LETTER TO THE EDITOR

Localisation criterion in the Cayley tree without electron–electron interactions

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Abstract. The electron localisation criterion for one impurity atom can be exactly derived for a Cayley tree network of atoms using the tight-binding approximation.

The Cayley tree or Bethe lattice is a convenient model lattice, since problems encountered in the theory of localisation of electrons in disordered systems (Abou-Chacra et al 1973, Thouless et al 1977, Anderson 1979) and in chemisorption theory (Haydock et al 1975, Van Santen and Toneman 1977) can sometimes be exactly solved for such a lattice.

In this Letter we will derive the exact expression for the local density of states of an impurity atom connected with a network of atoms as in the Cayley tree.

The network of the Cayley tree is sketched in figure 1. Its particular feature is that any two intersections on it can be interconnected in only one way. On each intersection we position one atomic orbital. We determine the local density of states using the tight-binding approximation in which electron–electron interactions are ignored. We will first derive the local density of states on an atom for the non-impurity case. The Hamiltonian has the matrix elements

\[ H_{ij} = \beta \quad (i \neq j; i \text{ and } j \text{ are neighbours}) \]

\[ = 0 \quad \text{otherwise.} \]

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Using the resolvent method (Haydock et al 1975, Van Santen and Toneman 1977, Van Santen 1972) one derives the help function \( g_0(z) \) when \( Z' = Z \):

\[
g_0(z) = \left\langle \varphi_0 \left| \frac{1}{z - H} \right| \varphi_0 \right\rangle = \frac{1}{z - Z' \beta^2 g_0(z)} \quad (Z' = Z)
\]

so that

\[
g_0(z) = \frac{z}{2Z\beta^2} \pm \frac{1}{2Z\beta^2} \sqrt{z^2 - 4Z\beta^2} \quad (-\text{sign if } z > 0)
\]

\[
+ \text{sign if } z < 0.
\]

(1)

\( Z' \) is the number of neighbours of atom 0; \( Z + 1 \) is the number of neighbours of the other atoms.

The solution for the ordered system when \( Z' = Z + 1 \) becomes

\[
g(z) = \left\langle \varphi_0 \left| \frac{1}{z - H} \right| \varphi_0 \right\rangle = \frac{1}{z - (Z + 1) \beta^2 g_0(z)}
\]

\[
= \frac{2Z(Z + 1)}{[(Z - 1)/(Z + 1)]z \pm \sqrt{z^2 - 4Z\beta^2}} \quad (Z' = Z + 1).
\]

(2)

If \( Z = 1 \) one gets the solutions of the linear chain.

The local density of states \( \rho(E) \) is defined as

\[
\rho(E) = -\frac{1}{\pi} \lim_{\epsilon \to 0} \text{Im} g(E + i\epsilon).
\]

(3)

Substitution of equation (2) into this equation gives

\[
\rho(E) = \frac{1}{2\pi} \frac{(Z + 1) [4Z\beta^2 - E^2]^{1/2}}{-E^2 + (Z + 1)^2 \beta^2} \quad (E^2 < 4Z\beta^2)
\]

\[= 0 \quad (E^2 > 4Z\beta^2).
\]

(4a)

(4b)

For \( Z = 1 \), expression (4a) reduces to the familiar expression for a linear chain which diverges at \( E = \pm 2\beta \).

For an impurity atom we introduce the matrix elements:

\[
H_{0i} = \beta' \quad \text{(i is a neighbour of 0)}
\]

\[
H_{00} = \delta.
\]

We will study the local density of states for arbitrary \( Z' \). The expression for the Green function becomes

\[
g'(z) = \left\langle \varphi_0 \left| \frac{1}{z - H'} \right| \varphi_0 \right\rangle
\]

\[
= \frac{1}{z - \delta - Z' \beta^2 g_0(z)}
\]

\[
= \frac{1}{z - \delta - (Z' \beta^2/2Z\beta^2) \{z \pm \sqrt{z^2 - 4Z\beta^2}\}}.
\]

(5)
The solution for the local density of states within the band becomes

$$\rho_0(E) = \frac{1}{\pi} \frac{[Z'\beta'^2(Z\beta^2 - Z'\beta'^2)](4Z\beta^2 - E^2)^{1/2}}{(E - \delta)^2 - \delta E'Z'\beta'^2/(Z\beta^2 - Z'\beta'^2) + Z'\beta'^4/(Z\beta^2 - Z'\beta'^2)}$$

$$E^2 \leq 4Z\beta^2.$$  

Solutions outside the band are found if:

**case (a)**

$$\frac{|2Z^{1/2}\beta|}{|2Z^{1/2}\beta| + |\delta|} > \frac{2Z\beta^2}{Z'\beta'^2}$$  \hspace{1cm} (two states)  

**case (b)**

$$\frac{|2Z^{1/2}\beta|}{|2Z^{1/2}\beta| - |\delta|} > \frac{2Z\beta^2}{Z'\beta'^2}$$  \hspace{1cm} (one state)  

and

$$\frac{|2Z^{1/2}\beta|}{|2Z^{1/2}\beta| + |\delta|} < \frac{2Z\beta^2}{Z'\beta'^2}.$$  

Interestingly, whereas the local density of states of the linear chain behaves very differently from that of the general case $Z > 1$, the conditions (7) and (8) are completely analogous for all values of $Z$.

It follows from calculation of the one-particle correlation function that expressions (7) and (8) are conditions for localisation. The one-particle correlation function is defined as

$$\rho_{ij} = -\frac{1}{\pi} \text{Im} \lim_{s \to +0} \left\langle \varphi_0 \left| \frac{1}{E - H' + i\epsilon} \right| \varphi_i \right\rangle$$

$$= \sum_{\alpha} c_0^\alpha c_j^\alpha \delta(E - E_\alpha).$$  

In equation (9) $c_0^\alpha$ and $c_j^\alpha$ are the coefficients of the atomic orbitals of the eigenfunctions of the network problem with eigenenergy $E_\alpha$. For a localised state at energy $E'$ equation (9) should decrease faster than $(1/Z)^{1/2}$ with increasing $j$.

In the Cayley tree there is only one route that connects 0 with $j$ (figure 2). Using Dyson's equations one derives:

$$g_{0j} = \left\langle \varphi_0 \left| \frac{1}{z - H'} \right| \varphi_j \right\rangle$$

$$= \left\langle \varphi_0 \left| \frac{1}{z - H'} \right| \varphi_1 \right\rangle \beta^{-1} g_0^{-1}(z)$$

$$= g'(z) \beta' \beta^{-1} g_0(z).$$

For values of $z^2 > 4Z\beta^2$ outside the band $\text{Im} \ g_0(z) = 0$, so:

$$\frac{\rho_{0j}^{(E')} + 1}{\rho_{0j}^{(E)}} = \beta g_0(E')$$

$$\left( E'^2 > 4Z\beta^2 \right)$$
Therefore
\[ \left| \frac{\rho_{0,j+1}}{\rho_{0,j}} \right| < \frac{1}{Z^{1/2}} \quad (Z \geq 1, |E'| > |2Z\beta|). \] (12)

Expression (12) shows that the states outside the band are exponentially localised.

It is of interest to study case (a) in the limit of strong localisation with \( Z' \beta'^2 / 2Z \beta^2 \gg 1 \) and \( E' = \pm \sqrt{Z' \beta'} \). Then
\[ \frac{\rho_{0,j+1}}{\rho_{0,j}} = \pm \frac{\beta}{\sqrt{Z' \beta'}}. \] (13)

So strong experimental decay with the exponential factor \( \ln(\sqrt{Z'/Z' \beta' \beta'}) \) is found. The factor \( Z^{1/2} \) is found when one calculates
\[ \rho_{0,j} = -\frac{1}{\pi} \text{Im} \lim_{\epsilon \to 0} \left( \varphi_0 \left| \frac{1}{E - H + i\epsilon} \right| \psi_j \right) \] (14a)
\[ = -\frac{1}{\pi} \text{Im} \lim_{\epsilon \to 0} g'(E + i\epsilon)\beta' Z^{j-1} \beta'^{-1} g'_{\lambda j}(E + i\epsilon) \] (14b)

with \( \psi_j \):
\[ \psi_j = \frac{1}{Z^{1/2}} \sum_{\alpha_l}^{z} \varphi_{\alpha_l}. \] (15)

Atoms \( \alpha_l \) are the neighbours in shell \( j \) of the atom in shell \( j - 1 \), that connects the atoms in shell \( j \) to atom 0.

For case (a) in the limit of strong localisation but now with \( |\delta/2Z^{1/2} \beta| \ll 1 \), the strong exponential factor with which the correlation function (14) decays becomes \( \ln |\beta'/\delta| \).
References

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