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The wavefunction envelope in one-dimensional random potentials

A MOOKERJEE and A M JAYANNAVAR*

S N Bose National Centre for Basic Sciences, DB-17, Sector I, Salt Lake City, Calcutta 700064, India

*International Centre for Theoretical Physics, Trieste, Italy

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Abstract. We propose a formalism for the study of mean resistance of a one dimensional chain of random potentials. We obtain the resistance as a function of the length of the chain. In the asymptotic limit, this is related to the wavefunction envelope. The formalism demands loss of translational symmetry, but is general enough to include potentials with spatial correlations which are not long ranged and also those whose randomness is inhomogeneous.

Keywords. One-dimensional random potentials; inhomogeneous disorder; wavefunction envelopes.

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The spectrum of random Hamiltonians has been a subject of intense study for the last two decades, following the pioneering work of Anderson (1958). Related to the above problem is the behaviour of the wavefunction for a given energy. One of the most interesting results in this connection is the fact that in one dimensional potentials even infinitesimal randomness in the potential leads to a pure point spectrum for almost all realisations of the potential, with exponentially decaying wavefunction envelopes (Kunz and Souillard 1980; Royer 1982; Delyon *et al* 1983). Delyon *et al* presented a formalism that allows generalization to random potentials which do not possess statistical homogeneity, or which have short ranged correlations in space. This is the subject matter of our study.

Several situations on non-homogeneous random potentials have been studied in the literature. A typical such potentials is $V(x) = f|x|^{-a}v(x)$, where $v(x)$ is a homogeneously random potential. The problem is closely related to the physically interesting problem of an independently random Kronig-Penny model in the presence of a uniform electric field, such that we have $V(x) = \Sigma v_n\, \delta(x-n) - Fx$ (Delyon *et al* 1983). For the former, Delyon *et al* have given a proof that almost surely

(i) if $0 < a < 1/2$, the entire spectrum is pure point with eigenfunction envelopes decaying as stretched exponentials of the form $\exp(-|x|^{-a})$. (ii) If $a = 1/2$, the spectrum is pure point with power law decaying states if $x > x_1$ and singularly continuous if $x < x_2$ in $|E| < 2$. (iii) If $a > 1/2$, the spectrum is absolutely continuous (Kotani 1986; Souillard 1986) with extended eigenstates.

In Kronig-Penny model Souillard finds that (i) $0 < F < F_1$ almost surely we have a point spectrum with power law decaying eigenstates. (ii) $F > F_2$ almost surely we have an absolutely continuous spectrum with extended states.

Vijaygovindan *et al* (1986) have studied the mean resistance of the same model.

They observe a smooth crossover from the power law to exponentially decaying states. The former is relevant at large fields and large lengths.

We shall develop a formalism to study the mean resistance of a one-dimensional potential. It would include non-homogeneously random potentials as well as those with spatially correlated potentials which are nevertheless without translational symmetry. A classic example of this is the Fibonacci chain (Mookerjee and Singh 1986). Our approach will be based on the invariant embedding principle (Chandrasekhar 1960; Bellman and Wing 1975). In particular, we shall use the variant used by Heinrichs (1986) involving the potential, rather than Kumar's (1985) version involving the potential derivatives.

The model Hamiltonian is given by

$$H = (-\hbar^2/2m)\,\mathrm{d}^2/\mathrm{d}x^2 + V(x)$$
$$V(x) = f(x)v(x) \tag{1}$$

where $f(x)$ is a non-random function which describes the non-homogeneity of the potential distribution (it is a constant for homogeneously random potentials). $v(x)$ is a Gaussian random function with

$$\langle v(x)\rangle = 0; \quad \langle v(x)v(x')\rangle = g(x-x'). \tag{2}$$

The disordered potential stretches from $x=0$ to $x=L$. A plane wave is incident at one end, partially reflected and partially transmitted. In our approach we address ourselves only to emergent quantities like the transmission and reflection coefficients. The complex amplitude reflection coefficient $R(x)$ obeys the Stochastic-Riccati equation

$$ik\frac{\mathrm{d}R(x)}{\mathrm{d}x} = V(x)[R(x)^2+1] - 2[k^2 - V(x)]R(x), \tag{3}$$

where k is the wavenumber of the incident wave related to the energy by $k=\sqrt{|E|}$ in atomic units (Bellman and Wing 1975).

