CRITICAL STRENGTH FOR IDEAL INCOMMENSURATE STRUCTURES

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A concise method is developed to show the following in one dimension: (a) If there is a sharp metal—insulator transition in an ideal sinusoidal incommensurate structure then \( W/V = 2 \). (b) There is an infinite dc conductivity of electrons in an ideal incommensurate structure for \( T = 0 \) if \( W/V < 2 \). (c) Addition of impurities which scatter between all pairs of \( k \) values may lead to a finite conductivity for \( W/V < 2 \). (It tends to zero as \( L \to \infty \)). The concept of duality used by Aubry is then extended to the general problem of localization and the breakdown of extended states is illustrated.

Recently, several distinct problems such as Bloch electrons in a magnetic field [1], electrons [2,3] and phonons [4,5] in incommensurate structures and the study of superconductivity on a network*1 [6] have been cast in the form of the eigenvalue problem

\[
(E - e_n) c_n + V c_{n+1} + V c_{n-1} = 0 ,
\]

where

\[ e_n = W \cos Qna . \]

If \( Q = 2\pi/\lambda \) and \( \lambda/a \) is irrational the two periods are said to be incommensurate. Under these conditions it has been shown by Aubry [7] that \( W_c/V = 2 \) is a critical value for a transition between extended and localized states. Many numerical calculations and other arguments support this conclusion [8–10]. In what follows we present a concise way of understanding this result and its implications.

In a tight binding representation one writes in coordinate space

\[
EI - H \equiv \begin{bmatrix}
E - e_{-1} & V \\
V & E - e_0 & V \\
& V & E - e_1
\end{bmatrix}.
\]

On Fourier transforming the periodic potential \( W \cos Qx \) one has

\[
V_{kk'} = \frac{1}{2} W \delta(k - k' + Q) + \frac{1}{2} W \delta(k - k' - Q) . \quad (4)
\]

Then in \( k \) space one has

\[
EI - H \equiv \begin{bmatrix}
E - e_k & \Delta \\
\Delta & E - e_{k+Q} & \Delta \\
& \Delta & E - e_{k+2Q}
\end{bmatrix} .
\]

Here \( \Delta = \frac{1}{2} W \) and \( e_k = J \cos k\alpha \) where \( J = 2V \).

Also as is well known a continued fraction expansion in coordinate space is

\[
G_{00} = \frac{1}{E - e_0 - \Sigma_{00}} ,
\]

where

\[
\Sigma_{00}^+ = \Sigma_{00}^- + \Sigma_{00}^+
\]

and

\[
\Sigma_{00}^+ = \frac{V^2}{E - e_1 - V^2} .
\]

*1 In this problem it is precisely the critical value of \( W \) which is of interest.

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Convergence of such an expression as (6) in the realm of real numbers means that \( \Sigma^+_{00} \) is real, and the states are local with an infinite lifetime. If it did not converge then \( \Sigma_{00} \) may have an imaginary part \( \text{Im} \Sigma_{00} = \hbar/\tau_L \neq 0 \), where \( \tau_L \) is the lifetime of the localized states, so that diffusion could then take place.

Similarly, for \( G_{kk} \) we have
\[
G_{kk} = \frac{1}{E - \varepsilon_k - \Sigma^+_{kk} - \Sigma^-_{kk}},
\]
where
\[
\Sigma^+_{kk} = \frac{\Delta^2}{E - \varepsilon_k + Q - \Delta^2} - \frac{\Delta^2}{E - \varepsilon_k + 2Q - \cdots} \tag{7}
\]
For \( k = 0 \) we notice a formal equivalence between the two continued fractions if
\[
\Delta \leftrightarrow V, \quad W \leftrightarrow J.
\]
Convergence of (7) means that plane waves are an adequate basis now (as local functions were previously) and thus one has extended states. If it does not converge we may think of the existence of an imaginary part \( \text{Im} \Sigma_{kk} = \hbar/\tau_E \) where \( \tau_E \) is the lifetime of extended states.

Let us suppose that we get convergence of \( \Sigma_{00} \) for \( W/V > q \) and we want to find \( q \). \( W \) which in coordinate space in coordinate is on the diagonal becomes \( \Delta = \frac{1}{2} W \) on the off-diagonal in \( k \) space. On the other hand, \( J = 2V \) in the diagonal terms in \( k \) space goes to \( V = \frac{1}{2} J \) on the off-diagonal in coordinate space.

The same convergence criteria as before now applies in \( k \) space, because of the formal equivalence of the continued fractions, i.e. convergence in \( k \) space takes place if
\[
|J/\Delta| > q \quad \text{or} \quad 2V/\Delta W > q \quad \text{or} \quad W/V < 4/q.
\]
Our results are summarized in table 1.

| Space Convergence | Implications | Convergence of
<table>
<thead>
<tr>
<th>condition</th>
<th></th>
<th>reality</th>
</tr>
</thead>
<tbody>
<tr>
<td>coordinate ( W/V &gt; q )</td>
<td>localization</td>
<td>( G_{rr} (r = 0) )</td>
</tr>
<tr>
<td>( k ) ( W/V &lt; 4/q )</td>
<td>extended</td>
<td>( G_{kk} (k = 0) )</td>
</tr>
</tbody>
</table>

extra off-diagonal matrix elements in \( k \) space favours localization.) As was shown, convergence in \( k \) space has the opposite interpretation to that in coordinate space and the critical strength was obtained thanks to the duality in the form of the hamiltonian under a Fourier transform. Up to now we have explained what essentially is the duality argument as used by Aubry. Let us discuss this more completely.

