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Localisation in disordered systems—I: The disordered spectrum

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Abstract. Starting from a definition of the localisation-delocalisation of electronic, wavefunctions in disordered systems based on the nature of the disordered spectrum, a delocalisation criterion identical to that of Abou-Chacra *et al* is recovered. The new derivation provides a very clear picture of the mechanism of delocalisation and brings out its incompatibility with the normalisability of wavefunctions at the transition.

Keywords. Localisation; disordered systems.

1. Introduction

In a recent paper Abou-Chacra *et al* (1973) have presented a localisation criterion on a Cayley tree which provides a very pleasing exposition of the localisation-delocalisation phenomenon within the Anderson tight-binding model of cellular disorder. It entirely avoids the use of the CPA and similar effective medium approximations inherent in the Economou-Cohen type criteria (Economou and Cohen 1972, Licciardello and Economou 1974). In view of the fact that these latter criteria ignore the effect of arbitrary large clusters which eventually *cause* localisation, serious doubt was cast on them (Haydock and Mookerjee 1974). The criterion of Abou-Chacra *et al* (henceforth AAT) was presented by the authors in a mathematically complex way and a clear picture of the mechanism of localisation-delocalisation was lacking. It is the purpose of this paper to approach the problem from an entirely different point of view. We shall eventually recover the AAT criterion in a manner that displays this transition in a transparent way.

2. The disordered spectrum

Let us begin by examining the spectrum of the self-adjoint Hamiltonian $\boldsymbol{H} \in \mathcal{H}$ of a disordered system. Corresponding to the operator $\boldsymbol{H}$ we may define the resolvent $\boldsymbol{R}(z) = (z\boldsymbol{I} - \boldsymbol{H})^{-1}$ where z is a complex number. The spectrum S is the set of singularities of $\boldsymbol{R}(z)$ in the complex z-plane. Hermiticity of $\boldsymbol{H}$ connected to the causality principle demands that S lies entirely on the real z-axis. We may also define the 'spectral family' operator $\boldsymbol{P}(e)$ where e lies in the spectrum S (Reisz and Nagy 1956) with properties: $\boldsymbol{P}^2 = \boldsymbol{P}$, $\boldsymbol{P}(+\infty) = \mathrm{I}$, $\boldsymbol{P}(-\infty) = 0$, $\boldsymbol{P}(e)\boldsymbol{P}(e') = \boldsymbol{P}(\min\{ee'\})$ and $f(\boldsymbol{H}) = \int f(e)\, \mathrm{d}\boldsymbol{P}(e)$. If we choose a tight-binding basis $\{|r_n\rangle\}$ for representations of operators on $\mathcal{H}$, the 'spectral measure' $m_n(e)$ is defined to be $\langle r_n | \mathbf{P}(e) | r_n \rangle$.

Consider first a finite system of N sites. The spectrum is a finite point set $\{e_i, i = 1, 2, \ldots, N\}$ on the real axis; that is, the function $R_{nn}(z)$ has N poles $\{e_i\}$ on the real z-axis with residues $\{c_i^n = |\langle r_n | e_i \rangle|^2\}$. The poles are non-dense in the sense that it is possible to enclose each e_i by open sets, say an open disc of radius r_e, such that for r_e sufficiently small the disc contains no other singularity of $R_{nn}(z)$. The spectral measure is a non-decreasing discontinuous step function with step discontinuities at $\{e_i\}$ of heights $\{c_i^n\}$ and the following hold:

$$\lim_{\delta \to 0} \operatorname{Im} R_{nn}(E + i\delta) = 0$$

for all E except a set of measure zero (1 *a*)

$$\int \lim_{\delta \to 0} \operatorname{Im} R_{nn}(E + i\delta)\, A(E, \delta)\, \mathrm{d}E > 0$$

if

$$\lim_{\delta \to 0} A(E, \delta) > 0 \text{ everywhere} \qquad (1\,b)$$

If we now let the system become infinitely large, $N \to \infty$, and the spectrum becomes an infinite set. It can behave in three distinct ways:

(I) A section (B) of the spectrum may contain a very large number of poles, but they still remain non-dense in the sense already described. The spectral measure remains a discontinuous step function and (1 *a*) and (1 *b*) continue to hold.

