Transport in quantum multi–barrier systems as random walks on a lattice

Emilio N. M. Cirillo
E_mail: emilio.cirillo@uniroma1.it

Dipartimento di Scienze di Base e Applicate per l’Ingegneria,
Sapienza Università di Roma, via A. Scarpa 16, I–00161, Roma, Italy.

Matteo Colangeli
E_mail: matteo.colangeli1@univaq.it

Dipartimento di Ingegneria e Scienze dell’Informazione e Matematica,
Università degli Studi dell’Aquila, via Vetoio, 67100 L’Aquila, Italy.

Lamberto Rondoni
E_mail: lamberto.rondoni@polito.it

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Politecnico di Torino, corso Duca degli Abruzzi 24, I–10129, Torino, Italy.

INFN, Sezione di Torino, Via P. Giuria 1, 10125 Torino, Italy.

Abstract. A quantum finite multi–barrier system, with a periodic potential, is considered and exact expressions for its plane wave amplitudes are obtained using the Transfer Matrix method [10]. This quantum model is then associated with a stochastic process of independent random walks on a lattice, by properly relating the wave amplitudes with the hopping probabilities of the particles moving on the lattice and with the injection rates from external particle reservoirs. Analytical and numerical results prove that the stationary density profile of the particle system overlaps with the quantum mass density profile of the stationary Schrödinger equation, when the parameters of the two models are suitably matched. The equivalence between the quantum model and a stochastic particle system would mainly be fruitful in a disordered setup. Indeed, we also show, here, that this connection, analytically proven to hold for periodic barriers, holds even when the width of the barriers and the distance between barriers are randomly chosen.

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1. Introduction

A variation of the Anderson model \cite{2} for disordered solids has been recently introduced and investigated in order to describe systems that are finely structured, but not macroscopic \cite{11,12,25}. In particular, for 1D chains of $N$ potential barriers, the large $N$ limit was performed in a way that prevents the application of standard techniques, such as Furstenberg type theorems \cite{13}. Numerically, it has been observed that such systems do not lead to localization, as indeed natural for systems whose length remains finite and fixed, when the number of barriers grows. Unlike the tight–binding model introduced by Anderson, the one of Refs. \cite{11,12,25} enjoys a purely off–diagonal disorder that affects the tunneling couplings among the wells, but not the energies of the bound states within the wells. In Refs. \cite{11,12}, it has been numerically shown that the $N \to \infty$ limit for the model there treated leads 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 Ref. \cite{25}, the transmission coefficient has been investigated for physically relevant numbers of potential barriers, referring to the scales of nano–structured sensors. In particular, the effect of compression has been numerically investigated, for different compression rules, finding that the rate of convergence to the behavior of the Kronig–Penney model \cite{10,18} strongly depends on the disorder degree; that compression induces a decrease of the transmission coefficient; and that a moderate number of barriers together with strong disorder imply high sensitivity to compression, which can be used for pressure sensors.

In search for a more detailed treatment of the model of Refs. \cite{11,12,25}, the present paper investigates the possibility of adopting an effective description, that replaces the original one with models that behave in an equivalent fashion, while being better suited for analytical treatment. The first case that ought to be investigated, in this respect, is the regular one, corresponding to the finite Kronig–Penney model. We show that the wave function time independent profile of the Kronig–Penney model can be associated with the stationary particle profile of independent random walkers with suitable hopping rates. For convenience, we deal with this model, using the language of the Zero Range Process (ZRP) \cite{4,5,15,19,20}. The regular quantum system considered here is the same as the one studied in Ref. \cite{10}, with $N$ potential barriers and fixed length $L$. Here, we focus on the connection between both regular and disordered quantum models of that kind with properly devised stochastic processes. This connection is established by introducing site-dependent hopping probabilities for the stochastic models, in terms of the parameters of the corresponding quantum systems. This connection allows the analysis of one of the models in terms of the other, which is particularly useful in the disordered cases.

