Quantum thermostatted disordered systems and sensitivity under compression

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Abstract
A one-dimensional quantum system with off diagonal disorder, consisting of a sample of conducting regions randomly interspersed within potential barriers is considered. Results mainly concerning the large \(N\) limit are presented. In particular, the effect of compression on the transmission coefficient is investigated. A numerical method to simulate such a system, for a physically relevant number of barriers, is proposed. It is shown that the disordered model converges to the periodic case as \(N\) increases, with a rate of convergence which depends on the disorder degree. Compression always leads to a decrease of the transmission coefficient which may be exploited to design nano-technological sensors. Effective choices for the physical parameters to improve the sensitivity are provided. Eventually large fluctuations and rate functions are analysed.

Keywords: disordered systems, compression, fluctuations, Kronig-Penny model, transfer matrix technique.

1. Introduction
Equilibrium and nonequilibrium thermodynamics are based on the vast separation between the space and time scales of the microscopic, mesoscopic and macroscopic physical realms. Such a separation of scales requires the systems of interest to be made of very large numbers of microscopic constituents and it allows the state of local thermodynamic equilibrium. In that state, microscopic fluctuations of physical quantities are negligible, so that the thermodynamic fields are defined and they are described by the thermodynamic laws. In certain small systems, pertaining e.g. to modern bio- and nano-technologies, the
separation of scales is not realized, and the physical properties of interest are characterized by fluctuations of size comparable to that of the average signals.

In this work, the investigation of Refs.\[2, 3\], concerning a variation of the Anderson model \[4, 5\] of disordered solids, is developed in order to account for the effects of compression on the electron transmission coefficient. Indeed, since Anderson’s paper, the study of electron transport has played a key role in the development of modern solid state physics, see for instance Refs. \[6, 7, 8\] and references therein. The systems of interest, here, are nanostructured devices made of an insulating matrix embedding randomly distributed drops of conducting material. Such complex objects can be represented by 1-dimensional models consisting of conducting regions delimited by $N$ randomly placed potential barriers, in which electrons are injected from one electrode at a given temperature $T$. The large $N$ limit is taken under the constraint that the sum of the $N$ barrier widths and the total length of the system remain constant as $N$ grows. This is at variance with models that grow in size with $N$.

Unlike usual models found in the literature \[5\], the one of Refs.\[2, 3\] enjoys a purely off-diagonal disorder \[9\] that affects the tunnelling couplings among the wells, but not the energies of the bound states within the wells. This is not the case of the original tight-binding model introduced by Anderson to describe localization phenomena in disordered solids \[4\], in which random fluctuations only concern the energy of a bound state. Furthermore, increasing the number of barriers leads, in the Anderson model, to the infinitely large system limit, while increasing $N$ in the model investigated here, produces finer and finer distributions of the same amount of conductor dispersed within the same amount of insulating material. Therefore, the two large $N$ limits do not describe the same situation: Anderson’s limit views the system of interest as macroscopic, i.e. very large compared to its microscopic constituents, while the limit of Refs.\[2, 3\] refers to system sizes that can be small compared to macroscopic objects. The relevant different mathematical constructions imply substantial differences, describing such different physical situations. While Anderson’s limit suits macroscopic objects, the limit of Refs.\[2, 3\] better describes systems at the mesoscopic scale.

In \[2, 3\], the $N \to \infty$ limit led to the conclusion that a large deviation principle holds for the fluctuations of the transmission coefficient, with a proper scaling for the rate function. In the present article, we focus on the behaviour of the transmission coefficient for physically relevant numbers of potential barriers, and we study the effects of compression, that can be realized in practice in numerous nanostructured devices.

Our findings are the following:

- We have extended the continuum limit results proposed in \[2\], observing that the rate of convergence of our model to the Kronig-Penny case \[10\] averaged over the energy strongly depends on the disorder degree.

- Unlike the Anderson model, our large $N$ limit implies no localization. Nevertheless, increasing the disorder degree at fixed $N$ leads to a substan-
tial reduction of the transmission coefficient, which may be viewed as a phenomenon in some sense analogous to localization.

- A mathematical framework of compression has been introduced and two different situations have been simulated and compared. In both cases, compression induces a decrease of the transmission coefficient.

- Analysing the relative percentage change of the transmission coefficient, an optimal configuration has been identified to design an effective sensor. It is found that a moderate number of barriers and strong disorder imply high sensitivity to compression.

- Fluctuations and rate function have been investigated, obtaining that they may be exploited to reveal the compression state of the system.

- A numerical scheme which does not suffer from overflow and Ω problem has been developed.

This article is organized as follows: Section 2 describes the mathematical model to be used for disorder and compression. Section 3 introduces our numerical results and it is divided in subsections concerning linear compression model and a generalized version. Section 4 deals with fluctuations and rate functions for systems under compression. Section 5 recapitulates the contents of the article and in the appendix the numerical scheme developed to tackle the issues raised by the range of energies and lengths of physical interest is explained.

2. The model

Consider a 1-dimensional system of length $L$, consisting of an array of $N$ potential barriers separating $N - 1$ potential wells, in equilibrium with one electrode that acts as an external thermostat at temperature $T$, cf. Fig. This means that the mean energy of the plane waves entering from the left boundary is $k_B T/2$. Let the wells have same width $\delta_N$, so that the total length of the $N - 1$ wells is $L_{\text{cond}} = (N - 1)\delta_N = \alpha L$, where $\alpha \in (0, 1)$, and let the widths of the $N$ potential barriers be picked at random with uniform distribution, to reach the total length $(1 - \alpha)L$ (cf. section 2.1 for details).

