should be the only ones worth looking for (i) in real

experiments, where the precise density measured by a given probe might well be ambiguous (for instance, neutron diffraction experiments with less than perfect resolution would presumably measure a coarse-grained magnetization) and (ii) in other complex frustrated systems, such as the problem of close-packing randomly-shaped tiles (possibly of relevance in the study of amorphous materials) where no a priori natural definition of the distance between states exists.

Our results are as follows: (a) we will show explicitly in mean field theory that the property of ultrametricity is invariant under metric-redefinitions, and (b) we will present numerical evidence that in the more realistic  $D = 2$  and  $D = 3$  Ising spin glass models not only is ultrametricity, if present, preserved, but a much stronger result may hold, namely that a wide variety of locally defined metrics are identical up to an overall scale factor. In this sense, the metric in the space of spin-glass states is almost unique, and the geometry universal.

The mean-field theory of spin-glasses is described by the long-range Sherrington-Kirkpatrick<sup>8</sup> Hamiltonian

$$\mathcal{H} = - \sum_{i,j=1}^N J_{ij} \sigma_i \sigma_j - H \sum_{i=1}^N \sigma_i \quad (3)$$

where the  $\sigma_i$  are Ising spins, and the  $J_{ij}$  are independent quenched random variables with a symmetric Gaussian distribution of variance  $1/\sqrt{N}$ . The property of ultrametricity was demonstrated<sup>1</sup> by calculating the average probability that three states  $a, b$  and  $c$  have mutual magnetization overlap  $z_1, z_2$  and  $z_3$ . Using the replica trick this can be written

$$P(z_1, z_2, z_3) = \lim_{n \rightarrow 0} \text{Tr}_{\sigma} \prod_{i < j} \int_{-\infty}^{\infty} dJ_{ij} \sqrt{\frac{N}{2\pi}} \cdot \exp\left(-\frac{NJ_{ij}^2}{2}\right) \exp\left[-\beta \sum_{e=1}^n \mathcal{X}(\sigma_i^e)\right] \\ \times \delta(q_{ab}(\sigma) - z_1) \cdot \delta(q_{bc}(\sigma) - z_2) \cdot \delta(q_{ca}(\sigma) - z_3) \quad (4)$$

where  $\text{Tr}_{\sigma}$  stands for a summation over all spin-configurations of the  $n$  replicas and the magnetization overlap of two real replicas is

$$q_{ab}(\sigma) = \frac{1}{N} \sum_i \sigma_i^a \sigma_i^b \quad . \quad (5)$$

Using standard saddle-point integrations, this is rewritten as

$$P(z_1, z_2, z_3) = \lim_{n \rightarrow 0} \frac{1}{n(n-1)(n-2)} \sum_{a \neq b \neq c} \delta(Q_{ab} - z_1) \delta(Q_{bc} - z_2) \delta(Q_{ca} - z_3) \quad (6)$$

where  $Q_{ab}$  is the  $n \times n$  matrix that minimizes the free energy. Below the transition temperature, it has the hierarchical form obtained by Parisi<sup>9</sup>

$$Q = \left( \begin{array}{c|ccc} q_1 & & & \\ \hline & q_1 & & \\ & & q_1 & \\ & & & q_1 \\ \hline q_2 & & & \\ \hline & q_3 & & \\ & \vdots & & \\ & & q_2 & \\ & & & q_1 \\ & & & & q_1 \\ & & & & & q_1 \\ & & & & & & \dots \\ \hline & & & & & & & m_1 \\ \hline & & & & & & & & m_2 \end{array} \right) \quad . \quad (7)$$

This is best described by the homogeneous tree shown in Fig. 1, and a *monotone non-increasing* and *positive* (for non-vanishing magnetic field  $H$ ) sequence  $q_i$ . It follows immediately from the hierarchical form of  $Q_{ab}$ , and Eq. (6), that  $P(z_1, z_2, z_3)$  vanishes unless the two smaller overlaps coincide. Thus all triangles in the space of pure states have their two bigger sides equal with probability one, which is the statement of ultrametricity.