If $R(x) = r(x)\exp[ip(x)]$ where $r(x)$ and $p(x)$ are real functions, then the Landauer (1970) expression for the resistance $\rho(x)$ in natural units of $(\hbar/e^2)$ is

$$\rho(x) = \frac{r^2(x)}{1-r^2(x)}. \tag{4}$$

The Riccati eq. (3) with the transformation (4) may be written as a pair of coupled non-linear stochastic equations

$$\frac{\mathrm{d}p(x)}{\mathrm{d}x} = -\frac{V(x)}{k}\left(r(x)+\frac{1}{r(x)}\right)\cos p(x) + 2\left(k-\frac{V(x)}{k}\right)$$
$$\frac{\mathrm{d}\rho(x)}{\mathrm{d}x} = -\frac{2V(x)}{k}(\rho(x)[\rho(x)+1])^{1/2}\sin p(x). \tag{5}$$

For deterministic potentials the phase $p(x)$ is a specific function of x. Equations (5) have in no way made use of the randomness in the potentials. Such equations have been used as the basis of elaborate numerical calculations on one dimensional quantum

wells both periodic as well as incommensurate. In random one-dimensional potentials, the phase $p(x)$ rapidly becomes random with increasing x and the phase memory is lost. The equations may then be decoupled by averaging over the random phase in addition to averaging over the different realizations of the potential. This has been implicitly done in all the work quoted above on random one-dimensional systems. The averaging is carried out using the Novikov theorem (Novikov 1964; Madhukar and Post 1977) for Gaussian random functions

$$\frac{\mathrm{d}}{\mathrm{d}x}\langle\rho(x)\rangle_{vp} = -(2/k)\langle V(x)F[V(x)]\rangle_{vp}$$

$$F[V(x)] = \sin p(x)\rho(x)[\rho(x)+1].$$

Note that $V(x)$ and $p(x)$ are not independently random functions but are related via the first of (5). Using (5)

$$\mathrm{d}F(x)/\mathrm{d}x = [V(x)/k][1+2\rho(x)] + 2[k - V(x)/k]\rho(x)[\rho(x)+1]\cos p(x).$$

It is at this point that we have to invoke randomness. In the second term above the factors $V(x)$, $\rho^2(x)$ and $\cos p(x)$ vary in a strongly correlated manner. In fact in systems where phase memory is retained, the pair of non-linear equations need to be solved. However, in systems where the phase memory is lost for large enough values of x (and this includes random variation in $V(x)$, homogeneous or otherwise, including short ranged order or not) phase averaging leads to this term dropping out, provided we apply the equations for large enough values of x. For periodic potentials this approximation is strictly untrue. For quasi-periodic systems, the validity of this assumption is uncertain

$$\langle \mathrm{d}F(x)/\mathrm{d}x\rangle = -[V(x)/k][1+2\rho(x)\rangle].$$

Thus,

$$F(x) = -(1/k)\int^x V(x')[1+2\langle\rho(x')\rangle\,\mathrm{d}x'$$

or

$$\langle \delta F/\delta V\rangle = -(1/k)[1+\langle\rho(x)\rangle].$$

Novikov's theorem states that

$$\langle V(x)F[V(x)]\rangle = \int^x \mathrm{d}x'\langle V(x)V(x')\rangle\langle\delta F/\delta V\rangle.$$

Using these equations and averaging over different realizations of the random potential, we obtain the basic equation for the averaged resistance $\langle\rho(x)\rangle = \bar{\rho}$

$$\mathrm{d}\bar{\rho}/\mathrm{d}x = (2/k^2)\int^x \mathrm{d}x' G(x,x')[1+2\bar{\rho}(x')]$$

where

$$G(x,x') = \langle V(x)V(x')\rangle = f(x)f(x')g(x-x') \tag{6}$$

$g(x-x') = \langle v(x)v(x')\rangle$ is the homogeneous part of the spatial correlations of the potential.

