Yang-Lee singularity and the mobility edge

1983 J. Phys. A: Math. Gen. 16 L243

(http://iopscience.iop.org/0305-4470/16/7/009)

J. Phys. A: Math. Gen. **16** (1983) L243–L248. Printed in Great Britain

LETTER TO THE EDITOR

Yang–Lee singularity and the mobility edge

Aharon Kapitulnik† and Yonathan Shapir‡

† Department of Physics and Astronomy, Tel Aviv University, Ramat Aviv, Tel Aviv 69978, Israel

‡ Department of Physics and Materials Research Laboratory, University of Illinois at Urbana–Champaign, 110 West Green St, Urbana, IL 61801, USA, and Laboratoire de Physique de L'Ecole Normale Supérieure, 24 rue Lhomond, 75231 Paris Cedex 05, France

Received 20 January 1983

Abstract. We give an exact mapping of the problem of an electron in a one-dimensional random potential onto a Yang–Lee model with random imaginary fields and random bonds. The resistance and inverse localisation length are given respectively by the partition function and the free energy of the spin model. The allowed states and the singular point of their density at the band edge are mapped onto the zeros of the partition function and the Yang–Lee edge.

Similar relations are found on a Bethe lattice near the critical point for the pure models. Extending naively to the random case, these relations reproduce the field theory of Harris and Lubensky with the expansion below eight dimensions.

In the presence of randomness, however, the two models differ for any dimension greater than one due to the interactive character of the spin model. This causes its density of states to vanish at the edge in contrast to the $\beta = 0$ of the non-interacting electronic model.

Since the original paper of Anderson (1958), many theoretical efforts have been invested in trying to reach better understanding of the motion of a particle moving in a random potential (for a review see Thouless 1974). Among those attempts, many have tried to relate the critical behaviour near the mobility edge to that of other known models. It is now well established that above two dimensions, the critical behaviour is described by a nonlinear, non-compact σ-model of matrices of the order $2n$ in the limit $n \to 0$ (Wegner 1979). This was also confirmed by scaling results (Abrahams *et al* 1979). On the other hand, the upper critical dimensionality was suggested to be eight (Harris and Lubensky 1981). Their model is in the same universality class as the Yang–Lee (YL) model (Yang and Lee 1952) with random imaginary fields (Parisi and Sourlas 1981, Lubensky and McKane 1981). Thus, the expansion in $\varepsilon = 8 - d$ is the same as for the YL model near six dimensions (Fisher 1978). However, this theory predicts there $\beta \neq 0$ for the exponent of the density of states as well as a singularity in the one-particle Green function and therefore probably has no real physical meaning.

The one-dimensional problem stands by itself. All states are localised for any degree of disorder (Thouless 1974) and for all energies except at the band edge of the non-random model (Azbel 1980, Kantor and Kapitulnik 1981), in particular at $E = 0$, if the randomness is purely off-diagonal. Recently, the dependence of the localisation length on the impurities concentration for different Fermi levels has been widely investigated (for recent reviews, see e.g. Erdos and Herndon 1982).

In the present letter we relate directly the one-dimensional (1D) electronic model to the 1D Ising model in an imaginary magnetic field, namely the 1D YL model, both in the random and non-random cases. We first show a simple correspondence between these two models in the non-random case. As a result, it will be shown that both models have the same spectrum of singularities, namely, allowed states and zeros of the partition function, respectively. The band edge of the extended states is the image of the YL edge in the spin model. This mapping follows from a direct correspondence between the transfer matrices of both models.

We start with the 1D Schrödinger equation for an electron having an energy $E = h^2k^2/2m$

$$-\frac{h^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}X^2}+\sum_{n=1}^{N} V_n(X-X_n)\psi=\frac{h^2k^2}{2m}\psi. \tag{1}$$

After being scattered from the potential at the site l (X_l), its wavefunction is

$$\psi_K(l)=\tau_l\,\mathrm{e}^{\mathrm{i}kX}+\rho_l\,\mathrm{e}^{-\mathrm{i}kX}. \tag{2}$$

The transfer matrix relating (τ_{l+1}, ρ_{l+1}) to (τ_l, ρ_l) is a general matrix of the form

$$T_{El}=\begin{pmatrix} A & B^* \\ B & A^* \end{pmatrix} \tag{2a}$$

where A and B are properties of the potential only and $|A|^2-|B|^2=1$ (an asterisk denotes complex conjugation). This matrix can be parametrised and rotated into

$$\tilde{T}=\begin{pmatrix} |A|\,\mathrm{e}^{\mathrm{i}\gamma} & (1-|A|^2)^{1/2} \\ (1-|A|^2)^{1/2} & |A|\,\mathrm{e}^{-\mathrm{i}\gamma} \end{pmatrix}. \tag{3}$$