(II) In another section ($\mathscr{E}$) the number of poles become so large that eventually they coalesce and become dense. That is, every neighbourhood of a pole, however small, always contains at least one other pole. $R_{nn}(z)$ from being non-analytic at points, becomes non-analytic on a *line*. Equation (1 *a*) no longer holds and $\lim_{\delta \to 0} R_{nn}(E + \mathrm{i}\delta)$ becomes non-zero on a set of finite measure. Hermiticity of H demands $R_{nn}(z) = R_{nn}^*(z^*)$ and this combined with the above property implies that on $\mathscr{E}$

$$\lim_{\delta \to 0^+} \operatorname{Im} R_{nn}(E + \mathrm{i}\delta) = -\lim_{\delta \to 0^+} \operatorname{Im} R_{nn}(E - \mathrm{i}\delta).$$

That is, this section of the spectrum is a branch cut of $R_{nn}(z)$. The spectral measure becomes a continuous, monotonically increasing function.

(III) In another section ($\mathscr{L}$) of the spectrum the poles may become dense but $\lim_{\delta \to 0} \operatorname{Im} R_{nn}(E + \mathrm{i}\delta)$ remains zero except on a set of measure zero (Thouless 1972). In other words, although the poles of $R_{nn}(z)$ become dense, the residues of the poles are significantly different from zero only on a set of measure zero. The spectral measure is continuous and non-decreasing, but it strictly increases only on a set of measure zero. Such pathological behaviour is called 'singular continuity'. At first glance it may be thought that such peculiar behaviour has nothing to do with physics, rather it is a mathematician's fanciful construction. However,

Ishii (1973) has proved that on a linear chain as soon as disorder is introduced the entire spectrum of an infinite system has this singular behaviour. It is well known that for an infinite linear chain *all* states are localised however small the disorder (Borland 1963). States in this regime will be connected to localised states.

In a periodic system the extended Bloch states correspond to a branch cut in $R_{nn}(z)$ and its poles correspond to bound states. Carrying over this idea into the disordered systems, we shall define the states in $\mathscr{E}$ as extended states (of course, no longer Bloch states), while those in B we whall call bound states. The section $\mathscr{L}$ basically consists of dense poles, but not a true branch cut. These states are similar in nature to bound states, but lie in a region of continuous density of states. These are exactly of the nature of localised states of the Mott-CFO model (figure 1).

3. The Cayley tree

Let us consider a system in which an electron moves on a Cayley tree of connectivity K. Each site has one possible energy level e_i which is a random variable. The hopping integral connecting nearest neighbours is V, which we may scale to 1. The eigenfunction $\psi(E)$ of the Hamiltonian

$$H = \sum_i \sum_j \{e_i \delta_{ij} + V_{ij}\} \tag{2}$$

is specified by a set of amplitudes $\{a_i(E)\}$ which obey the equation

$$(E - e_i)\, a_i(E) - \sum_{j(i)} a_j(E) = 0 \tag{3}$$

Here $j(i)$ are the nearest neighbours of i. Let us define N_i as the nearest neighbours of i which lie in a shell *away* from the chosen origin. The origin has $K+1$ nearest neighbours away from it and all subsequent sites have K such neighbours. If we now define $r_{ji}(E)$ as the ratio $a_j(E)/a_i(E) j \notin N_i$ we immediately get from eq. (3)

$$r_{ji}(E) = 1/\{E - e_j - \sum_{k \in N_j} r_{kj}(E)\}; \quad E - e_0 - \sum_{j \in N_0} r_{j0}(E) = 0 \tag{4}$$

On the Cayley tree, suppose S_n denotes the set of vertices at a distance 'n' away from an arbitrary chosen origin (the 'nth shell'), then there are in all $K^{n-1}(K+1) \sim K^n$ points on it for large n, and only *one* path leading to each such point from the origin. Because of the absence of closed polygonal paths, the contributions of these K^n paths to the configuration averaged quantities are *independent*.

