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Localization in Quasi-1D Systems: Perturbation Theory and Scaling.

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Abstract. – A perturbative study of the localization length in the Anderson model on strips is presented. It is shown that in the neighbourhood of those energies corresponding to the opening of a new channel, a certain rearrangement of the perturbation expansion significantly improves the accuracy of the prediction. Moreover, the localization length scales in a way which is reminiscent of the strictly 1D behaviour, but is nevertheless different.

The simplest model describing the behaviour of an electron on a disordered lattice is the one due to Anderson:

$$H_{\mathrm{A}} = \sum_{\langle ij \rangle} |i\rangle\langle j| + \mu \sum_i V_i |i\rangle\langle i| , \tag{1}$$

where $\langle ij \rangle$ denotes summation over nearest-neighbouring sites only and V_i, the site energies, are uncorrelated random numbers sharing the same distribution of variance $\overline{V^2}$. The eigenstates of this model were rigorously shown to be exponentially localized in 1D and quasi-1D systems (1) [1,2]. Moreover, the finite-size scaling theory of localization [3] predicts that all states are localized in 2D and that a metal-insulator transition takes place in 3D for large enough disorder, μ. On the other hand, it appears that a complete picture on the variation of the localization length with energy is hard to obtain. Aside from the numerical approach, there are very few other methods available [4]. One of them is the perturbation theory (PT) developed in ref. [5] and [6]. Unfortunately, this method only works as long as no more than one channel is open and therefore for strips of width $M \gg 1$ it fails for almost the entire energy band, $|E| \leqslant 2 + 2\cos(\pi/(M+1))$ (2). The purpose of this letter is to show that

(1) While a 1D lattice is an infinitely long row of evenly spaced atoms, a quasi-1D lattice has several such rows. A quasi-1D system which is embedded in 2D is referred to as a strip.

(2) See however the results obtained at $M = 2$ in a tight-binding–like model with random fluxes by Avishai *et al.* [7].

despite the failure of PT, it nevertheless provides a good qualitative description of the localization length, ξ, in the vicinity of the opening of a new channel. This agreement suggests that an appropriate modification of the formalism could give quantitative predictions for ξ.

We start with a brief summary of the results in ref. [6]. The PT is constructed in terms of $2M \times 2M$ transfer matrices, M_α, associated with the α-th column of the strip, $\alpha = 1, \ldots, N$ and $N \to \infty$. The localization length is related to the Lyapunov exponents, γ_i, of the infinite product

$$P = \prod_{\alpha=1}^{N} M_\alpha \,. \tag{2}$$

In fact, if $\mathrm{Re}\,\gamma_i \geqslant \mathrm{Re}\,\gamma_{i+1}$, then ξ is the inverse of the real part of the smallest positive Lyapunov exponent. On the other hand, $\sum_{i=1}^{p} \gamma_i$ is given by the rate of growth of the p-dimensional volume enclosed by p different $2M$-vectors, $\boldsymbol{W}_{i,N}$, such that $\boldsymbol{W}_{i,N} = P\boldsymbol{W}_{i,0}$. In the limit of weak disorder, one assumes that

$$M_\alpha = A + \mu B_\alpha \,, \tag{3}$$

where A is the transfer matrix of the periodic lattice and B_α is a random matrix with elements that have vanishing average, $\overline{B_{ij}} = 0$. Then

$$\sum_{i=1}^{p} \gamma_i = \sum_{i=1}^{p} \log \lambda_i - \frac{\mu^2}{2} \sum_{i=1}^{p} \sum_{j=1}^{p} \frac{\overline{B_{ij} B_{ji}}}{\lambda_i \lambda_j} + O(\mu^3), \tag{4}$$

where λ_i are the eigenvalues of the unperturbed transfer matrix, A, ordered such that

$$|\lambda_1| \geqslant |\lambda_2| \geqslant \ldots \geqslant |\lambda_k| \geqslant \ldots \geqslant |\lambda_{2M}| \,, \tag{5}$$

and B_{ij} are the matrix elements of B in the diagonal representation of A. If in eq. (5) the $\geqslant$ signs are replaced by $>$, we refer to it as the *non-degeneracy condition*. The $O(\mu^4)$ terms in eq. (4) (not shown) include certain double sums which run *along* the strip (see eq. (23) in ref. [6]) and converge only if the non-degeneracy condition is satisfied.