The paper is organized as follows. In Section 2 we illustrate our model, which consists
of a 1D sequence of \( N \) regularly placed conducting and insulating regions, and we solve the time independent Schrödinger equation for the density of particles, at the center of each conducting region, as a function, in particular, of \( N \) and of the energy of the particles \( E \). We observe that the transport of particles is approximately ballistic when the energy \( E \) is sufficiently higher than a reference energy \( E_0 \).

In Section 3, we summarize the fundamental properties of the Zero Range Process, and we show how the parameters of the quantum and of the stochastic process can be tuned so that their profiles coincide. In Section 4 we test numerically the validity of our method comparing the Monte Carlo results with the exact expressions. We show that our technique also applies to the case of random environments, for which no general ergodic–like results seem to have been so far developed. In particular we show that, for sufficiently large \( N \) and \( L \) fixed, the quenched ZRP averaged profiles tend to stationary regular ones, implying, also, that in the equivalent quantum model no localization occurs. This happens because our large \( N \) limit is not of the standard hydrodynamic kind; rather, it is meant to describe small systems. Conclusions are drawn in Section 5.

2. The quantum multi–barrier model

Consider a 1D medium consisting of \( N \) identical potential barriers of width \( \gamma \delta \) separated by a distance \( \delta \), cf. Fig. 2.1. The total length of the system is

\[ L = (1 + \gamma)\delta N \]  

(2.1)

and the position of the left side of the \( n \)–th barrier is given by:

\[ \ell_n = n\delta(1 + \gamma) \quad \text{with} \quad n = 0, \ldots, N. \]  

(2.2)

For the potential barrier, we take \( V(x) = V > 0 \) for \( x \in [\ell_{n-1}, \ell_{n-1} + \gamma \delta], \ n = 1, \ldots, N, \) and 0 for the other positions \( x \). The zero potential regions can be interpreted as electrically conducting regions and the potential barriers as made of a given insulating material. As in Refs. [10, 12, 25], the total length \( L \), and the fraction \( \gamma \) of insulating to conducting material are fixed, while the number of barriers \( N \) can be varied to represent more or less finely structured media. Therefore, the width of the conducting regions is given by

\[ \delta \equiv \delta_N = \frac{1}{1 + \gamma N} \frac{L}{N}. \]  

(2.3)

Like \( \delta_N \), most of the quantities introduced in this paper depend on \( N \), but for sake of notation simplicity we omit to explicitly note it where there is no risk of confusion.
In Ref. [10], it was found that a single barrier of height

\[ E_0 = \frac{\gamma}{1 + \gamma} V \]  

leads to the same asymptotic transmission coefficient of the Kronig–Penney model in the \( \gamma, L - \text{continuum limit} \), namely, when all the parameters of the model are kept fixed but the number of barriers \( N \) which tends to infinity. The potential \( E_0 \), which was there called zero point energy in Ref. [10], will be used also here to discriminate various transport regimes.

We now write the stationary Schrödinger equation in units such that the constant \( \hbar^2 / 2m \) (\( m \) the mass of the electron) equals 1, denoting by a prime the space derivatives:

\[ -\psi''(x) + V(x)\psi(x) = E\psi(x) \quad . \]  

\[ (2.5) \]

![Figure 2.1: Schematic representation of the finite Kronig–Penney model.](image)

As in Ref. [10], the solution corresponding to positive energy, \( E > 0 \), can be written as

\[ \psi(x) = \begin{cases} 
C_1e^{ikx} + D_1e^{-ikx} & x \leq 0 \\
A_ne^{zx} + B_ne^{-zx} & \ell_{n-1} < x < \ell_{n-1} + \gamma\delta \\
C_{n+1}e^{ikx} + D_{n+1}e^{-ikx} & \ell_{n-1} + \gamma\delta \leq x \leq \ell_n \\
C_N+1e^{ikx} + D_N+1e^{-ikx} & x > \ell_N
\end{cases} \]  

where \( n = 1, \ldots, N \), \( k = \sqrt{E} \), and \( z = \sqrt{V - E} \). The boundary conditions provide the real constants \( C_1 \) and \( D_{N+1} \), below simply denoted by \( C \) and \( D \) respectively. The remaining coefficients \( C_n \) and \( D_n \), that respectively represent the amplitudes of the waves entering and being reflected from the left boundary of the \( n \)-th barrier, are then computed in terms of \( C \) and \( D \), imposing the continuity of both the wave function and its first derivative.