Let all potential barriers have same constant height $V(x) = V$, and let their boundary points be denoted by $x = x_0, ..., x_{2N-1}$. For fixed barrier width, we would have a variation of the Kronig-Penney model [10]. In a steady state, the microscopic behavior of the electrons in this environment is given by the time independent Schrödinger equation:

$$\frac{d^2}{dx^2} \psi = \frac{2m}{\hbar^2} (V - E) \psi, \quad x \in [0, L]$$

(1)

where $m$ is the mass of an electron, and $\hbar$ is the reduced Planck constant. Denoting by $U_l$ the $l$-th region, for $l \in \{0, 2, ..., 2N\}$, the solutions of eq. (1) for
\[ E < V \] have the form:

\[
\psi_l(x) = \begin{cases} 
A_{2l} e^{ikx} + A_{2l+1} e^{-ikx} & \text{for } x \in U_l \text{ and even } l \ (i.e. \ for \ V(x) = 0) \\
A_{2l} e^{-ix} + A_{2l+1} e^{ix} & \text{for } x \in U_l \text{ and odd } l \ (i.e. \ for \ V(x) = V)
\end{cases}
\]

with \( k = \sqrt{2mE/\hbar} \) and \( z = \sqrt{2m(V - E)/\hbar} \). The boundary conditions prescribe \( A_0 > 0 \) for the amplitude of the plane wave entering from the left boundary, and \( A_{4N+1} = 0 \) since no wave enters or is reflected from the right boundary. The steady state current is defined by [11],

\[
j_l(x) = \frac{\hbar}{2mi} \left[ \psi_l(x)^* \left( \frac{d}{dx} \psi_l(x) \right) - \left( \frac{d}{dx} \psi_l(x)^* \right) \psi_l(x) \right] = j_l^{tr}(A_{2l}) - j_l^{ref}(A_{2l+1}),
\]

where \( j_l^{tr}(A_{2l}) = \hbar k |A_{2l}|^2 / m \) denotes the current transmitted from the \((l - 1)\)-th barrier on the left and \( j_l^{ref}(A_{2l+1}) = \hbar k |A_{2l+1}|^2 / m \) denotes the current reflected from the \((l + 1)\)-th barrier. Considering eqs. (2) and (3), we get the following definition for the transmission coefficient \( S \) across the system:

\[
S(N) = \frac{j_{2N}^{tr}(A_{4N})}{j_0^{tr}(A_0)} = \frac{|A_{4N}|^2}{|A_0|^2}.
\]

To numerically compute the coefficient \( S \) as a function of the various parameters of the model, it is convenient to rewrite eq.(1) in terms of the characteristic quantities, introducing \( \tilde{x} = x/L, \ \tilde{\psi} = \psi \sqrt{L}, \ \tilde{E} = E/E_T \) and \( \tilde{V} = V/E_T \), with \( E_T = K_b T \), which is twice the mean kinetic energy of the plane waves entering from the left thermostat. Further, introducing the scalar parameter \( \gamma = \hbar^2 / (2mL^2E_T) \), the expression for the dimensionless wave vectors takes the form: \( \tilde{k} = \sqrt{\tilde{E}} / \sqrt{\gamma} \) and \( \tilde{z} = \sqrt{\tilde{V} - \tilde{E}} / \sqrt{\gamma} \).

In the following, we refer only to dimensionless quantities, but for sake of simplicity, we omit the hat over the corresponding symbols. Hence, the dimensionless form of eq.(1) reads:

\[
\frac{d^2}{dx^2} \psi(x) = \frac{1}{\gamma} (V - E) \psi(x), \quad x \in [0, 1].
\]
2.1. Mathematical treatment of disorder

We introduce disorder in our systems by picking the dimensionless potential barrier widths, $\hat{\lambda}_i$, $i = 1, ..., N$, from a given probability distribution $\rho(\lambda) d\lambda$. We begin with a uniform distribution:

$$\rho(\lambda) = \frac{1}{1 - 2\eta}, \quad \lambda \in [\eta, 1 - \eta], \quad \eta \in (0, 1/2),$$

where, for a given $L$, $\eta$ is chosen in order to avoid physical nuisances, such as barriers widths smaller than single atoms. The smaller is $\eta$, the larger is the support of the probability density function $\rho(\lambda)$, thus a measure of the disorder degree is given by the value of $\eta$. The empirical mean width for a single realization of the disorder is a random variable denoted by:

$$\hat{\lambda}_N = \frac{1}{N} \sum_{i=1}^{N} \hat{\lambda}_i. \quad (6)$$

The weak law of large numbers implies that $\hat{\lambda}_N$ converges in probability to the mean $\langle \hat{\lambda} \rangle$, in the large $N$ limit.