The YL reduced Hamiltonian is

$$-\beta H = K\sum_{(i\ i+1)} S_iS_{i+1}+\mathrm{i}h\sum_i (S_i+S_{i+1}). \tag{4}$$

It has a similar transfer matrix

$$T_{\mathrm{YL}}=(2\sinh^2 K)^{1/2}\tilde{T}. \tag{5}$$

Then if we identify

$$A=[2\sinh(2K)]^{-1/2}\,\mathrm{e}^{K} \qquad \text{and} \qquad \gamma = 2h$$

γ is given simply by $ka+\delta$ where δ is the phase shift of the potential and a is the lattice constant.

All the properties of the special states as a function of k are therefore similar. The same singular behaviour in the spectrum occurs for both models at the band edge defined by the relation (see e.g. Hori 1968)

$$\mathrm{Tr}\,\tilde{T}=0. \tag{6}$$

In the random case, we cannot perform an overall rotation to the canonical form of $\tilde{T}$, since the matrices do not commute in general. However, the mapping between the models and their critical behaviour is completely independent of the particular representation. In order to demonstrate the local correspondence in the random case, we choose a slightly different approach introduced by Azbel (1980) and Abrahams and Stephen (1980).

Based on (1) they defined the quantities

$$r_l^+ = (1/\tau_l)\exp[-ik(X_{l+1}-X_l)], \qquad r_l^- = (\rho_l/\tau_l)\exp[-ik(X_{l+1}+X_l)]. \tag{7a, b}$$

The same quantities, but for a sequence of L scatterers such as R_L^+ and R_L^-, follow the recursion relation

$$\begin{pmatrix} R_l^+ \\ R_l^- \end{pmatrix} \begin{pmatrix} r_l^+ & r_l^{-*} \\ r_l^- & r_l^{+*} \end{pmatrix} \begin{pmatrix} R_{l-1}^{+*} \\ R_{l-1}^{-*} \end{pmatrix}. \tag{8}$$

Using the Landauer (1970) formula, the resistance R of the chain is given by

$$R = |R_L^-|^2. \tag{9}$$

It is now a straightforward calculation to show that (see also Azbel 1980)

$$R_L^{S_N} = C \sum_{\substack{\{S_l\} \\ l=1,L-1}} \exp\Big(\sum_{l=1}^{L} K_l S_l S_{l-1} - i\tfrac{1}{2} \sum_{l=1}^{L} h_l (S_l + S_{l-1}) \Big) \tag{10}$$

where S_l are spin variables that can take the values ± 1, $K_l = \frac{1}{4}\ln[(1+A_l^2)/A_l^2]$ and $h_l = (ka_l + \delta_l)$. Here A_l and δ_l are the scatterer's amplitude and phase shift, respectively, as discussed before, $a_l = X_{l+1} - X_l$ and C is the normalisation constant, which depends only on the boundary conditions and the overall combination of amplitudes.

Formula (10) shows that we can describe the scattering properties of an electron in a 1D random potential by an Ising YL partition function. As the relation between them is local, it is applicable to any 1D potential with random distances and random scatterers (characterised by their amplitudes and phase shifts). In particular, we see that random distances induce random imaginary fields, while random scatterers result in both random fields and random bonds.

As mentioned by Azbel (1980) this relation yields (except for a set of measure zero) a resistance growing exponentially with the length. The well known result (Abrahams *et al* 1979, Abrahams and Stephen 1980) that the typical resistance may be very different from its average follows naturally from the fact that all the moments of the partition function grow exponentially. Meaningful statistics may be extracted only for an additive function, e.g. the free energy. In the electronic case its absolute value is proportional to the inverse localisation length.

Once the partition sum grows more slowly than exponentially, we have a diverging localisation length and therefore a critical point. Two cases where this occurs are worth mentioning: the zero-field and the pure limit. When only random bonds are present (with no random or homogeneous field), the matrices commute and the problem is solvable. For the electron problem, it will correspond to correlated random distances and phase shifts such that $h_l = 0$. Alternatively, this may be realised in a Kronig–Penny (1931) model where equally spaced δ-functions with different random strengths form the potential (Kantor and Kapitulnik 1981). At the band edge ($ka = 0$, π, etc) the resistance does not grow exponentially with the length but rather with its square (Kantor and Kapitulnik 1981, Azbel and Soven 1982). The second-quantised formulation of this case yields the well studied pure off-diagonal randomness with $E = 0$ (see e.g. Shapir *et al* 1982 and references therein). Note that in many random cases the gap is filled with the tail of localised states (Thouless 1974). Similar effects in the spin model are the origin (at higher dimensions) of the Griffiths singularities (Griffiths 1969, Bray and Moore 1982, Schwarz *et al* 1982).