It is clear from a logical point of view that it is still possible that there exists a narrow region about \( W_c/V = 2 \) where neither completely extended nor completely localized states exist. This is because we did not prove that the continued fraction actually converges for \( W/V > 2 \) in coordinate space, nor has a proof been given previously. However, there is a preponderance of numerical results supporting this conclusion. We have shown that if the transition is sharp it necessarily occurs at \( W_c/V = 2 \). Furthermore, the argument holds for all incommensurate values of \( Q \) and all values of \( E \) for which there are states. This is in agreement with the results of Soukoulis and Economou [2]. Furthermore, their result that the inclusion of two cosines with different periodicities can lead to a mobility edge is in agreement with our argument that the addition of other matrix elements in \( k \) space has a localizing effect.

From here on one can try to understand localization in a disordered one-dimensional system. First of all, one can imagine that there are repeating disordered unit cells of length \( L \). Taking the Fourier transform of the potential leads to many \( k \) values bounded by \( k_{\text{min}} = 2\pi/L \) and \( k_{\text{max}} = 2\pi/a \). If the potential is truly random the Fourier transform contains almost every multiple of \( k_{\text{min}} \). The limit is then taken for \( L \to \infty \) and the off-diagonal elements in \( k \) space become dense. Then one expects that the states should be localized in the limit \( L \to \infty \) (though extended for any finite \( L \)).

There is a different way of stating the above statement, which we checked numerically.
Since the unit cells repeat, the continued-fraction can be closed off, each unit cell contains site energies $(e_1 \ldots e_L)$:

\[
\Sigma^+ = \frac{V^2}{E - e_1 - V^2} = \frac{V^2}{E - e_2 - V^2} = \cdots = \frac{V^2}{E - e_L - \Sigma^+}
\]

Because this is a sequence of linear fractional transformations (with a group property under substitution) it always reduces to quadratic form:

\[A_L(\Sigma^+)^2 + B_L(\Sigma^+) + C_L = 0.\]

On calculating $\text{Im } \Sigma^+ = (\hbar/\tau_L)^+$ one verifies for a model in which $e_l \in [-\frac{1}{2} W, \frac{1}{2} W]$ uniformly that $\langle \text{Im } \Sigma \rangle \propto e^{-L/\lambda}$ as $L \to \infty$ in agreement with localization theory. Here localization is achieved by a breakdown of extended states $L \to \infty$. Here $\langle \rangle$ indicates a configuration average. Note that $\lambda(W)$ is not really a localization length since one is here working with a sequence of ordered lattices. It is better to interpret it as a scaling length.

For a single incommensurate cosine that imaginary part predictably did not attenuate as $L$ increases, for $W/V < 2$. The jump discontinuities in the cosine at the boundaries of the cell should have no influence as $L \to \infty$. For $W/V > 2$ that attenuation does take place but in a complicated manner that cannot be simply expressed with an exponential.

The convergence properties with a potential of the form $\Sigma^+_M A_l \cos Q_l x$ can be analyzed in $k$ space by adding constant off-diagonal elements $A_1, A_2, \ldots$. Our argument implies that each successive term added $(M \to M + 1)$ increases “extension” in $k$ space, i.e. increases localization in coordinate space. This may be considered a Fourier approximation to an even potential, and increasingly higher harmonics will be needed to describe short range disorder.

The argument is clearest if the series $\Sigma^+_l A^2_l$ diverges. We give below the approximate values for the transition at $E = 0$ for the following potentials which illustrate the effect.

\[
E_n = W \cos 2n: \quad W_c/V = 2,
\]

\[
E_n = W \cos 2n + W \cos 4n: \quad W_c/V = 1,
\]

\[
E_n = W \cos 2n + W \cos 4n + W \cos 6n: \quad W_c/V = 0.4.
\]

This also reinforces the conclusion of Aubry, that discontinuous incommensurate potentials would lead to localized states.

In summary we show how localized states can arise from a breakdown of extended states and the duality idea helps to understand this effect. The addition of impurities reduces the one dimension conductivity to zero as $L \to \infty$, because $\text{Im } \Sigma = \hbar/\tau \to 0$ as $L \to \infty$ in $x$ space (lifetime of local states becomes infinite).

We note finally that the calculations of $\text{Im } \Sigma^+_{00}$ are facilitated; that simple recursion relations may be found when performing the linear fractional transformations.

If we represent one such transformation with

\[Z = \frac{a_1 W + a_2}{a_3 W + a_4} = f(W),\]

it may be represented by a matrix

\[
\begin{pmatrix}
a_1 & a_2 \\
a_3 & a_4
\end{pmatrix}
\]

The composition of the transformations is simply reduced to multiplying $2 \times 2$ matrices. Thus, it is easy to calculate the coefficients $A_L B_L$ and $C_L$ of the quadratic equation up to the length $L$ of the unit cell.

The result $\text{Im } \Sigma^+_{(E=0)} = V \exp[-L/\lambda(W)]$ was obtained by averaging over 500 systems in one dimension and we found that this expression is adequate in fitting the data.

This method of calculating the lifetime of local states may also be extended to stripes or bars with repeating cells. Instead of a quadratic equation one gets a matrix-Ricatti equation. We will present further details of such calculations in a separate publication.

References