After the $N$ widths have been generated, the total length of the sample may exceed or be smaller than the desired value, therefore we rescale all lengths introducing the parameter

$$c_N = \frac{L(1 - \alpha)}{N\hat{\lambda}_N}$$

so that $\lambda_i = c_N \hat{\lambda}_i$ and

$$\sum_{i=1}^{N} \lambda_i = \sum_{i=1}^{N} \frac{L(1 - \alpha)}{N\hat{\lambda}_N} \hat{\lambda}_i = L(1 - \alpha) = L_{ins} \quad (8)$$

Let us denote by $\Lambda_N = \{\lambda_1, ..., \lambda_N\}$ the set of barrier widths. Among the possible realizations of $\Lambda_N$, the regular barrier distribution $\Lambda_B = \{\lambda_B, ..., \lambda_B\}$ plays a crucial role, since it corresponds to the Kronig-Penney model, the continuum limit of which has been considered in Ref.\[10]. We call periodic the case of $\Lambda_B$.

Considering an observable $A$, defined as a function of a given realization of barriers, and denoting by $\Omega = \{\Lambda^{(1)}_N, \Lambda^{(2)}_N, ..., \Lambda^{(\ell)}_N\}$ a set of realizations, the corresponding ensemble average is given by:

$$\langle A \rangle_{\Omega} = \frac{1}{\ell} \sum_{i=1}^{\ell} A \left( \Lambda^{(i)}_N \right). \quad (9)$$

We are interested in the observable $S$, which is also a function of the energy $E$ of the incoming particle, of the potential height $V$ and of the temperature $T$ that determines the distribution of the particles energies: $S = S(\Lambda_N; V, E, T)$. Averaging over the particles energy gives the coefficient

$$S(\Lambda_N; V, T) = \int_0^\infty S(\Lambda_N; E, V, T) f_{eq}(E) dE, \quad (10)$$
where the Maxwellian probability density
\[ f_{eq}(E) = \sqrt{\frac{1}{\pi E}} e^{-\frac{E}{E}} \] (11)
is used to represent the electrode on the left as a classical heat reservoir.

2.2. Sample compression

Because of externally exerted pressure, the sample length may be reduced by an amount \( \Gamma \), so that its length is given by \( L_{\text{compr}} = L - \Gamma \). If the insulator is \( e.g. \) polymeric and the conductor is \( e.g. \) metallic, we may in first approximation assume that the length reduction only concerns the potential barrier widths. In any event, introducing the ratio \( r \) for the effect of compression on the two materials, we may write:

\[ L_{\text{ins,compr}} = L_{\text{ins}} - \Gamma \cdot r \] \hspace{1cm} (12)
\[ L_{\text{cond,compr}} = L_{\text{cond}} - \Gamma \cdot (1 - r) \] \hspace{1cm} (13)
\[ L_{\text{ins,compr}} + L_{\text{cond,compr}} = L_{\text{compr}} \] \hspace{1cm} (14)

where the index \( \text{compr} \) denotes the lengths regarding the compressed state. For instance, the case \( r = 1 \) describes the situation in which only the insulator is affected by the compression. Introducing the parameter \( \alpha_{\text{compr}} = L_{\text{cond,compr}} / L_{\text{compr}} \), the compressed state can be described by the function

\[ f_{\Gamma,r} : (L, \alpha, \Lambda_N, V) \rightarrow (L_{\text{compr}}, \alpha_{\text{compr}}, \Lambda_N, \text{compr}, V_{\text{compr}}) \] (15)

that associates the old system, characterized by \( (L, \alpha, \Lambda_N, V) \) with the compressed system characterized by \( (L_{\text{compr}}, \alpha_{\text{compr}}, \Lambda_N, \text{compr}, V_{\text{compr}}) \), where the notation indicates that the compression modifies the realization of the barrier widths and, consequently, that it may affect the potential height.

One possibility for the variation of the potential under compression is that the area under a barrier, \( i.e. \) barrier width times barrier height, is constant. The idea is that the compression leads to higher insulator density, hence to an increase of the potential. The specific form of the increase is irrelevant here, since other rules may be simply implemented in our framework.

One may ask whether the compression introduces disorder also in the potential strength, because of different increments in barriers of different widths. Using our rule, this does not happen. Indeed, consider a system composed by two barriers of width \( \lambda_1 \) and \( \lambda_2 \) divided by a conduction region whose length is \( \delta \). One has

\[ L = \lambda_1 + \lambda_2 + \delta \, , \quad L_{\text{ins}} = \lambda_1 + \lambda_2 \, , \quad L_{\text{cond}} = \delta \, , \quad \alpha = \frac{\delta}{\lambda_1 + \lambda_2 + \delta} \] (16)

Compressing the system by a quantity \( d \), and distributing the compression with ratio \( r \), one gets:

\[ L_{\text{compr}} = \lambda_1 + \lambda_2 + \delta - d \, , \quad L_{\text{ins,compr}} = \lambda_1 + \delta - d \cdot r \] \hspace{1cm} (17)
\[ L_{\text{cond,compr}} = \delta - d \cdot (1 - r) \, , \quad \alpha_{\text{compr}} = \frac{\delta - d \cdot (1 - r)}{\lambda_1 + \lambda_2 + \delta - d} \] (18)
Observe that the widths $\lambda_1$ and $\lambda_2$ arise from the normalization of realizations $\hat{\lambda}_1$ and $\hat{\lambda}_2$ picked at random from the chosen distribution of widths. Then, we may write

$$\lambda_i = \frac{L(1 - \alpha)}{N\lambda_N} \hat{\lambda}_i, \quad i = 1, 2 \quad (19)$$

