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## RENORMALIZATION GROUP METHOD FOR VIBRATIONAL BEHAVIOR IN MIXED CRYSTALS

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**Abstract-** The renormalization group method has been applied to investigate vibrational properties of a diatomic mixed crystal. It has been found that there exists a fixed point which separates the one mode behavior from the two mode behavior. This transition depends on concentration, force constants and mass ratios.

It is shown that a fixed point exists which separates the extended mode behavior from a localized one which is interpreted as a transition from the one mode to two mode behavior.

We propose here a new criterion based on the renormalization group method (R.G), this gives an unstable fixed point of transition from one mode to two mode behavior.

We find a transition from one mode behavior to two mode behavior for given mass ratios and force constants (therefore the same crystal) as depending on concentration (Fig. 2). This fact is able to explain qualitatively the transition found experimentally in InSbAs. We perform the renormalization group transformation in one dimension and (with one force constant  $K_X^X$ ) for  $d=3$  we use the Migdal Kadano point moving, technique.

Our R.G. Transformation consists in comparing the eigenvalues, coupling constants and probability distribution of the initial lattice with those of a new one of spacing  $S( S>1)$  times larger than the original.

We consider the mixed crystal  $AB_zC_{1-z}$ .  $M_A$  is the constant mass and the random mass  $M_z(1)$  is  $M_B$  with probability  $z$  or  $M_C$  with probability  $1-z$ ,

We define a disorder parameter (The root mean square deviation of the optical mode normalized by the effective coupling between the nearest cells). We study the transformation  $\lambda \rightarrow \lambda'$  for a change of the scale of the lattice constant  $a \rightarrow Sa$ .

The function  $R(\lambda)$  describes the transition from one mode to two mode behavior.

We can physically explain this claim as follows: the apparition of a localised mode is the condition for a two mode behaviour. For a localised mode, distant regions are uncoupled for our effective chain (the correlation function decreases exponentially). We calculate the coupling constant between distant cells as a coupling adjacent cells in a given state of the R.G. transformation; increasing the size of the cell during the transformation, we obtain a decrease of  $t_{\text{eff}}^{(d=3)}$  an increase of  $\lambda$  and therefore  $R(\lambda) \rightarrow 0$ . ( $t_{\text{eff}}$  is the coupling constant between the cells).

For a one mode behavior (one type of oscillation) a long correlation exists and  $t_{\text{eff}}^{(d=3)}$  decreases slowly relatively to the decrease of the root mean square deviation of the oscillation frequencies,  $\lambda$  decreases and  $R(\lambda) < 0$ .

The fixepts  $R(\lambda)=0$  occur at  $\lambda=0$ ,  $\lambda=\infty$  (one mode, two mode) and the unstable fix point at  $\lambda=\lambda_c \neq 0$ ,  $[R(\lambda) > 0 \text{ for } \lambda > \lambda_c \text{ and } R(\lambda) < 0 \text{ for } \lambda < \lambda_c]$  which describes the point of transition from one mode to two mode behaviour.

For a given  $z, \epsilon$ , we find  $\lambda_c$  for which  $R(\lambda_c)=0$  and respectively the value of  $\mathcal{J}_c$ . ( $\lambda = \lambda(z, \epsilon, \mathcal{J})$ ).

We plot a graph  $\epsilon, \mathcal{J} (\mathcal{J} = \mathcal{J}_c)$  for constant  $z$  and a graph of  $z, \mathcal{J} (\mathcal{J} = \mathcal{J}_c)$  for constants  $\epsilon$ .

Fig. 1 shows our results for  $Z=0.5$  which are compared to the M.R.E.I. and C.P.A. models. Fig. 2 shows the results for  $\epsilon=1$ , which might explain the behaviour of the crystal  $\text{InSb}_z\text{As}_{1-z}$  whose  $\epsilon=1.06$  and  $\mathcal{J}=0.38$  and has been found to behave one mode for  $Z=0.25$  and two mode for  $Z=0.85$ .