We are now ready to show that the property of ultrametricity is robust under redefinitions of the metric, of type (2).<sup>10</sup> Instead of a general proof, which would be tedious and not particularly illuminating, we will restrict ourselves here to two examples where the observable  $\mathcal{O}_i$  is (a) the local molecular field, and (b) the energy density; these can then be readily generalized.

#### (A) LOCAL MOLECULAR FIELD

The field-overlap of two real replicas is defined as

$$q_{ab}^{(h)} \equiv \frac{1}{N} \sum_i \left( \sum_j J_{ij} \sigma_j^a \right) \left( \sum_k J_{ik} \sigma_k^b \right) .$$

To calculate the average probability that three states  $a, b$  and  $c$  have mutual field-overlaps  $z_1, z_2$  and  $z_3$ , we substitute  $q_{ab}^{(h)}$  for  $q_{ab}$  in Eq. (4), and then replace in turn  $J_{ij}$  and  $q_{ab}(\sigma)$  (for  $a \neq b$ ) by their saddle-point values  $\frac{\beta}{N} \sum_{i=1}^n \sigma_i^a \sigma_i^b$  and  $Q_{ab}$  respectively. The result is the same as Eq. (6), but with the saddle point matrix  $Q$  replaced by

$$Q^{(h)} = \beta^2 (Q + \mathbf{1})^3$$

where  $\mathbf{1}$  is the identity matrix. Now matrices of the Parisi-form (7) are closed under addition and multiplication, as can be easily seen by inspection. That

monotonicity of  $q_i$  is preserved under multiplication follows from the trivial inequality  $x\tilde{x} + y\tilde{y} \geq x\tilde{y} + \tilde{x}y$  if  $x \geq y$  and  $\tilde{x} \geq \tilde{y}$ . Thus the matrix of field-overlaps  $Q^{(h)}$  has the same hierarchical form as the saddle-point matrix  $Q$ , which suffices to establish the ultrametricity of the space of states in the new metric.

## (B) ENERGY DENSITY

The energy-overlap of two replicas is

$$q_{ab}^{(E)}(\sigma) = \sum_i \left( \sum_j J_{ij} \sigma_i^a \sigma_j^a \right) \left( \sum_k J_{ik} \sigma_i^b \sigma_k^b \right) .$$

Going through the same steps as before, we arrive at the joint probability of mutual energy-overlaps of a triplet given by Eq. (6) with  $Q$  now replaced by

$$Q_{ab}^{(E)} = \beta^2 \sum_{c,d=1}^n (Q + \mathbf{1})_{ac} (Q + \mathbf{1})_{bd} M_{abcd}$$

where  $M_{abcd}$  is the one-site average<sup>11</sup>

$$M_{abcd} = \left( \text{Tr}_{\sigma} \sigma^a \sigma^b \sigma^c \sigma^d \exp \left[ \frac{1}{2} \sum_{e,f} Q_{ef} \sigma^e \sigma^f \right] \right) / \left( \text{Tr}_{\sigma} \exp \left[ \frac{1}{2} \sum_{e,f} Q_{ef} \sigma^e \sigma^f \right] \right) .$$

To show that  $Q^{(E)}$  has the same hierarchical structure as  $Q$ , note that the invariance-group of the latter is the direct product of the permutation groups of  $m_{i_A}/m_{i_A-1}$  branches at each branching-point  $A$  on the tree:

$$Q_{ab} = Q_{\pi(a)\pi(b)} ; \quad \pi \in \bigotimes_{\substack{\text{branching} \\ \text{point } A}} P_{m_{i_A}/m_{i_A-1}} .$$

When  $a$  runs over all  $n$  replicas so does  $\pi(a)$  and hence, by a change of dummy variables it follows that  $Q^{(E)}$  has the same symmetry-group, and thus also the

same hierarchical structure (7) as the Parisi matrix. It remains to prove that its entries are larger the more they are nested. This can be shown with the use of lengthy to prove but straightforward inequalities<sup>12</sup> for the ferromagnetic hierarchical model with Hamiltonian  $\mathcal{H} = \frac{1}{2} \sum_{a,b} Q_{ab} \sigma^a \sigma^b$  which is a generalization of the long-range Dyson ferromagnet. The positivity of  $Q_{ab}$  is crucial here.