If the area under each barrier is kept constant under compression, we have

$$\lambda_i V = \lambda_{i,\text{compr}} V_{i,\text{compr}}, \quad i = 1, 2 \quad (20)$$

which, thanks to eq.(19) can be rewritten as:

$$\frac{L(1 - \alpha)}{N\lambda_N} \hat{\lambda}_i V = \frac{L_{\text{compr}}(1 - \alpha_{\text{compr}})}{N\lambda_N} \hat{\lambda}_{i,\text{compr}} V_{i,\text{compr}}, \quad i = 1, 2 \quad (21)$$

This implies:

$$V_{1,\text{compr}} = V_{2,\text{compr}} = \frac{V}{L_{\text{compr}}(1 - \alpha_{\text{compr}})} \quad (22)$$

The reasoning can be easily extended to any numbers of barriers. It follows that the heights of the potential barriers depend only on the compression level and on the ratio $r$, not on the realization of the microscopic disorder.

### 3. Numerical results

The solution (2) of eq.(1) must be subjected to the classical BenDaniel-Duke boundary conditions on the generic $l$-th node, with $l \in \{0, 1, ..., 2N - 1\}$, which require the continuity both of the wave function and of its first derivative at each node:

$$\begin{align*}
\psi_l(x_l) &= \psi_{l+1}(x_l) \\
\psi_l'(x_l) &= \psi_{l+1}'(x_l)
\end{align*} \quad (23)$$

where $x_l = \sum_{i=1}^{(l/2)} \lambda_i + \delta_{l \text{ even}}$, if $l$ is even, and $x_l = \sum_{i=1}^{(l+1)/2} \lambda_i + \delta_{l \text{ odd}}$ if $l$ is odd, where $\lambda_i$ denotes the random width of the $i$-th barrier. With this notation, eq.(23) may be written as:

$$\begin{align*}
M_0(x_0) \cdot \begin{pmatrix} A_0 \\ A_1 \end{pmatrix} &= M_1(x_0) \begin{pmatrix} A_2 \\ A_3 \end{pmatrix} \\
M_2(x_1) \cdot \begin{pmatrix} A_2 \\ A_3 \end{pmatrix} &= M_3(x_1) \begin{pmatrix} A_4 \\ A_5 \end{pmatrix} \\
M_4(x_0) \cdot \begin{pmatrix} A_4 \\ A_5 \end{pmatrix} &= M_5(x_0) \begin{pmatrix} A_6 \\ A_7 \end{pmatrix}
\end{align*} \quad (24)$$

where the support matrices $M_{2l}$ and $M_{2l+1}$ have been introduced, and

$$M_{4N-2}(x_{2N-1}) \cdot \begin{pmatrix} A_{4N-2} \\ A_{4N-1} \end{pmatrix} = M_{4N-1}(x_{2N-1}) \begin{pmatrix} A_{4N} \\ A_{4N+1} \end{pmatrix} \quad (24)$$
For $E < V$, these 2x2 matrices of coefficients $M_{2l}(x_l)$ and $M_{2l+1}(x_l)$ read:

$$M_{2l}(x_l) = \begin{pmatrix} e^{ikx_l} & e^{-ikl} \\ ik e^{ikx_l} & -ik e^{-ikl} \end{pmatrix} \quad \text{and} \quad M_{2l+1}(x_l) = \begin{pmatrix} e^{-zx_l} & e^{zx_l} \\ -ze^{-zx_l} & z e^{zx_l} \end{pmatrix}$$ (25)

for even $l$, and

$$M_{2l}(x_l) = \begin{pmatrix} e^{-zx_l} & e^{zx_l} \\ -ze^{-zx_l} & z e^{zx_l} \end{pmatrix} \quad \text{and} \quad M_{2l+1}(x_l) = \begin{pmatrix} e^{ikx_l} & e^{-ikx_l} \\ ik e^{ikx_l} & -ik e^{-ikx_l} \end{pmatrix}$$ (26)

for odd $l$. Assuming that the amplitude of the incoming wave $A_0$ is known, and imposing $A_{4N+1} = 0$, since there is no reflection at the right boundary, these equations constitute a set of $4N$ equations in $4N$ variables, for which the support matrices $M_{2l}$ and $M_{2l+1}$ allow us to write:

$$\begin{pmatrix} A_0 \\ A_1 \end{pmatrix} = M_0^{-1} \cdot M_1 \cdot M_2^{-1} \cdot M_3 \cdots M_{4N-2}^{-1} M_{4N-1} \cdot \begin{pmatrix} A_{4N} \\ 0 \end{pmatrix} = M \begin{pmatrix} A_{4N} \\ 0 \end{pmatrix}$$ (27)

where $M$ denotes the product of the $M_i$. It follows that

$$A_0 = M_{11} A_{4N}$$ (28)

where $M_{11}$ is the first entry of $M$. Consequently, eq.(1) may be written as:

$$S = \frac{A_{4N}' A_{4N}}{A_0 A_0} = \frac{1}{|M_{11}|^2}$$ (29)

which is, in principle, a simple and efficient expression for the transmission coefficient. In practice, however, the range of energies and lengths of nanotechnological interest make eq.(29) hardly of any use for numerical calculations. For instance, $L = 500nm$ and energy of the order of $E_T$ at room temperature imply that the dimensional variable $z$ ranges between 100 and 1000, which make overflow the entries of the matrices $M_i$, see e.g. Ref.[12] for overflow and $\Omega$ problems.