We mention that our approximation might change the value of the unstable fixed point  $\lambda = \lambda_c$  (to smaller  $\lambda_c$ ) and as a result the function  $Z = Z(\mathcal{J})$  (Fig. 2), appears to be shifted upwards for  $\mathcal{J}$  close to 1, as approximation involves less disorder.

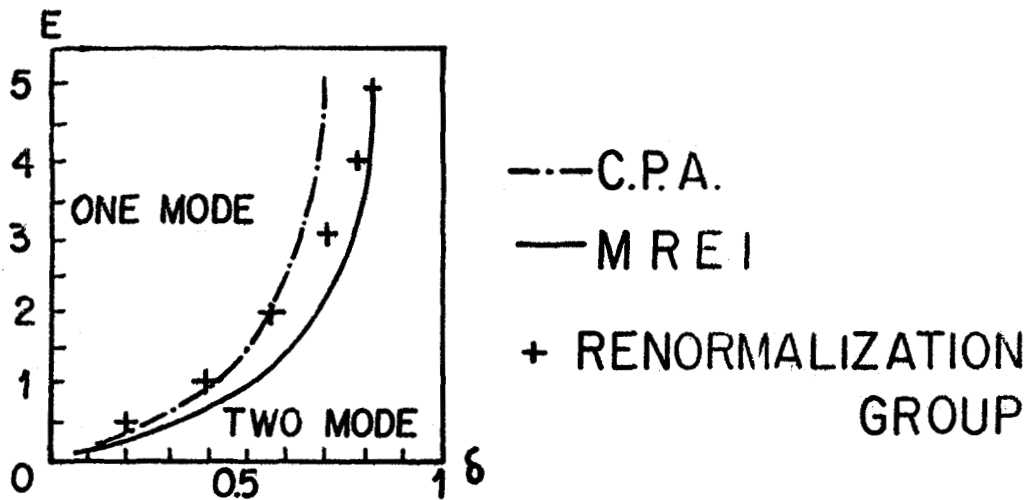


Fig. 1:- Mode behaviour  $\epsilon = \epsilon(\delta)$  for  $Z=0.5$

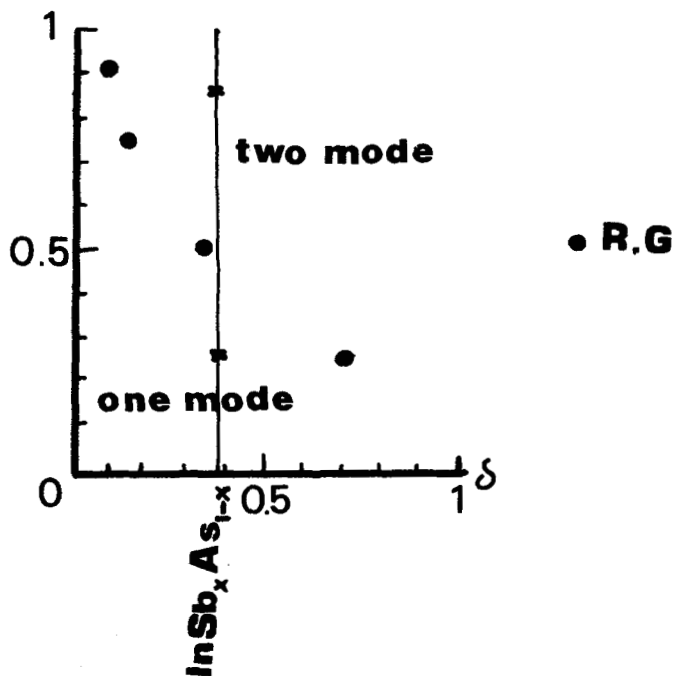


Fig. 2:- Mode behaviour for  $Z=Z(\delta)$  for  $\epsilon=1$