The above examples can be easily generalized to other gauge-invariant definitions of the metric. The invariance of ultrametricity is a consequence of the fact that the distance  $d_{ab}^{(\mathcal{O})}$  of two states is a monotone increasing function of their magnetization distance alone:<sup>13</sup>  $d_{ab}^{(\mathcal{O})} = f^{(\mathcal{O})}(d_{ab})$ . In mean field theory the functions  $f^{(\mathcal{O})}$  are in general complicated.

We will now present numerical evidence that in the more realistic two- and three-dimensional spin glass models (a)  $d_{ab}^{(\mathcal{O})}$  are still monotone functions of  $d_{ab}$ , and (b) for several  $Z_2$ -odd densities  $\mathcal{O}_i$  these functions are, surprisingly, straight lines. Hence, such changes of metric amount to a simple rescaling that preserves not only the notion of ultrametricity, but all other geometric features (such as the distribution of overlaps) as well.

Our numerical simulations were done on the IBM 3081 at SLAC. We studied the frustration models with Hamiltonian (3), but with  $J_{ij}$  being  $\pm 1$  with equal probability for nearest neighbors on a  $D = 2$  square, and  $D = 3$  cubic lattice, and zero otherwise. Our lattices varied in size from  $16^2$  to  $54^2$  and from  $8^3$  to  $14^3$ ; we used periodic boundary conditions, and mostly zero magnetic field  $H$ . We slowly cooled several replicas, typically 50, of the same sample down to some low temperature, that ranged from  $\beta = 0.8$  to  $\beta = 3.0$ , and then in each replica we measured the densities of magnetization ( $m_i$ ), molecular field ( $h_i$ ), energy ( $E_i$ ),

coarse-grained magnetization ( $m_i^c$ ) and a composite operator ( $c_i$ ), where  $m_i^c$  is the average magnetization over an elementary square or cube of the lattice with  $i$  at its lower left corner, and for the composite operator we took:

$$c_i = \left\langle \frac{1}{2D} \left( \sum_{\substack{\text{nearest} \\ \text{neighbors } j}} J_{ij} \sigma_j \right)^2 \sigma_i \right\rangle .$$

The averages were taken over a few hundred Monte-Carlo sweeps. Finally we measured the distances  $d^{(O)}$  between each replica and some randomly chosen fixed replica, for each of the above densities  $O$ , as well as the self-overlaps  $q_{EA}^{(O)}$ .

Consistency checks included verifying that the internal energy of our states agreed with previous simulations,<sup>14</sup> near the freezing temperature. We also verified that self-overlaps are to a good approximation state-independent and self-averaging, and used their fluctuations to estimate error bars. We made no attempt to establish the presence or absence of an equilibrium transition, for which much better data already exists,<sup>15</sup> for all we know our states could be metastable.

In Figs. 2 and 3 we present typical distributions of  $(d_{ab}^{(O)2}, d_{ab}^2)$  with  $O = h$  and  $c$  for a  $D = 2$  sample, and  $O = h$  and  $m^c$  for a  $D = 3$  sample, at zero external field. The little squares indicate the areas in which the points  $(q_{aa}^{(O)}, q_{aa})$  fall for all replicas  $a$ . Assuming state-independent self-overlaps, the square sizes can be used as estimates of the corresponding error bars. Within these error bars, the distributions are one-dimensional curves, that are remarkably well fitted by straight lines. Due to the global  $Z_2$  invariance, there is a reflection symmetry about the point  $(q_{EA}^{(O)}, q_{EA})$ ; thus the slopes of the straight lines are the ratios of the corresponding self-overlaps, whose values we found to be essentially independent of lattice size, sample, and to a good approximation temperature below



$1/\beta = 1$ ; they are given on the figures. Note that if gauge non-invariant additions to the metric self-average to zero, one would expect  $q_{EA}^{(m^c)}/q_{EA} = 8$  in three dimensions, which is consistent with the “experimental” value. Let us stress, that although our data shows no statistically significant deviations from linear laws, we know of no theoretical argument that would exclude such deviations.