To overcome these difficulties, we have developed a numerical scheme which relies uniquely upon the scattering matrix, and that is described in the Appendix.

For our numerical results, if not otherwise stated, we refer to $L = 500nm$, which is a length suitable for present nanotechnology, to $V = 3$ for the dimensionless potential, and to $\alpha = 10/11$, meaning that the insulator length amounts to the fraction 1/11 of the total sample length.

Figure 2 shows the common behaviour of the ensemble average $\langle S(\Lambda N; V, T) \rangle_{\Omega}$ as a function of the number of barriers $N$, computed over different realizations of the microscopic disorder. The maximum value $N = 400$ is determined by the fact that for $L = 500nm$, one obtains barrier widths of the order of $10^{-10}m$, below which the physical significance is lost. The right panel of Figure 2 concerns the behaviour of $\langle S(\Lambda N; V, T) \rangle_{\Omega}$ for small values of $N$.

Let us understand as greater disorder the situation in which the support of the uniform distribution of widths $\rho$ is wider, i.e. the case in which $\eta$ is smaller. Then, Fig 2 shows that the periodic case enjoys the highest transmission coefficient, and that growing disorder implies a decay of $\langle S \rangle_{\Omega}$.
At the same time, the growth of $N$ at fixed disorder degree makes $\langle S \rangle_\Omega$ increase, apart from a minimal decrease at small $N$. The periodic case, in particular, reaches a plateau at $N \approx 200$; in other words the periodic case attains within physically relevant scales the maximum transmission coefficient that the model allows and that remains throughout the physically relevant range. The disordered cases, on the other hand, may also reach a plateau, but presumably at scales that exceed the physically relevant ones. Therefore, in their cases, larger $N$, i.e. finer structures, correspond to higher $\langle S \rangle_\Omega$.

This statement agrees with Ref. [10], in which a closed formula for the asymptotic behavior of the transmission coefficient in the periodic case has been given:

$$\hat{S} = \lim_{N \to \infty} S_N = \left[ 1 + \frac{E^2}{4E} \left( \frac{\sin(L\sqrt{E - E})}{\sqrt{E - E}} \right)^2 \right]^{-1}$$  \hspace{1cm} (30)

As we are interested in the average with respect to the energy distribution, we
numerically computed

$$S_B = \int_E I_{eq}(E) \left[ 1 + \frac{E^2}{4E} \left( \frac{\sin(L\sqrt{E-E})}{\sqrt{E-E}} \right)^2 \right]^{-1}$$

(31)

for different disorder intensities. Setting the parameters given at the beginning of this section we get $S_B = 0.4178$, while $\langle S(\Lambda_{400}; V, T) \rangle_\Omega = 0.4076$, and $\langle S(\Lambda_{10}; V, T) \rangle_\Omega = 0.4150$, with $\lambda \in [0.4, 0.6]$. For $\lambda \in [0.1, 0.9]$, we get instead $\langle S(\Lambda_{7.10}; V, T) \rangle_\Omega = 0.4073$

We conclude that in the large $N$ limit our model tends to the Kronig Penney model, with a rate of convergence that depends on the disorder degree. This confirms the results of Ref. [2], although for highly disordered cases the asymptotic properties do not suit the nanotechnological interests. These observations mean that there are no localization effects in our model, unlike the case of the Anderson model. The origins of this discrepancy may be traced back to the fact that Anderson’s model is based on a discrete tight binding Hamiltonian, that we do not have, and to the inapplicability in our model of Furstenberg’s theorem, from which localization depending on the first Lyapunov exponent follows [13],[14]. While the sequence of barriers of Anderson’s model increases by adding new barriers without modifying the previous ones, adding a barrier in our construction alters the preceding barriers in order to keep unchanged the insulator amount, cf. eq.(8). The hypothesis of Furstenberg’s theorem are thus violated and we are in a framework that has been little investigated so far.

3.1. Linear compression model and design optimization for sensor devices

Suppose now that our samples have been compressed according to the model described in section 2.2.

Figure 3 shows that increasing the compression percentage leads in our model to a mild decrease of $S$, for large $N$, and to an equally mild increase for small $N$. The cross-over between the two regimes grows with the disorder. Note that the growth of the disorder also seems to move forward, away form the physically interesting region, the asymptotic regime.

Figure 4 shows the dependence of $\langle S(\Lambda_{400}; V, T) \rangle$ on the compression percentage. More precisely, Fig 4(a) and 4(b) corresponds to Fig 3(a) and Fig 3(b), while Fig 4(c) and Fig 4(d) refer to the same setting, but $r=1$. It is evident that the reduction of the transmission coefficient is linear as a function of the compression factor. Furthermore table 1 allows us to conclude that for given disorder, the absolute value of the rate of decrease, $a$, increases with $r$, the fraction of compression attributed to the insulator. For fixed $r$, the absolute value of $a$ decreases if the disorder is higher. The increment of $a$ for growing $r$ means that the increment of the potential height is more significant than the reduction of $L_{ins}$.

Figure 5 shows the behaviour of the probability current defined by eq. (3) for different temperatures. Being the problem time independent, the current
is constant along the system and it is sufficient to compute it at one of the extreme. For the sake of simplicity, we have fixed $A_0 = 1$ in the simulations.