The non-random case is recovered after setting $h_l = h$ and $K_l = K$, i.e. the same values for all the scatterers. We then get the known density of states (density of zeros in the Yang and Lee (1952) model)

$$g(h) = (2\pi)^{-1}(\sin h)/(\sin^2 h - e^{-4k})^{1/2}$$

as well as all the other results which followed from the direct correspondence (e.g. by rotating all the matrices uniformly) described above.

It is very tempting to extend the relations to higher dimensions. The natural way is to relate the Green functions to the spin–spin correlations. Indeed, in 1D the complex local magnetisation is related to the difference in the amplitudes of the electron described by the incoming and outgoing channels. It is also given by the derivative of the free energy with respect to the uniform field (energy). In particular, the magnetisation diverges at the allowed states (namely in the band) and its singular part is proportional to the density of states. However, already in 2D, one immediately sees that the 'equations of motions' which relate correlation functions of the spin model at different points are highly nonlinear and non-local in the presence of a magnetic field, in contrast to the inhomogeneous Schrödinger equation. This explains why although the pure electronic model is soluble in any dimension (with $(E - E_c)^{(d-2)/2}$ type singularity at the band edge), the pure YL model is an interacting system with non-classical exponents below six dimensions (Fisher 1978) and so far has no exact solution (except for 1D). It is interesting to note that some critical properties of the *random* YL model in $D-2$ and $D-3$ are probably known by their correspondence to the $D-2$ pure model (Parisi and Sourlas 1981). This is an exceptional example where the random model is more tractable than its pure counterpart. However, these results only confirm that the YL random behaviour is unrelated to the mobility edge singularity (i.e. they have $\beta \neq 0$) at these dimensions.

The complexity already arises on strips which are infinite in one direction but with finite width L (Fisher 1980). The YL transfer matrix has $2^L \times 2^L$ elements while the electronic one is only of order $2L \times 2L$. On these strips the electronic model must therefore be described by a 1D chain of generalised spins with $N = 2L$ components. The resulting model will be discussed elsewhere (Shapir and Kapitulnik, to be published).

The YL and electronic models become related again at higher dimensions. The limit $D \to \infty$ may be achieved on a Bethe lattice (see e.g. Müller-Hartmann and Zittartz 1974). The pure YL problem on a tree has been solved (Bessis *et al* 1976) as well as the pure electronic model on that lattice (Thorpe and Wearie 1971, Dancz and Edwards 1973). With the same mapping as for 1D, the two models have the same type of singularity, $(h - h_c)^{1/2}$, for the density of states near the same edge which is related to the coordination number of the tree. The YL model becomes linear and local near its critical point due to the 1D character (no loops) of this lattice. This is easily shown by considering another equivalent model, namely the monomer–dimer model (Shapir 1982). It is straightforward to show that the monomer–monomer correlation in this model obeys, on the tree, the same recursion relations as the electronic Green function (Thorpe and Wearie 1971), though this relation *cannot* be pursued when random fugacities are assigned to the monomer. We thus confirm that the two models share the same singular behaviour in the pure case, for high enough dimensions.

Including fluctuations, it has been shown (Fisher 1978) that the YL model has $D_c = 6$ with expansion in $\varepsilon = 6 - D$. The effect of random imaginary fields is to shift the critical dimensionality (Imry and Ma 1975) to $D_c = 8$ with the same $\varepsilon = 8 - D$

expansion (Parisi and Sourlas 1981). The effect of random bonds is completely similar since along the critical line $H_c = H_c(K)$, random couplings would result in local random fields. This is consistent with the relation between the crossover exponents for both cases: $\alpha = \gamma$ for this model.

So far these relations seem to explain in a natural way why the field-theoretical results of Harris and Lubensky (1981) coincide with the random YL exponents near 8D (Lubensky and McKane 1981). However, their field theory predicts a vanishing density of states at the mobility edge due to the singularity in the 'diagonal' sector of their order parameter, i.e. $\langle Q^{++}(E)\rangle = (G^{+}(E+\mathrm{i}0))^2$. It has been suggested that higher correlation functions may become singular deeper in the gap due to attraction of the effective potential (M Stone, private communication, see also Parisi 1982). Wegner (1981) has advanced other arguments as to why the cut has to extend into the gap with no singularity in the density of states. In 5D this has been confirmed from numerical simulations (Kirkpatrick 1981). Finally, very recently, Kunz and Souillard (1982) have proved that for a wide class of potentials the density of states is analytic on the Bethe lattice although a mobility edge exists.