In Figs. 2 and 3, on the same scale as  $[d^{(h)}]^2$ , we have also plotted  $[d^{(E)}]^2$ , to show that the energy-density fluctuations from one state to another are relatively small. A more detailed analysis showed that: (a) in two dimensions, the  $[d^{(E)}]^2$  curve fluctuates a lot with quenched disorder, and approaches the horizontal axis with increasing lattice size. It might thus be the case that in the thermodynamic limit all states have the same energy distribution, except on a set of measure zero; a much better scaling analysis, on larger lattices, is necessary in order to address this issue. (b) In three dimensions, the  $[d^{(E)}]^2$  curves seem to converge to the symmetric shape shown in Fig. 4(a). The symmetry under reflections about  $d = q_{EA}$  is due to the fact that  $E_i$  is  $Z_2$ -even, and can be lifted in the presence of a magnetic field, as shown in Fig. 4(b). Our statistics are not good enough to determine the functional form of these curves, although we can safely say that, up to reflections, they are monotone increasing and hence preserve the notion of ultrametricity.

In conclusion, we have presented analytic (in mean field theory) and numerical (in the  $D = 2$  and  $D = 3$  spin glass models) evidence, that the notion of ultrametricity is invariant under redefinitions of the distance between states. We have also presented evidence that in the  $D = 2$  and  $D = 3$  models, the choice of metric is to a large extent unique.

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11. The reader unfamiliar with calculations in the framework of Parisi's replica symmetry breaking can consult for instance: M. Mézard and M. Virasoro, *J. Physique* **46**, 1293 (1985); also J.R.L. De Almeida and E. J. Lage, *J. Phys. C* **16**, 939 (1982).
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13. Note that this is not true for arbitrary single configurations of spins.
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## FIGURE CAPTIONS

Fig. 1. The tree describing Parisi's hierarchical replica symmetry breaking ansatz. The entry  $Q_{ab} = q_i$  depends only on the level  $i$  of the nearest common ancestor of  $a$  and  $b$ . The bifurcation number of all branches at the  $i^{\text{th}}$  level is  $m_i/m_{i-1}$ .

Fig. 2. Plots of  $[d^{(h)}]^2$ ,  $[d^{(c)}]^2$  and  $[d^{(E)}]^2$  versus the magnetization distance  $d^2$ , for 50 replicas of a typical  $2D$   $24 \times 24$  sample at  $\beta = 2.1$ . The little squares indicate where the corresponding self-overlaps for all 50 states fall. The slopes are the ratios of self-overlaps; the quoted errors are due to fluctuations from sample to sample. The energy fluctuations  $[d^{(E)}]^2$  may be vanishing in the thermodynamic limit.

Fig. 3. Plots of  $[d^{(h)}]^2$ ,  $[d^{(m^c)}]^2$  and  $[d^{(E)}]^2$  versus  $d^2$  for a typical  $3D$   $12 \times 12 \times 12$  sample at  $\beta = 2.1$ .

Fig. 4. (a) A typical  $[d^{(E)}]^2$  versus  $d^2$  curve at external field  $H = 0$ . Crosses and dots represent data from a  $10 \times 10 \times 10$  and  $12 \times 12 \times 12$  sample respectively. In the insert, (b) a magnetic field  $H = 1$  has been switched on, and the symmetry of the curve around  $d^2 = q_{EA}$  has been lifted.