Equation (4) holds for any product of random matrices of the form given in eq. (3). On the other hand, in the particular case corresponding to the Anderson model, eq. (1), the two matrices, A and B, take on a block form with blocks of size $M \times M$:

$$A = \begin{pmatrix} E\boldsymbol{I} - \boldsymbol{T}_H & -\boldsymbol{I} \\ \boldsymbol{I} & \boldsymbol{0} \end{pmatrix}, \qquad B_\alpha = \begin{pmatrix} \boldsymbol{V}_\alpha & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} \end{pmatrix}, \tag{6}$$

where $\boldsymbol{I}$ and $\boldsymbol{0}$ are the corresponding identity and null matrix, respectively, $(\boldsymbol{T}_H)_{ij} = \delta_{i,j+1} + \delta_{i,j-1}$ and $(\boldsymbol{V}_\alpha)_{ij} = -V_{i,\alpha}\delta_{i,j}$. Notice that the indices of the Anderson model have been now redefined: while each index of eq. (1) was running over all the sites, here the first index of $V_{i,\alpha}$ runs across the strip, $1 \leqslant i \leqslant M$, while the second one counts the sites along the strip, $1 \leqslant \alpha \leqslant N$. Moreover, we have assumed rigid boundary conditions on the edges of the strip.

The zeroth-order approximation to the Lyapunov exponents is given by the eigenvalues of the matrix A. These satisfy the relation

$$\lambda_k + \lambda_k^{-1} = E - 2\cos q_k \,, \tag{7}$$

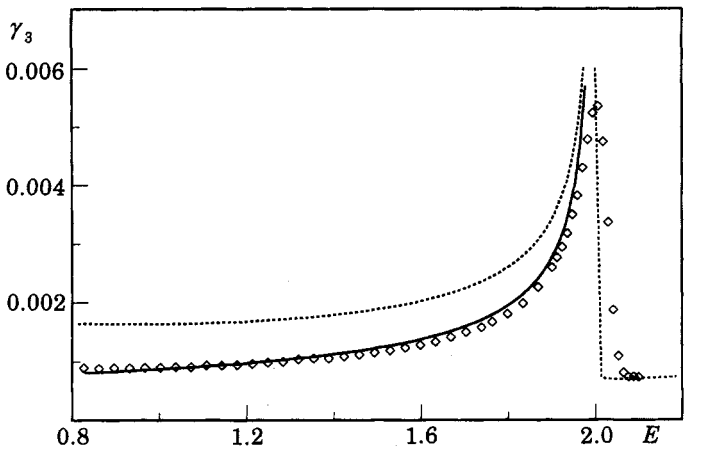

Fig. 1. – The inverse localization length; comparison of numerical results (◇), perturbation theory (dashed line) and scaling (continuous line) at $M = 3$ and $l = 2$. The $V_{i,\alpha}$ are chosen from a distribution which is uniform between -1 and 1. Moreover, $\mu = 0.2$ and we used $N = 2 \cdot 10^7$ in the numerics. The scaling regime ends at $E \simeq 1.4$.

where

$$q_k = \frac{\pi j}{M+1}, \qquad 1 \leqslant j \leqslant M, \tag{8}$$

and the j's are ordered such that condition (5) is satisfied. In order to obtain the higher-order terms of the perturbation expansion, one has to substitute eq. (6) into eq. (4). Then

$$\sum_{i=1}^{p} \gamma_i = \sum_{i=1}^{p} \log \lambda_i - \frac{2\mu^2 \overline{V^2}}{(M+1)^2} \sum_{i=1}^{p} \sum_{j=1}^{p} \frac{\sum_{k=1}^{M} [\sin(kq_j) \sin(kq_i)]^2}{(\lambda_i - \lambda_i^{-1})(\lambda_j - \lambda_j^{-1})} + O(\mu^3). \tag{9}$$