We next focus on possible optimal choices for the design of effective sensor devices. From this point of view, it is convenient to examine the relative percentage change of the transmission coefficient under compression, rather than the absolute variation investigated previously. In the following, the relative percentage change is defined as $\Delta(\beta) = \frac{|\langle S(\Lambda_N, \beta) \rangle - \langle S(\Lambda_N, 0) \rangle|}{\langle S(\Lambda_N, 0) \rangle}$, where $\beta \in [0, 100]$ is the compression percentage. In particular, we look for good choices for the number of barriers $N$ and for the disorder degree, in order to have a high sensitivity to compression, i.e. large relative percentage change $\Delta(\beta)$ under compression.

Guided by the behaviour of $\langle S(N) \rangle$ described by figures 3, we have considered three possible optimal choices for the variable $N$, that are a) small number of barriers, $N \approx 10$; b) high number of barriers, $N = 400$; c) intermediate number of barriers, $N \approx 150$.

Table 2 (see appendix) summarizes the most interesting values of $\Delta(\beta)$ for these different $N$, disorder degree and ratio $r$. The results show that even tough for $N = 400$ we have the maximum absolute drop of the transmission
coefficient under compression, the maximum relative drop is attained for smaller numbers of barriers. In fact, especially for strong disorder degree, we have that in the range $N \approx 100 \sim 200$, $\Delta(\beta)$ is significantly larger than for $N = 400$. For very low $N$, we have a large relative drop of $S$ which might be in theory exploited. Nevertheless since $S$ is very small in absolute value, there might be difficulties to measure the corresponding low currents. Considering the ratio, the higher is $r$, the greater is $\Delta(\beta)$ as we would expect. For $r = 1$ and $\beta = 10$ results are not shown, because that corresponds to a negative insulator length, cf. (12).

We observe that the higher the disorder, the higher the relative percentage change $\Delta(\beta)$, if the other parameters are fixed. Therefore in spite of all the other possible choices, randomness enhances the sensitivity to compression.

For this reason, we have also simulated a system in which not only the barriers but also the wells are random. With $\lambda \in [0.1, 0.9]$, and a weak disorder for the wells $\delta \in [0.4, 0.6]$. Fig 6 shows the behaviour of the transmission
Table 1: For fixed $r$, the absolute value of $a$ decreases if the disorder is higher, meaning a minor variation of $\langle S(\Lambda_{100}; V, T) \rangle$ as the compression percentage grows. Similarly, the absolute value of $a$ decreases if $r$ decreases at a constant disorder degree.

| $\rho(\lambda)$ | $r = 1$ | $r = 0.6$ |
|------------------|---------|-----------|
| [0.4:0.6]        | $-2.629 \cdot 10^{-3}$ | $-2.276 \cdot 10^{-3}$ |
| [0.35:0.65]      | $-2.589 \cdot 10^{-3}$ | $-2.126 \cdot 10^{-3}$ |
| [0.3:0.7]        | $-2.381 \cdot 10^{-3}$ | $-1.812 \cdot 10^{-3}$ |
| [0.1:0.9]        | $-1.340 \cdot 10^{-3}$ | $-9.667 \cdot 10^{-4}$ |

Figure 5: Behaviour of $\langle j(\Lambda_N; V, T) \rangle$ as $N$ increases for the first model of compression with $r = 0.6$ and different compression percentages. Left panel $T = 300K$, right panel $T = 170K$.

coefficients for this system. We observe that the behaviour changes since $\langle S \rangle$ is flat and almost vanishing for $N < 100$ and then it grows quickly suggesting a faster rate of convergence to the periodic case than the fixed wells width case. Nevertheless the relative percentage change remains similar, even tough the crossover zone restricts, as well as the interval of moderate $N$ values for which the relative percentage change is significant. Therefore, introducing randomness in the wells widths does not appear to improve the sensitivity.

All things considered, the optimal design choice for a compression sensor whose barriers height grows linearly with compression, requires a number of barriers $N \approx 100 \sim 200$, strong disorder only for the barriers width and ratio $r$ close to one. Nevertheless the absolute variation of the transmission coefficient is small.

3.2. Generalized compression model

The numerical results of section 3.1 show that a model of compression that preserves the area of the potential barriers produces a limited decrease of the transmission coefficient under compression. We therefore propose and numerically test another possibility. In particular we consider the following rule for the potential height:
Figure 6: Comparison of the transmission coefficient. On the left side disorder is present only in the barrier widths. On the right the barriers widths are strongly disordered, while the wells widths are weakly disordered.

\[ V_{\text{compr},a} = V \left( \frac{L(1-\alpha)}{L_{\text{compr}}(1-\alpha_{\text{compr}})} \right)^2 = V \left( \frac{L(1-\alpha)}{L_{\text{ins,compr}}} \right)^2 = V \left( \frac{L(1-\alpha)}{L_{\text{ins}} - L \cdot r \cdot \beta \frac{100}{1000}} \right)^2 \]

where \( \beta \) is the compression percentage. In this case, the potential increases as \( \frac{1}{(C-\beta \frac{100}{1000})^2} \) for \( \beta \frac{100}{1000} \rightarrow C \), where \( C = \frac{L_{\text{ins}} \cdot L \cdot r}{100} \).