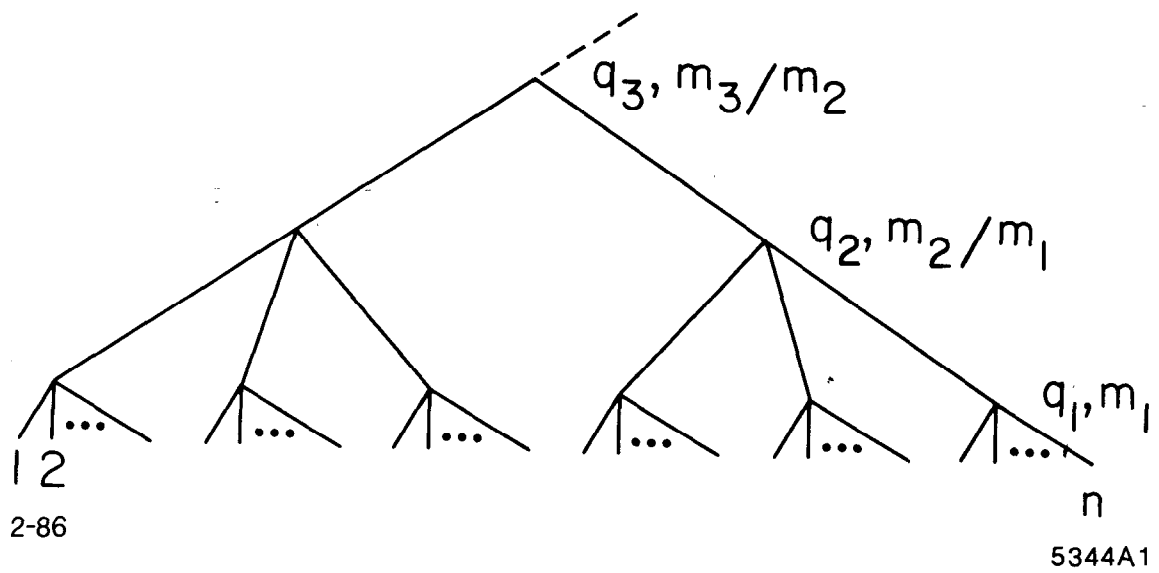


Fig. 1