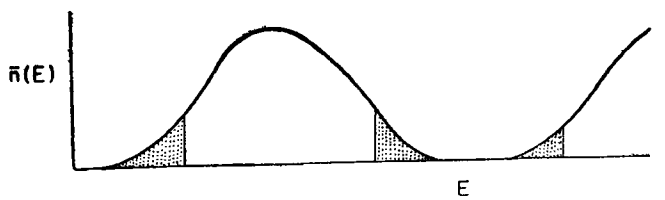

Figure 1. The Mott-CFO model showing density of electronic states in a disordered semi-conductor. The shaded portion indicates the localised states.

Further, because of the macroscopic homogeneity of configuration averaged quantities, these contributions are independent of the path chosen. Let us label one such path P_s by (0, 1, 2, ..., n) and let N_i' denote those vertices in N_i not lying on P_s. Define now

$$A_i(r_{i+1,i}) = \int \dots \int |r_{i+1,i}, r_{i+2,i+1} \dots | P(r_{i+1,i}, r_{i+2,i+1} \dots) \, dr_{i+2,i+1} \dots \tag{5}$$

The ratios $r_{ji}(E)$ are *dependent* variables as shown in eq. (4); we can, however, break up the joint probability density as:

$$P(r_{i+1,i} | r_{i+2,i+1}) \, P(r_{i+2,i+1}, r_{i+3,i+2} \dots)$$

The ratio $r_{i+1,i}$ depends *only* of $r_{i+2,i+1}$ because of the Cayley tree topology. In general lattices it may depend on other ratios and this simple decomposition vital to the development will not strictly hold subsequently. Substituting this into eq. (5) we obtain

$$A_i(r_{i+1,i}) = \int |r_{i+1,i}| P(r_{i+1,i} | r_{i+2,i+1}) \, A_{i+1}(r_{i+2,i+1}) \, dr_{i+2,i+1} \tag{6}$$

Let us define

$$w_i = E - e_i - \sum_{j \in N_i'} r_{ji};$$

then referring back to eq. (4),

$$\begin{aligned} P(r_{i+1,i} | r_{i+2,i+1}) &= \int \delta(r_{i+1,i} - [w_i - r_{i+2,i+1}]^{-1}) \, Q(w_i) \, dw_i \\ &= Q(r_{i+2,i+1} + 1/r_{i+1,i})/r_{i+1,i}^2 \end{aligned}$$

where $Q(w_i)$ is the probability density of the variable w_i. Putting this value of the conditional probability back in eq. (6) we obtain the difference-integral equation

$$A_i(r_{i+1,i}) = \int \frac{1}{|r_{i+1,i}|} Q(r_{i+2,i+1} + 1/r_{i+1,i}) \, A_{i+1}(r_{i+2,i+1}) \, dr_{i+2,i+1} \tag{7}$$

Suppose we want to evaluate the average of a quantity like $|a_n(E)/a_0(E)| = |r_{10}r_{21} \dots r_{nn-1}|$ for sufficiently large n. This in essence measures the average space evolution of the modulus amplitudes away from the origin and should, for localised states, decrease faster than K^n. The average of such a quantity for sufficiently large n can be deduced from eq. (7) as $\lambda^n \phi$ where λ and ϕ are the largest eigenvalue and corresponding eigenfunction of the integral equation

$$\lambda A(x) = \int |x|^{-1} Q(y + 1/x) \, A(y) \, dy \tag{8}$$

4 Delocalisation criterion

Let us now concentrate on the off-diagonal resolvent $R_{on}(z)$. It is to be noted that as functions of z, the off-diagonal and diagonal terms of the resolvent representation have identical singularities (on the spectrum of H). In terms of the energy eigenstates it may be expressed as

$$R_{on}(E_n) = \int a_0(E_s)\, a_n(E_s)\,(E - E_s)^{-1}\, dm(E_s) \tag{9}$$

Thus $R_{on}(E)$ diverges whenever E lies on the energy spectrum. Near $E = E_s$ $R_{on}(E) \sim a_0(E_s)\, a_n(E_s)/(E - E_s)$. Given R is sufficiently large, in an interval I_s around E_s given by $|E - E_s| < |a_0(E_s)\, a_n(E_s)|/R$ $|R_{on}(E)| > R$.