Clearly, inside the band, $|E| \leqslant 2 + 2\cos(\pi/(M+1))$, the non-degeneracy condition is not satisfied and this leads to the failure of PT. The degeneracy in absolute value of the unperturbed eigenvalues, λ_i, can be lifted by adding a small imaginary part to the energy, $E \to E + i\varepsilon$. While for large enough ε the PT is recovered, its prediction now refers to the $\gamma_M \equiv \xi^{-1}$ of an Anderson model with complex energy rather than that of the actual, physically relevant, model. On the other hand, if the minimal ε required for agreement, ε_c, is not too large, one could hope that $\gamma_M(\varepsilon_c)$ is a good estimate of $\gamma_M(0)$. Such hope, which was also expressed in ref. [6], is unfortunately not supported by numerical results. Although throughout most of the band, to lowest order in μ, $\gamma_M = K_M \mu^2$, we find large disagreement in the value of K_M between the prediction of PT and numerics (see fig. 1) (3). Moreover, there are energies in the band, $E_l = 2 + 2\cos(l\pi/(M+1))$, $l = 1, \ldots, M$, where the PT prediction for K_M is diverging. These correspond to the opening of a new channel, $\lambda_{M-l+1} = 1$ for $E > 0$. In what follows, we refer to the terms entering K_M that diverge at E_l as *resonant*. It is natural to expect that, in the neighbourhood of E_l, PT fails in an even more extreme way.

(3) We use K_M to denote the M-dependent coefficient of μ^2 in the Taylor expansion of γ_M around $\mu = 0$. Notice that, when $M \to \infty$, $K_M(E) \to K(E)$.

Indeed, due to the largeness of the resonant terms, the perturbation expansion needs to be rearranged such as to give these terms a certain priority over the non-resonant ones [5]. In other words, one is trying to balance the largeness of the resonant terms with the smallness of disorder. The expected rearrangement of PT is of the form

$$\gamma_M = \mu^{\alpha_1} f_{\alpha_1}(x_1) + \mu^{\alpha_2} f_{\alpha_2}(x_2) + \dots , \tag{10}$$

where $\alpha_1 < \alpha_2 < \dots < \alpha_i < \dots$, $x_i = t\mu^{\beta_i}$ and $t \equiv E - E_l \ll 1$. This approach was used in ref. [5] for $M = 1$ in the neighbourhood of the band edge, $E = 2$. It was shown there that $\alpha_1 = 2/3$, $x_1 = t\mu^{-4/3}$ and, asymptotically,

$$f_{\alpha_1}(x) \simeq \sqrt{x} - \frac{\overline{V^2}}{8x} - \frac{5}{128}\frac{\overline{V^2}^2}{x^{5/2}} + \dots . \tag{11}$$

We refer to $f_{\alpha_1}(x)$ as the *scaling function*. It turns out that one can further relax the non-degeneracy condition such that, for a single open channel, PT converges as well. Accordingly, for the $M = 1$ case PT is convergent for all E and in this sense it is quite special. This enabled Derrida and Gardner [5] to include in eq. (11) the resonant $O(\mu^4)$ terms of PT. Notice, however, that for $x < 0$ the first and third terms in eq. (11) are purely imaginary and therefore do not contribute to ξ.