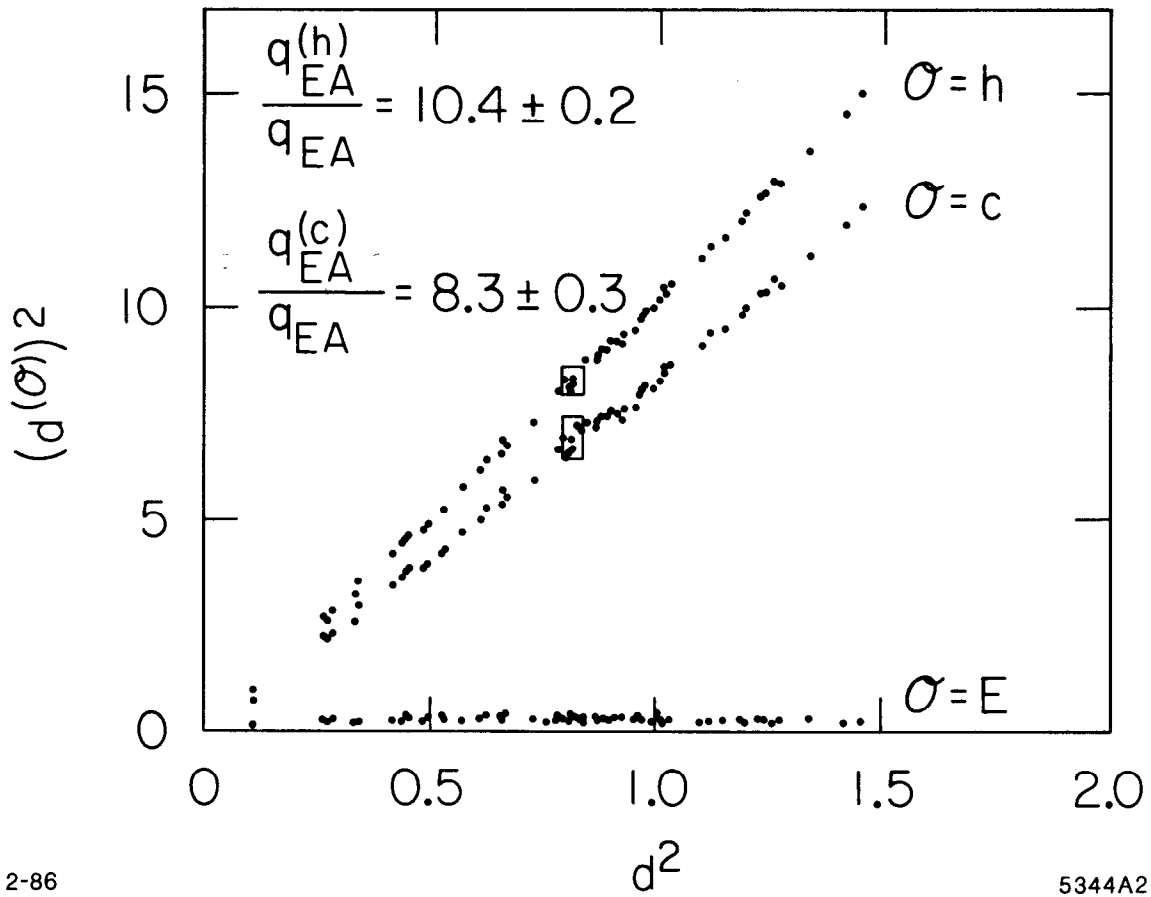


Fig. 2

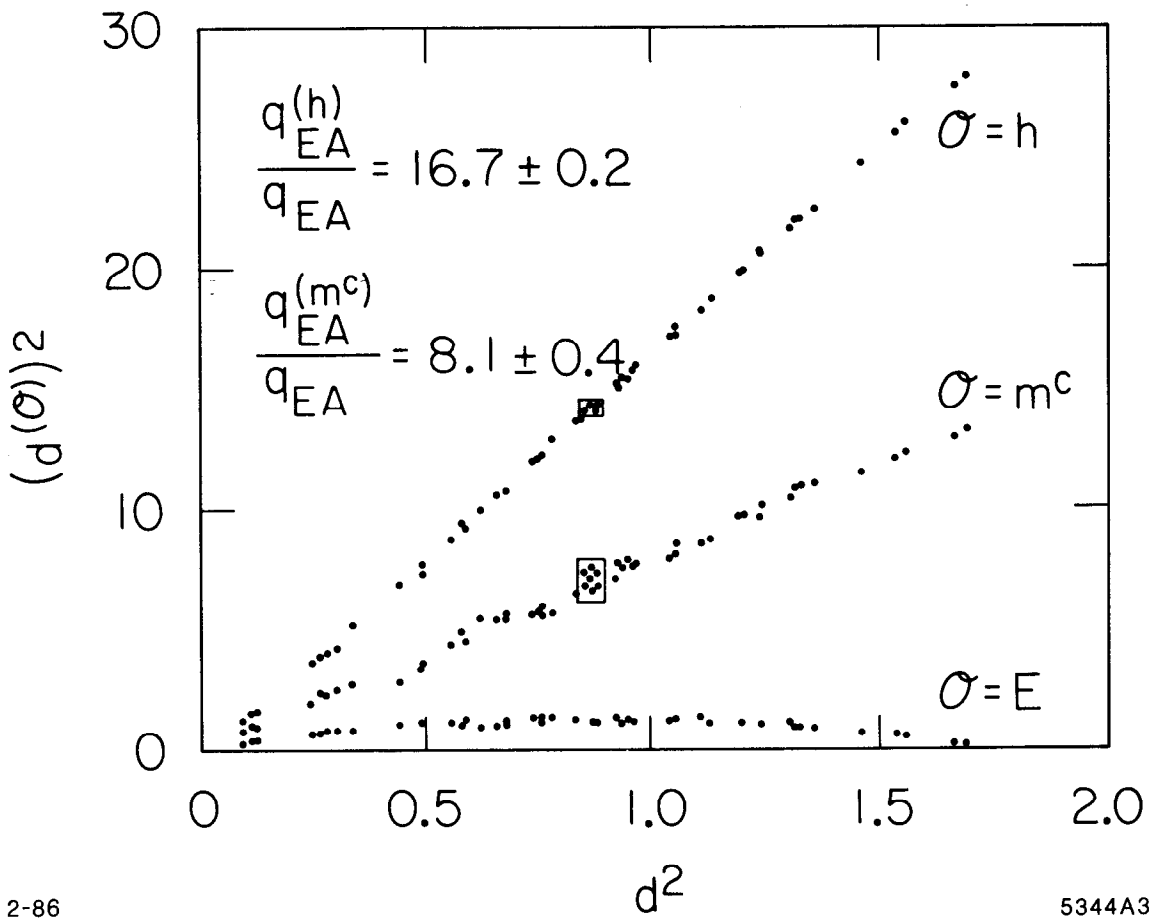