We thus observe that due to its interactive character, the random YL model differs from the localisation problem in all dimensions greater than one (including the Bethe lattice on which they may be related only in the pure limit). This is also in accordance with recent results concerning many-electron systems, in which interactions, as well as randomness, are taken into account. New singularities then occur in the one-particle Green function and the density of states does vanish at the mobility edge, (see e.g. Fradkin 1982 and references therein).

In conclusion, we have shown a one-to-one mapping of the electron in a random potential problem onto the random YL model in one dimension. The same relation holds between the two models near the critical point on a Bethe lattice without randomness. The YL model, being a nonlinear (interacting) system, is more complicated than the electronic one for all dimensions greater than one. The question of whether it can be formulated as a relatively simple many-body interacting model is currently under investigation.

We would like to thank A Aharony for valuable comments and critical reading of the manuscript. Discussions with M Ya Azbel, D J Bergman, M Schwarz and E Fradkin are also acknowledged. This work was supported by the US–Israel BSF (Jerusalem) at Tel Aviv University and by the NSF under Grant 80-20250 at the University of Illinois. YS is grateful for the warm and kind hospitality of G Toulouse, J Vannimenus and all the members of the Groupe de Physique des Solides at Ecole Normale Supérieure, where part of this work was done (during a visit made possible by a Joliot–Curie Fellowship). AK is grateful for the support of a grant from the KFK, Karlsruhe, Germany.

References

Abrahams E, Anderson P W, Licciardello D C and Ramakrishnan T V 1979 *Phys. Rev. Lett.* **42** 673
Abrahams E and Stephen M J 1980 *J. Phys. C: Solid State Phys.* **13** L377
Aharony A, Imry Y and Ma S-K 1976 *Phys. Rev. Lett.* **37** 1364
Anderson P W 1958 *Phys. Rev.* **109** 1492
Azbel M Ya 1980 *Phys. Rev.* B **22** 4045
Azbel M Ya and Soven P 1982 *Phys. Rev. Lett.* **49** 751

Bessis J D, Drouffe J M and Moussa P 1976 *J. Phys. A: Math. Gen.* **9** 2105
Bray A J and Moore M A 1982 *J. Phys. C: Solid State Phys.* **15** L765
Dancz J and Edwards S F 1973 *J. Phys. C: Solid State Phys.* **6** 3413
Erdos P and Herndon R C 1982 *Adv. Phys.* **31** 65
Fisher M E 1978 *Phys. Rev. Lett.* **40** 1610
—— 1980 *Prog. Theor. Phys. Suppl.* **69** 19
Fradkin E 1982 *Proc. Ecole d'Eté de Physique Théorique, Les Houches 1982* (Amsterdam: North-Holland) to be published
Griffiths R B 1969 *Phys. Rev. Lett.* **23** 17
Harris A B and Lubensky T C 1981 *Phys. Rev.* B **23** 2640
Hori J 1968 *Spectral Properties of Disordered Chains and Lattices* (Oxford: Pergamon)
Imry Y and Ma S-K 1975 *Phys. Rev. Lett.* **35** 1399
Kantor Y and Kapitulnik A 1981 *Solid State Comm.* **42** 161
Kirkpatrick S 1981 in *Proc. Conf. Disordered Systems and Localization, Rome 1981* ed C Castellani, C Di Castro and C Pelik (Berlin: Springer) p 280
Kronig R de L and Penny W G 1931 *Proc. R. Soc.* A **130** 499
Kunz H and Souillard B 1982 *The Localization transition on the Bethe Lattice, preprint*
Landauer R 1970 *Phil. Mag.* **21** 863
Lubensky F C and McKane A F 1981 *J. Physique Lett.* **42** L331
Müller-Hartmann E and Zittartz J 1974 *Phys. Rev. Lett.* **15** 893
Parisi G 1982 *Proc. Ecole d'Eté de Physique Théorique, Les Houches 1982* (Amsterdam: North-Holland) to be published
Parisi G and Sourlas N 1981 *Phys. Rev. Lett.* **46** 871
Schwarz M, Shapir Y and Aharony A 1982 *Tel Aviv University preprint*
Shapir Y 1982 *J. Phys. A: Math. Gen.* **15** L433
Shapir Y, Aharony A and Harris A B 1982 *Phys. Rev. Lett.* **49** 486
Thorpe M F and Wearie D 1971 *Phys. Rev.* B **10** 3518
Thouless D J 1974 *Phys. Rep.* C **13** 24
Wegner F 1979 *Z. Phys.* B **35** 207
—— 1981 in *Proc. Conf. Disordered Systems and Localization, Rome 1981* ed C Castellani, C Di Castro and L Peliti (Berlin: Springer) p 191
Yang N C and Lee T D 1952 *Phys. Rev.* **87** 404, 410