Again, it is to be remarked that for every power \( p \), the rule

\[ V_{\text{compr}} = V \left( \frac{L(1-\alpha)}{L_{\text{ins}} - L \cdot r \cdot \beta \frac{100}{1000}} \right)^p \]

does not introduce any disorder in the potential heights. Taking \( p > 1 \), compression makes the potential increase significantly more than in the case analysed in the previous section, thus we expect the transmission coefficient to drop much faster as a function of disorder. This is confirmed by Fig.7.

In Fig.8 a polynomial regression is shown, to find the decay rate of the transmission coefficient under compression, with the new potential barriers. We observe a linear decrease of \( S \) with the compression factor for a wide compression range, followed by a nonlinear, milder decay regime at high compressions. Clearly the absolute value of \( a \) is larger than the counterpart for the linear compression model. This indicates that the selection of the material plays a determinant role for the physical properties of the system, and that a non-linear behaviours of the potential height with compression are to be preferred.

4. Fluctuations and rate functions

In [2, 3], the authors studied the decay of fluctuations as \( N \) increases, they identified micro, meso and macroscales and checked the validity of a large deviation principle (LDP). It is therefore interesting to check how the fluctuations are...
affected by compression. In Fig. 7 we plot $\sqrt{\langle (S - \langle S \rangle_{\Omega})^2 \rangle}/\langle S \rangle_{\Omega}$ for different percentages of compression. We observe that compression enhances the relative size of fluctuations, and it does so more efficiently at small $N$. On the contrary, growing $N$ implies smaller fluctuations relative size.

Introducing the variable $X_N = \frac{S_N}{\langle S_N \rangle}$, which is the transmission coefficient normalized to its expected value, approximated by the empirical mean, and denoting by $\rho_N(X)$ the probability distribution of $X_N$, we can write

$$\langle S \rangle_{\Omega} = \int S \rho_N(X) dX$$

and we may consider now the behaviour under compression of the rate function $\Xi(x)$, \cite{13,14,15} defined by:

$$\lim_{N \to \infty} -\frac{\log \rho_N(x)}{N} = \Xi(x)$$

Figure 7(a) shows that, in accord with Fig. 7(b), the probability distribution covers a wider range of values under larger compression rates. Therefore, also the properties of the fluctuations can be used to reveal the compression state. Furthermore, this can be done more efficiently for higher disorder.
5. Conclusion and future developments

In the present article we have investigated the behaviour of a thermostatted disordered system under compression. Our results indicate that for physically relevant $N$, the randomness of the barrier widths leads to a decrease of the transmission coefficient, which is more significant for stronger microscopic disorder. Considering the large $N$ limit, we have shown numerically that our model behaves similarly to the large $N$ limit of the Kronig-Penny model recently studied in [10] and we have expanded that work considering energy averages. We have then shifted our attention to compressed systems, providing a mathematical framework suitable for real cases and amenable to experimental tests. For two compression models we find that compression causes a decrease of $S$. Modifying the degree of freedom $p$, which represents the power law followed by the potential heights under compression, our numerical simulations show that for quite a large interval of compression percentages, the decrease can be assumed to be linear. Furthermore for the linear compression model we have extensively
investigated the relative percentage change of the transmission coefficient, identifying the best possible configuration for effective sensors. Eventually we have noticed that compression increases the fluctuations of $S$, as shown by a probability density and rate function estimation. This effect may be used to reveal the compression state of the sample.

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Appendix

Appendix 1. Numerical scheme: the transfer matrix and scattering matrix techniques

To overcome the numerical difficulties described in section 2, we have developed a numerical scheme that relies uniquely upon the scattering matrix. If the transfer matrix relates linearly the wave amplitudes on the left side with the wave amplitudes on the right side, the scattering matrix relates linearly the amplitudes of wave exiting the barrier potential with the amplitudes of the wave entering the barrier potential. Therefore, considering a single barrier, the following relations hold:

\[
\begin{pmatrix} A_4 \\ A_5 \end{pmatrix} = M_3^{-1}M_2M_1^{-1}M_0 \begin{pmatrix} A_0 \\ A_1 \end{pmatrix} = T \begin{pmatrix} A_0 \\ A_1 \end{pmatrix} = \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} \begin{pmatrix} A_0 \\ A_1 \end{pmatrix} \quad (1)
\]

\[
\begin{pmatrix} A_4 \\ A_1 \end{pmatrix} = S \begin{pmatrix} A_0 \\ A_5 \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} A_0 \\ A_5 \end{pmatrix} \quad (2)
\]

It is straightforward to verify that:

\[
S = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} = \begin{pmatrix} T_{11}T_{22} - T_{12}T_{21} & T_{12} \\ -T_{11} & T_{22} \end{pmatrix} \quad (3)
\]

Since all the components of \( T \) scale at most as \( e^{zd} \), \( S_{12}, S_{21}, S_{22} \) are bounded. \( S_{11} \) might instead explode, because the numerator scales as \( e^{2zd} \). Nevertheless, introducing

\[
a_1 = (1 - \frac{z}{ik})(1 - i\frac{k}{z}) \quad a_2 = (1 + \frac{z}{ik})(1 + i\frac{k}{z}) \quad (4)
\]

\[
a_3 = (1 - \frac{z}{ik})(1 + i\frac{k}{z}) \quad a_2 = (1 + \frac{z}{ik})(1 - i\frac{k}{z}) \quad (5)
\]

one finds that the leading term of the numerator of \( S_{11} \) is \( (a_1a_2 - a_3a_4)e^{2zd} \).