Fig. 3

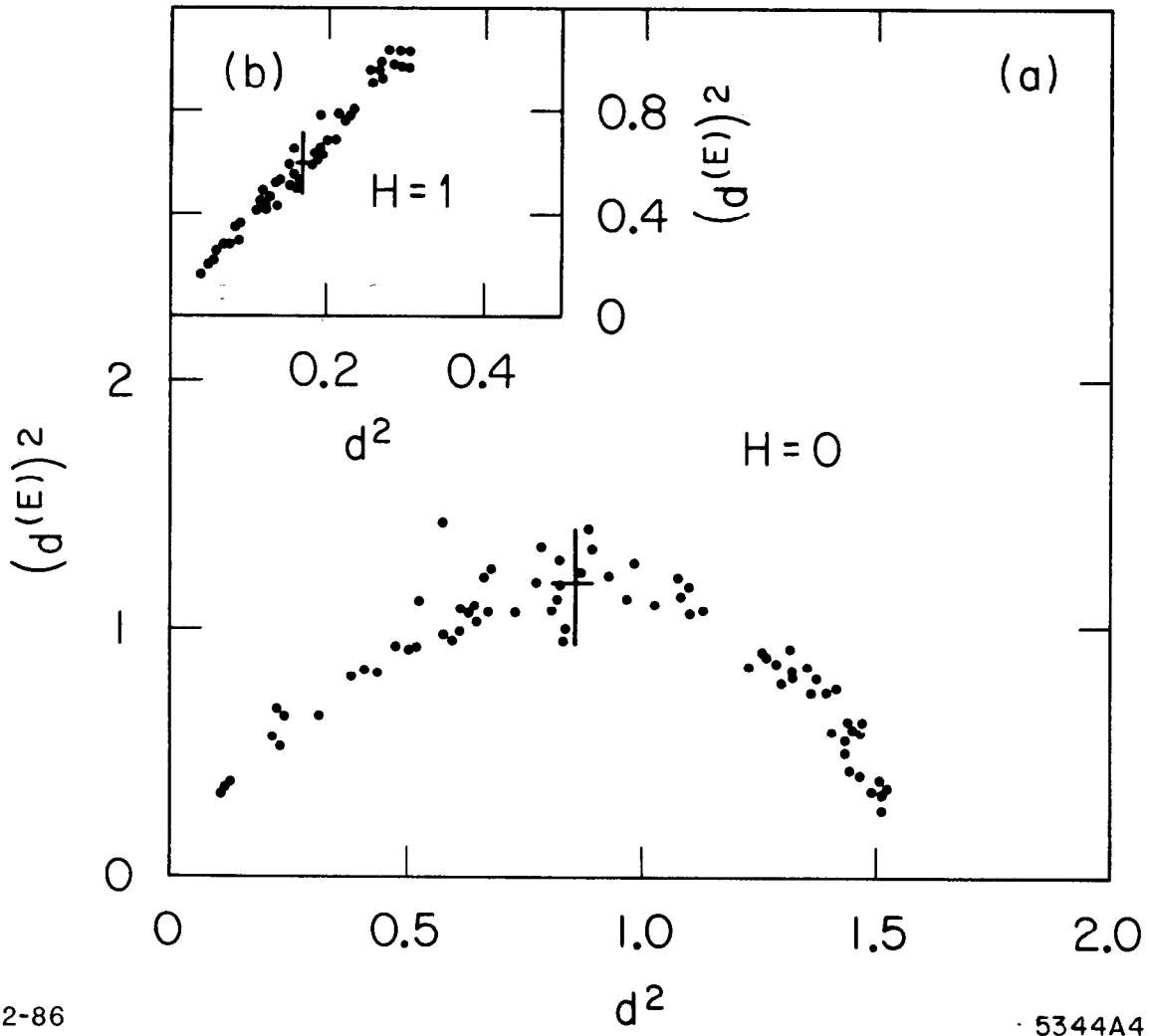


Fig. 4