Let us now apply the scaling approach to the $M > 1$ case. Here, when $|E| < E_2$, the $O(\mu^4)$ terms are ill-behaved for real energies, $\varepsilon = 0$. It is however natural to expect that the $O(\mu^4)$ terms do not affect the $O(\mu^2)$ behaviour. Therefore, in the following derivation and the corresponding numerical computation, we set $\varepsilon = 0$ and only consider the PT up to $O(\mu^2)$. Moreover, since the energies under consideration are in the vicinity of E_l, the non-resonant terms of eq. (9) can be neglected. In order to bring the remaining terms to the form of eq. (10), one needs to find the scaling variable, x_1, for which α_1 is minimal. In practice, we assume that eq. (9) includes at least two terms of the asymptotic expansion of f_{α_1} and, accordingly, compare all pairs of terms. Given the power of t in a term, ν, and that of μ, τ ($\tau = 0$ or 2), one has to find α and η, such that: 1) $\alpha + \eta = \tau$, 2) the value of α is the same for both terms, 3) the ratio between the η's of the two terms is the same as that between the ν's. The pair of terms with the smallest value for α determines α_1, $\alpha_1 = \alpha$. Finally, $\beta_1 = \tau - \alpha_1$.

Using the prescription described in the previous paragraph, we find that, in the neighbourhood of the band edge, $E = E_1$, α_1 and β_1 are the same as for $M = 1$ and

$$f_{\alpha_1}(x) \simeq \sqrt{x} - \frac{3\overline{V^2}}{16(M+1)x} + \dots . \tag{12}$$

Asymptotically, the agreement between this scaling function and the corresponding numerical results is better than the precision of the latter. On the other hand, for E_l with $l > 1$, $\alpha_1 = 4/3$, while the form of the scaling variable, x_1, is once again unchanged. The real part of the corresponding scaling function is for, $x_1 < 0$,

$$\mathrm{Re} f_{\alpha_1}(x) \simeq$$

$$\simeq \frac{\overline{V^2}}{8(M+1)\sqrt{\sin\frac{\pi(l+1)}{2(M+1)}\sin\frac{\pi(l-1)}{2(M+1)}\left(1 - \sin\frac{\pi(l+1)}{2(M+1)}\sin\frac{\pi(l-1)}{2(M+1)}\right)}\sqrt{-x}} + \dots . \tag{13}$$

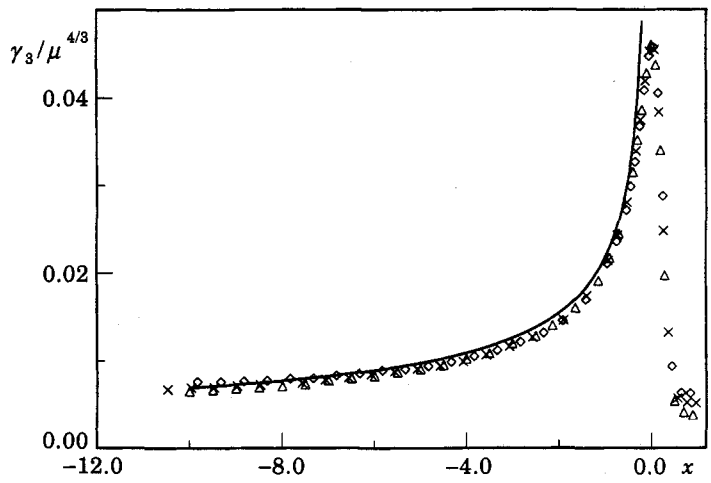

Fig. 2. – Scaling of γ_M. Parameters are the same as in fig. 1, except for μ which is 0.1 (△), 0.15 (×) and 0.2 (◇). The continuous line represents the scaling curve given by eq. (13). The scaling regime ends at $x \simeq -5$ for $\mu = 0.2$ and at $x \simeq -8$ for $\mu = 0.15$. On the $x > 0$ side, scaling holds only up to $x \simeq 0.4$.

