LOCALIZED EIGENSTATES IN DISORDERED SYSTEMS: APPLICATION TO PHONONS*

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The recently developed localization function method is applied to the problem of lattice vibrations in isotopically disordered systems with nearest neighbor coupling. Higher value eigenfrequencies correspond to higher degree of localization. Under a crude approximation explicit results are obtained, which are in qualitative agreement with available calculations.

ANDERSON [1] introduced the idea that the eigenstates of a tight-binding random model are extended or localized depending on whether or not the renormalization perturbation expression [1] (RPE) for the self energy [1] Δ_0 diverges. Recently Anderson's method has been extended and improved [2] to the point where a localization function $L(E)$ has been introduced such that $L(E) > 1$ (< 1) if the energy E lies in the regions of extended (localized) states. At the energies E_c, where $L(E_c) = 1$, the nature of the eigenstates changes abruptly from localized to extended.

The purpose of this communication is to report some results obtained by applying similar ideas to the problem of lattice vibrations in a system with nearest neighbor coupling only and in the case where randomness is introduced by allowing the mass of every particle to be a statistically independent random variable.

The equation governing the displacement u_n of the nth particle of mass m_n is

$$\omega^2 m_n u_n = - \sum_m{}' k_{nm} \cdot (u_m - u_n),\qquad (1)$$

where k_{nm} is a 3×3 matrix describing the coupling of the oscillation of the nth-particle with that of the mth-particle; ω is the eigenfrequency of the oscillation. Equation (1) can be written as

$$(K - \omega^2 m_n) u_n = \sum_m{}' k_{nm} u_m \qquad (2)$$

where $K = \sum_m{}' k_{nm}$ is a 3×3 matrix independent of n due to the assumed peiodicity of the coefficients k_{nm}; the summation in (1) and (2) is over nearest neighbors. For the tight binding approximation in the electronic case considered in reference 2 the corresponding equation is

$$(E - \epsilon_n) c_n = \sum{}' V_{nm} c_m, \qquad (3)$$

where the electronic wave function is given by $|\psi> = \sum_n c_n |n>$, $|n>$ are Wannier functions localized around each site of the lattice, E is the energy eigenvalue and the Hamiltonian is assumed to be $<n|H|m> = \epsilon_n \delta_{nm} + V_{nm}$, with ϵ_n random variables and V_{nm} equal to V for nearest neighbors and zero otherwise.

By comparing equations (2) and (3) one sees that ϵ_n and $m_n \omega^2$ are corresponding quantities. The same analysis [2] that led to the proof of the

existence of a localization function for equation (3) can be repeated for equation (2) and the resulting localization function, L, would depend on ω^2 through the combination $\omega^2 \Delta m$, where Δm is a measure of the spread of the distribution of m_n. In general, larger values of $\Delta m \omega^2$ correspond to smaller values of L, although not always in a monotonic way.[2] Thus larger values of the eigenfrequency ω correspond to larger degree of localization. The fact that k_{nm} in equation (2) are matrices makes any quantitative calculation of L along the lines used[2] for equation (3) impossible. For this reason and in order to obtain some explicit results, it shall be assumed from now on that u_n is scalar and that k_{nm} is a constant number k for every nearest neighbors n, m. Then equation (2) becomes

$$(Zk - \omega^2 m_n)u_n = k \sum_m{}' u_m , \qquad (2')$$

where Z is the number of nearest neighbours. One does not expect that such a model can describe quantitatively a real 3-D motion. However, it is expected that the qualitative features of this simple model are present in the realistic case described by (2). The reason is that, in the corresponding electronic case, there is ample evidence[3] that the band mixing always present in realistic cases does not alter the basic qualitative features present in the one-band model.[4]

Figure 1 exhibits a typical behavior[2] of the localization function pertinent to equation (3) in the case where the quantity ϵ_n has a terminating distribution function centered and peaked at ϵ_0 with a total width W. The trajectory of the mobility edge E_c, where $L(E_c) = 1$, has been plotted (shown as dashed line) in the $E' - W$ plane, where $E' = E - \epsilon_0$. The lines $A'C$ and AC' are the trajectories of the band edges in the same plane according to Lifshitz[5] argument. L is larger than 1 in the unshaded region of the spectrum (extended states) and smaller than 1 in the shaded region. (localized states).

Let us now assume that the masses m_n in (2') possess a terminating distribution function centered and peaked at m_0 with total width Δm. By simple inspection of equations (3) and (2') one sees that problem (2') reduces to (3) if one

makes the substitutions

$$Zk = E, \quad \omega^2 m_n = \epsilon_n, \quad \omega^2 m_0 = \epsilon_0, \quad \omega^2 \Delta m = W,$$

$$k = V, \quad Zk - \omega^2 m_0 = E' \qquad (4)$$

From (4), eliminating ω^2 between the 4th and the 6th equation, we obtain

$$E' = ZV - \frac{m_0}{\Delta m} W . \qquad (5)$$

Thus as ω^2 varies one moves along the straight line (5) in the $E' - W$ plane. This line starts from the point $A(ZV, 0)$ and its slope depends on the ratio $\Delta m/m_0$, i.e. $\tan \phi = \Delta m/m_0$, where ϕ is defined in Fig. 1. Since $m_n \geqslant 0$, $m_0 - \Delta m/2 \geqslant 0$; and consequently $\phi \leqslant \phi_{max} = \tan^{-1} 2$. The frequency corresponding to any point D in the plane is given by

$$\omega^2 = \frac{(AD)}{(AA')} \cdot \frac{2Zk}{(m_0^2 + \Delta m^2)^{\frac{1}{2}}}$$