Since \( a_1a_2 - a_3a_4 = 0 \), we conclude that all the components of \( S \) are bounded.

Suppose now that the scattering matrix \( \hat{S} \) links linearly the wave amplitudes that enter and exit a sequence of \( N \) barriers, while \( S \) describes the scattering
process through the \((N+1)th\) that is added to the system. The following relations allow us to construct a unique scattering matrix for the whole system.

\[
A_{4N} = \hat{S}_{11} S_{11} A_0 + \left( \frac{\hat{S}_{11} S_{12} \hat{S}_{22}}{1 - S_{12} \hat{S}_{21}} + \hat{S}_{12} \right) A_{4N+1} \tag{6}
\]

\[
A_1 = \left( S_{21} + \frac{S_{22} \hat{S}_{21} S_{11}}{1 - S_{12} \hat{S}_{21}} \right) A_0 + \frac{S_{22} \hat{S}_{22}}{1 - S_{12} \hat{S}_{21}} A_{4N+1} \tag{7}
\]

Once we have the total scattering matrix, it is easy to compute the transmission coefficient through

\[
S = \frac{|A_{4N}|^2}{|A_0|^2} = |S_{11}|^2 \tag{8}
\]

The scheme illustrated here has the advantage of being numerically stable and not subjected to overflow problems. Nevertheless, this advantage comes at the cost of having to deal with non linear relations, which require a greater computational effort than the simpler matrix multiplications of Eq (27). Given the present day computer facilities, this is not a serious hindrance.
Appendix 2. Relative percentage change under compression

| Periodic case $N = 400, r = 0.6$ | $\beta = 2$ | $\beta = 4$ | $\beta = 6$ | $\beta = 8$ | $\beta = 10$ |
|----------------------------------|-------------|-------------|-------------|-------------|-------------|
| $\Delta(\beta)$                 | 1.08        | 1.95        | 3.29        | 4.65        | 5.65        |
| $\lambda \in [0.4; 0.6]$        | $\beta = 2$ | $\beta = 4$ | $\beta = 6$ | $\beta = 8$ | $\beta = 10$ |
| $\Delta(\beta)$                 | 1.16        | 2.54        | 3.72        | 5.17        | 6.64        |
| $\lambda \in [0.4; 0.6]$        | $\beta = 2$ | $\beta = 4$ | $\beta = 6$ | $\beta = 8$ | $\beta = 10$ |
| $\Delta(\beta)$                 | 1.70        | 3.19        | 4.6         | 6.28        |             |
| $\lambda \in [0.3; 0.7]$        | $\beta = 2$ | $\beta = 4$ | $\beta = 6$ | $\beta = 8$ | $\beta = 10$ |
| $\Delta(\beta)$                 | 1.73        | 3.2         | 4.88        | 6.56        | 8.14        |
| $\lambda \in [0.3; 0.7]$        | $\beta = 2$ | $\beta = 4$ | $\beta = 6$ | $\beta = 8$ | $\beta = 10$ |
| $\Delta(\beta)$                 | 1.10        | 2.54        | 4.66        | 6.83        | 9.10        |
| $\lambda \in [0.1; 0.9]$        | $\beta = 2$ | $\beta = 4$ | $\beta = 6$ | $\beta = 8$ | $\beta = 10$ |
| $\Delta(\beta)$                 | 1.47        | 4.18        | 5.65        | 7.4         | 10.18       |
| $\lambda \in [0.1; 0.9]$        | $\beta = 2$ | $\beta = 4$ | $\beta = 6$ | $\beta = 8$ | $\beta = 10$ |
| $\Delta(\beta)$                 | 2.78        | 5.81        | 8.14        | 11.24       |             |
| $\lambda \in [0.1; 0.9]$        | $\beta = 2$ | $\beta = 4$ | $\beta = 6$ | $\beta = 8$ | $\beta = 10$ |
| $\Delta(\beta)$                 | 1.98        | 6.00        | 10.71       | 19.10       | 28.17       |
| $\lambda \in [0.1; 0.9]$        | $\beta = 2$ | $\beta = 4$ | $\beta = 6$ | $\beta = 8$ | $\beta = 10$ |
| $\Delta(\beta)$                 | 3.7         | 12.22       | 29.18       | 52.99       |             |
| $\lambda \in [0.1; 0.9]$        | $\beta = 2$ | $\beta = 4$ | $\beta = 6$ | $\beta = 8$ | $\beta = 10$ |
| $\Delta(\beta)$                 | 5           | 7.92        | 40.76       | 94.88       |             |
| $\lambda \in [0.1; 0.9]$        | $\beta = 2$ | $\beta = 4$ | $\beta = 6$ | $\beta = 8$ | $\beta = 10$ |
| $\Delta(\beta)$                 | 2.6         | 7.75        | 15.19       | 23.82       |             |
| $\lambda \in [0.4; 0.6]$        | $\beta = 2$ | $\beta = 4$ | $\beta = 6$ | $\beta = 8$ | $\beta = 10$ |
| $\Delta(\beta)$                 | 42.56       | 71.29       | 89.16       | 95.09       | 91.37       |

Table 2: Relative percentage variation for different configurations.