For $x_1 > 0$, however, all the resonant terms in eq. (9) are imaginary. We find that eq. (13) represents a significantly better approximation to ξ than PT alone (see fig. 1). Moreover, the numerical results of fig. 2 support the scaling indicated by eq. (13). Nevertheless, a certain difference between the scaling prediction and numerics persists arbitrarily far into the asymptotic regime and is a remaining consequence of the failure of PT. In the case of fig. 2 for example, for $\mu = 0.1$ and $x \in (-10, -5)$, this difference, Δ, satisfies $\log \Delta = a \log(-x) + b$ with $a = -0.5 \pm 0.2$ and $b = -6.5 \pm 0.4$. This indicates that the discrepancy is due to a small error in the coefficient of $(-x)^{-1/2}$ in eq. (13). Qualitatively, the behaviour at other M's and l's such that $l > 1$ was found to be similar. Although the agreement between theory and numerics becomes gradually worse as either M or l increase, it is always much better than the prediction of PT.

Clearly, the range of validity of eq. (13) is limited (see fig. 2). At small enough $|x|$, it fails since it is a first term in an *asymptotic expansion*. On the other hand, at $|x| > |x_c(\mu)|$, the scaling argument fails simply because t is no longer small. In the large-$|x|$ extreme, the range of validity is extended by the fact that eq. (13) is at the same time of the PT form, $\gamma_M = \mu^2 g(E) + \ldots$. In order to properly illustrate the breakdown of scaling at large $|x|$, one needs to enlarge the $x \in (-9, -4)$ range in fig. 2. Although this is not shown here, notice that, while the $\mu = 0.1$ symbols stay roughly parallel to the theoretical line for $x < -3$, the $\mu = 0.2$ symbols at $x \simeq -5$ begin to slightly deviate upwards from the numerical scaling curve. This can be interpreted as the saturation which is expected when approaching E_3, which for $\mu = 0.2$ is at $x = -12.09$. Since for $\mu = 0.15$ E_3 corresponds to $x = -17.74$, it is only at large values of x, $x \simeq -8$, that the corresponding saturation occurs. Finally, for $\mu = 0.1$, $x(E_3) = -30.47$ and the saturation occurs outside the range of x depicted in fig. 2. We find that $x_c(\mu) \propto \mu^{-4/3}$ and, therefore, scaling breaks at fixed t, t_c. Furthermore, our numerics seems to indicate that t_c grows with M. Since, on the other hand, $\Delta E_l \equiv E_{l+1} - E_l$ decreases with M, we conjecture that, for wide enough strips, scaling holds throughout the band.

One can further use the approach described above to study the behaviour of the higher

Lyapunov exponents as well. We find that in the vicinity of E_l all γ_j with $M - l + 1 \leqslant j \leqslant M$ scale with the same scaling variable. While for $M - l + 1 < j \leqslant M$, $\alpha_1 = 4/3$, when $j = M - l + 1$, $\alpha_1 = 2/3$. Appropriate scaling functions have also been obtained. The rest of the positive Lyapunov exponents are non-vanishing in the $\mu \to 0$ limit and, accordingly, do not scale.

In summary, we found that, to lowest order in μ, the inverse localization length, γ_M, behaves as $\gamma_M \propto \mu^{\alpha}$, where as one lowers the energy from $E > E_1$ towards the centre of the band, $\alpha = 0, 2/3, 2, 4/3, 2, 4/3, \ldots$. This represents a generalization of the $M = 1$ behaviour where the above-mentioned sequence stops after the first three terms, $\alpha = 0, 2/3, 2$. It should be stressed that the behaviour of γ_M for $\varepsilon > 0$ is quite different. In particular, for $\varepsilon > \varepsilon_c(E)$, we have found agreement between PT and the numerical calculation which was done at this particular value of ε. A major task, which will make the PT significantly more useful, remains to obtain an upper bound on ε_c. This, in turn, will allow to estimate the size of the error bar on the prediction of PT. In an earlier work along similar lines, Dorokhov [8] has reached, to lowest order in μ and M^{-1}, a semi-empirical formula, $\xi = Ml/2$. Here, however, l, that can be loosely interpreted as a mean free path, has its own M, and E, dependence including the large decrease in ξ at E_l. Moreover, in ref. [8] the difficulties arising from the $O(\mu^4)$ terms were ignored.

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