Hence, for the phonon problem, the line (5) corresponds to the ω^2 axis and the scale on it is proportional to $(m_0^2 + \Delta m^2)^{\frac{1}{2}}$. From Fig. 1 we see that, when $\Delta m = 0$, $\phi = 0$ and all eigenstates are extended as they should be. For $\Delta m \neq 0$, $\phi \neq 0$ and there is always a critical eigenfrequency ω_B,

$$\omega_B^2 = \frac{(AB)}{(AA')} \frac{2Zk}{(m_0^2 + \Delta m^2)^{\frac{1}{2}}} , \qquad (6)$$

separating the localized states ($\omega > \omega_B$) from the extended states ($\omega < \omega_B$). As $\Delta m \to \infty$, $\omega_B \to 0$ and all eigenstates become localized. The above discussion shows that the V-plots in Fig. 1 (and Fig. 2) are very useful tools in presenting properties not only of electronic disordered systems[6] but of vibrational random systems as well.

For small randomness (small ϕ in Fig. 1) localization appears at high frequencies and near the band of the edge. This seems to be a common characteristic of numerical calculations in complicated disordered systems.[7]

If the distribution of the mass is a Lorentzian, the trajectory of E_c in Fig. 1 is approximately a semicircle[2] and explicit results for ω_c can be obtained.[2,8]
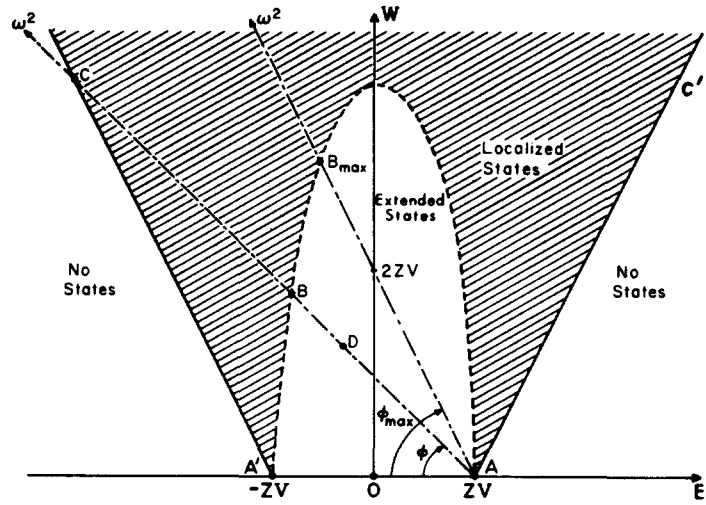
We consider now the binary alloy case where

FIG. 1. Trajectories of the band edges (solid lines) and mobility edges (dashed lines). For the electronic case, W is the total width of the distribution around the value ϵ_0 (see text) and E' is the energy measured from ϵ_0. For the phonon case the frequency axis is a straight line starting from the point A and making an angle ϕ with the E' axis; $\phi = \tan^{-1} \Delta m / m_0$ (see text).
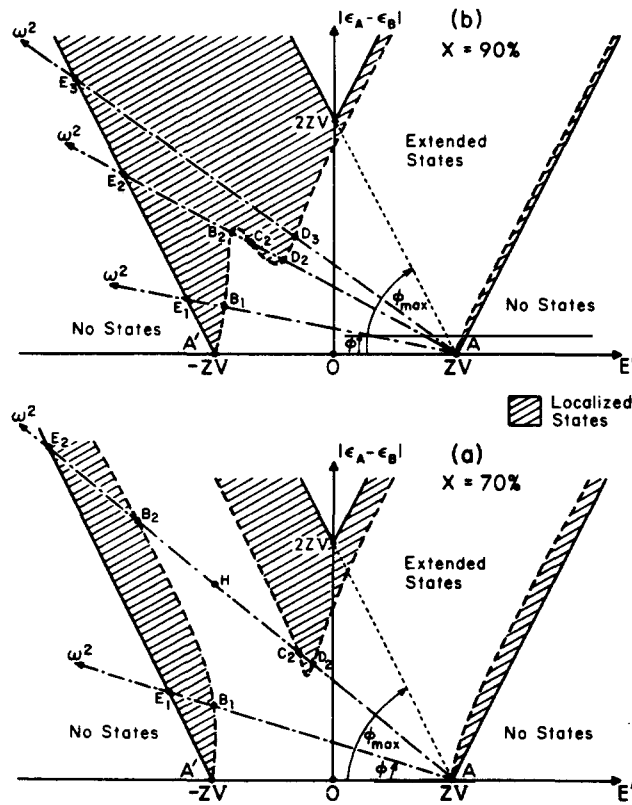