Suppose now L be the event such that it is possible to find an energy value E which lies *outside* the union of all such intervals I_s corresponding to all the eigenenergies E_s. We have

$$P(L) = \prod_s \{1 - n(E)\,|a_0(E_s)\, a_n(E_s)|/R\}$$

Let us start with a large but finite Cayley tree of size up to n shells, n being very large. There are on the whole $\sim K^n$-eigenenergies. So

$$P(L) \simeq \exp\{-n(E) \sum_{s=1}^{K^n} |a_0(E_s)\, a_n(E_s)|/R\}$$

Since n is very large, and eventually we aim to look at $n \to \infty$, it is immaterial where we choose the origin of the Cayley tree. If we so choose it that it coincides with the maximum amplitude of the wavefunction $\psi(E)$, and further scale the amplitudes in terms of $|a_0(E_s)| = 1$, then

$$P(L) \simeq \exp[-n(E)\, K^n \{K^{-n} \sum_{n=1}^{K^n} |a_n(E_s)|\}/R]$$

But the term inside the { } is exactly the kind of average we have been speaking about in section 3. The sum takes into account all intermediate values for r_{21}, ... $r_{n,n-1}$, there being $\sim K^n$ such possibilities. For large n, therefore, this expression takes the form

$$P(L) \simeq \exp\{-n(E)\,(K\lambda)^n/R\} \tag{10}$$

Let us now make the system infinite, $n \to \infty$. The two possibilities are: (*I*) If $\lambda K > 1$, then in the energy region in which this holds it is impossible to find an energy value E lying outside the union UI_s. This is only possible if the eigenenergies in this region form a continuous branch cut of $R_{0n}(z)$. By our definition, this criterion corresponds to extended states. (II) If $\lambda K < 1$, then we are certain to find an energy value E outside the union UI_s. Even if the energies are dense, the measure of UI_s on which $|R_{on}| > R$, however large, is of the order $1/R$, however small. These can correspond only to localised or bound states.

The delocalisation criterion is therefore $\lambda K > 1$. This is exactly the AAT criterion. Equation (8) is the AAT integral equation. The argument used here is similar to the argument used for linear chain by Thouless (1972). In fact the $(K\lambda)$ measures the rate of decay of the wavefunction amplitude modulus on succeeding shells and can be related to the range of localisation parameter in the region $\lambda K < 1$.

5. Comments

The most important factor to note here that it is $|a_n(E_s)|$ and not $|a_n(E_s)|^2$

which enters the criterion (10). We expect that in the delocalised region the wavefunction should be un-normalisable on the average, similar to Bloch states in periodic systems. That is $\langle \int |\psi(E)|^2 \mathrm{d}V \rangle$ should not be finite. In tight-binding formalism this implies $\sum_n \langle |a_n(E)|^2 \rangle$ should diverge. Our criterion for delocalisation $\lambda K > 1$, involving as it does $|a_n(E)|$ is not incompatible with normalisable wavefunction (since $\langle |a_n(E)| \rangle^2 \neq \langle |a_n(E)|^2 \rangle$). This discrepancy was noted by Abou-Chacra *et al* (1973). They noted that even in the delocalised regime the wavefunction near the transition remains normalisable. Thouless and Last (1973) point out that the above criterion relates to the breakdown of exponentially localised states. They propose an intermediate regime of 'power-law' localised states. This suggestion, however, must remain speculative until more convincing arguments establish it. We could, of course, construct a criterion based on the divergence or otherwise of $\sum_n \langle |a_n(E)|^2 \rangle$. This would clarify the picture. This problem is under consideration and will be reported in a subsequent communication.

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