We shall now apply the above equation to different situations of interest

(1) Let $f(x)=f$, and $g(x-x')=\delta(x-x')$. This occurs if we have a purely homogeneously random potentials with no short ranged correlations at all. Here $d\bar{\rho}/dx = (2f^2/k^2)(1+\bar{2}\rho)$, with $\bar{\rho}=0$ at $x=0$. This gives

$$\bar{\rho}(x)=(1/2)[\exp(x/x_0)-1] \quad \text{with } x_0=k^2/f^2. \tag{7}$$

This result is identical with that of Kumar (1985), although a different embedding technique is used.

(2) The inhomogeneously random potential with $f(x)=f|x|^{-a}$ and $g(x-x')=\delta(x-x')$ (studied by Souillard), so that

$$d\bar{\rho}/dx=(2f^2/k^2)|x|^{-2a}(1+2\bar{\rho}) \quad \text{with } \bar{\rho}=0 \text{ at } x=0$$

(a) for $0<a<1/2$ $\bar{\rho}=(1/2)[\exp(c|x|^{1-2a})-1]$ with the factor $c=(4f^2/k^2)\{1/(1-2a)\}$. The average resistance diverges non-ohmically and the resistivity is infinite. This is characteristic of localized states and pure point spectra. Since, for large x, $\rho \simeq 1/T(x)$ where $T(x)$ is the transmission coefficient, which itself reflects the decay of the wavefunction envelope decay, the above expression indicates that this decay is of the stretched exponential type. This result is identical to that of Souillard but based on completely different arguments. (b) for $a=1/2$, if $\bar{\rho}=\rho_0$ at $x=x_0$ $\bar{\rho}=(1/2)[(1+2\rho_0)\cdot(x/x_0)^{4f^2/k^2}-1]$ again, using the above arguments, the wavefunction decay is power law, agreeing with Souillard's result. (c) For $a>1/2\bar{\rho}=(1/2)[(1+2\bar{\rho}_0)\exp\{(2f^2/k^2)\cdot|x|^{1-2a}\}-1]$ since $a>1/2$, $\bar{\rho}$ becomes a constant as x becomes large. Thus the resistivity vanishes. This is characteristic of extended states and absolutely continuous spectra.
(3) Finally we wish to apply the ideas of (6) to a homogeneously random potential with $f(x)=f$, but $g(x-x')=(1/a)\exp\{-a(x-x')\}$ so that $1/a$ is a measure of the extent of spatial correlation (or short ranged order) of the potentials. In (6) we change the variable $\bar{\rho}$ to $y=(1+2\bar{\rho})$ and take the Laplace transform of both sides

$$s\tilde{y}(s)=2\tilde{g}(s)\tilde{y}(s) \quad \text{or} \quad \tilde{y}(s)=1/[s-g(s)]. \tag{8}$$

For our case $\tilde{g}(s)=(2f^2/k^2a)(s+a)$ which leads to the solution $\tilde{y}(s)=(1/2)[(1+a/D)\cdot(s-s_1)+(1-a/D)(s-s_2)]$ where $s_1=(D-a)/2$ and $s_2=(D+a)/2$ and $D=[a^2+16(f^2/ak^2)]^{1/2}$. Inverse transform yields

$$\bar{\rho}(x)=(1/2D)[s_2\exp(s_1x)+s_1\exp(s_2x)-1] \tag{9}$$

for large values of x, $\bar{\rho}=(s_2/2D)\exp(x/x_0)$, where $x_0=1/s_1$. Thus although the potentials have an extent of spatial correlations, the result is substantially similar to the case (1) without any spatial correlation. We have shown that short ranged order does not destroy localization in a one-dimensional system and we still have exponentially decaying wavefunction envelope and pure point spectra.

The aim of the present communication is to study the mean resistance of linear random systems as a means of examining the wavefunction envelopes. We propose (6) as the basis of further study. The examples quoted illustrate that the results of this analysis agree substantially with more detailed and involved mathematical analysis of the same problems. The added advantage is that in the process we also have information about the physical response of the one-dimensional systems.

Conjectures have been made about the spectrum of quasi-crystalline one-dimensional systems (Valsakumar and Ananthakrishna 1986). Such one-dimensional systems have potentials which lack translational symmetry and long ranged correlations, but whose correlations are different from random one-dimensional systems. We propose to make confirmatory studies on the basis of this formalism.

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