FIG. 2. Trajectories of the band edges (solid lines) and mobility edges (dashed lines) for the binary alloy case for two different values of the concentration x. E' is the energy for the electronic case measured from $(\epsilon_A + \epsilon_B)/2$ (see text). For the phonon case the frequency axis is a straight line starting from the point A and making an angle ϕ with the E' axis; $\phi = \tan^{-1} 2(M - m)/(M + m)$ (see text).

each m_n can take two values m or M with probability $1 - x$ and x respectively, where x is the concentration of the heavy mass (M) particles. The corresponding electronic problem is the one where ϵ_n can take two values ϵ_B or ϵ_A with probability $1 - x$ and x respectively, $(\epsilon_A > \epsilon_B)$. The phonon problem is equivalent to the electronic one if we make the substitutions

$$E = Zk, \quad \epsilon_A = \omega^2 m, \quad \epsilon_B = \omega^2 m, \quad V = k,$$

$$\epsilon_A - \epsilon_B = \omega^2(M - m), \quad E' = Zk - \omega^2 \frac{(M + m)}{2} \quad (7)$$

Figure 2 is the analogue of Fig. 1 for the binary alloy case. The trajectories of the band edges (solid lines) were drawn according to Lifshitz[5] argument; the trajectories of the mobility edges E_c (dashed lines) were calculated according to the coherent potential approximation[6] of the function $F(E)$ introduced in references 2 and 4; $F(E)$ always underestimated the regions of localized states. The ω^2 axis is again a straight line starting from the point A and making an angle ϕ with the E' axis (Fig. 2) given by

$$\phi = \tan^{-1} \frac{2(M - m)}{-M + m} \quad (8)$$

and the scale is proportional to $[(M - m)^2 + \frac{1}{4}(M + m)^2]^{\frac{1}{2}}$. From Fig. 2 one can see that, as the quantity $(M - m)/(M + m)$ increases from zero, a critical frequency ω_B appears such that the eigenstates with eigenfrequency larger (smaller) than ω_B are localized (extended). As $(M - m)/(M + m)$ increases further ω_B varies and at a certain critical value of the mass ratio two additional critical frequencies, ω_C, ω_D, appear such that the regions $0 \leqslant \omega < \omega_D$ and $\omega_C < \omega < \omega_B$ correspond to extended states while the regions $\omega_D < \omega < \omega_C$ and $\omega_B < \omega$ correspond to localized states. As $(M - m)/(M + m)$ continues to increase, there are two possibilities presented in Figs. 2a and 2b depending on whether or not the concentration x of the large mass is smaller or larger than a critical value x_c of x, (which in the present case is calculated to be $x_c \doteq 83$ per cent). If $x < x_c$ (case of Fig. 2a), the difference $\omega_B - \omega_C$ remains always finite as $(M - m)/(M + m)$ increases and there are always extended states in the interval $[\omega_C, \omega_B]$. On the other hand, if $x > x_c$ (Fig. 2b), there is another critical value of the mass ratio such that the

critical frequencies ω_C, ω_B merge together eliminating the extended states of the interval $[\omega_C, \omega_B]$. This corresponds to the Anderson transition[1,2] in the electronic case. Let us consider the case where m is kept constant and $M \to \infty$. Then $\phi \to \phi_{max}$ and $\omega_D \to 0$. On the other hand, ω_B, ω_C (case $x < x_c$) approach some finite limits. Thus as $M \to \infty$, if $x > x_c$, all 'phonons' become localized, while, if $x < x_c$, there are two critical frequencies ω_C, ω_B such that the states in the interval $[\omega_C, \omega_B]$ are extended and the states in the intervals $[0, \omega_C]$ $[\omega_B, \omega_E]$ are localized, where ω_E is the band edge.

This last case can be important, since it implies a temperature dependence of the form $e^{-E_c/kT}$ for transport coefficients depending on phonons, like, for example, the thermal conductivity in non-magnetic insulators. The activation energy E_c is directly related with the critical frequency ω_c, $E_c = \hbar\omega_c$.

The analysis of the nature of the localized states presented in reference 4 as well as the verification of the existence of a critical concentration x_c by percolation[9] theory can be carried on unaltered for the phonon case. It can be shown[4] that $x_c = 1 - P_c$, where P_c is the critical percolation probability.[9] The present analysis predicts a quite drastic change in the character of the eigenstates corresponding to the upper part of the spectrum as the concentration of the light masses $1 - x$ passes through the critical percolation probability P_c. This is exactly what was observed in the numerical calculations of Payton and Visscher.[10] The results presented in Fig. 2 are also capable of explaining[8] features present in Taylor's calculations.[11]

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Die kürzlich entwickelte Lokalisierungsfunktionsmethode wirde auf Gitterschwingungen in isotop gestörten Systemen mit Kopplung zum nächsten Nachbarn angewendet. Der Grad der Lokalisierung ist umso höher, je grösser die Eigenfrequenz ist. Mit einer groben Approximation kann man explizite Resultate bekommen, die qualitativ mit bisher bekannten Ergebnissen übereinstimmen.