As in [10], we introduce the notation

\[ \Delta(a) = \begin{pmatrix} e^a & 0 \\ 0 & e^{-a} \end{pmatrix}, \quad \forall a \in \mathbb{C} \]  

\[ (2.7) \]
and we observe that
\[ \Delta(a)^{-1} = \Delta(-a), \quad \Delta(a)\Delta(b) = \Delta(a + b), \quad \Delta(0) = I, \quad \det(\Delta(a)) = 1, \quad \forall a, b \in \mathbb{C} \quad (2.8) \]
where \( I \) denotes the identity. Moreover, we set
\[ T(a, b) = \begin{pmatrix} e^{ab} & e^{-ab} \\ ae^{ab} & -ae^{-ab} \end{pmatrix}, \quad \forall a, b \in \mathbb{C} \quad (2.9) \]
and we remark that for any \( a, b, c \in \mathbb{C} \)
\[ T(a, b) = T(a, 0)\Delta(ab), \quad T(a, b + c) = T(a, b)\Delta(ac), \quad \det(T(a, b)) = -2a, \quad (2.10) \]
and
\[ T(a, 0)^{-1} = T(1/a, 0)^{\dagger}/2 \quad (2.11) \]
where \( ^{\dagger} \) denotes matrix transposition.

With such notation, the continuity of the wave function and its first derivative at the points \( \ell_n \) and \( \ell_n + \gamma \delta \) can be written as
\[ T(ik, \ell_n) \begin{pmatrix} C_{n+1} \\ D_{n+1} \end{pmatrix} = T(z, \ell_n) \begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix} \]
and
\[ T(z, \ell_n + \delta \gamma) \begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix} = T(ik, \ell_n + \delta \gamma) \begin{pmatrix} C_{n+2} \\ D_{n+2} \end{pmatrix} \]
for \( n = 0, 1, \ldots, N - 1 \). Equivalently, using (2.8) and (2.10), we have
\[ \begin{pmatrix} C_{n+1} \\ D_{n+1} \end{pmatrix} = \Delta(-ik\ell_n)T(ik, 0)^{-1}T(z, 0)\Delta(z\ell_n) \begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix} \]
and
\[ \begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix} = \Delta(-z\delta \gamma)\Delta(-z\ell_n)T(z, 0)^{-1}T(ik, 0)\Delta(ik\ell_n)\Delta(ik\delta \gamma) \begin{pmatrix} C_{n+2} \\ D_{n+2} \end{pmatrix}. \]
Furthermore, \( \Delta(-z\delta \gamma) \) commutes with \( \Delta(-z\ell_n) \), hence one can write:
\[ \begin{pmatrix} C_{n+1} \\ D_{n+1} \end{pmatrix} = \Delta(-ik(\ell_n - \delta))M\Delta(ik(\ell_{n+1} - \delta)) \begin{pmatrix} C_{n+2} \\ D_{n+2} \end{pmatrix} \quad (2.12) \]
for \( n = 0, \ldots, N - 1 \), where
\[ M = \Delta(-ik\delta)T(ik, 0)^{-1}T(z, 0)\Delta(-z\delta \gamma)T(z, 0)^{-1}T(ik, 0). \quad (2.13) \]
Iterating (2.12) it is possible to relate $C_1$ and $D_1$ to $C_{n+1}$ and $D_{n+1}$, as follows:

$$
\begin{pmatrix}
C \\
D_1
\end{pmatrix} = \Delta(ik\delta)M^n\Delta(ik(\ell_n - \delta))
\begin{pmatrix}
C_{n+1} \\
D_{n+1}
\end{pmatrix}
$$

(2.14)

for $n = 2, \ldots, N - 1$. Then, using (2.13), the entries of the $2 \times 2$ matrix $M$ are found to be:

$$
\begin{align*}
M_{11} &= \cos(k\delta) \cosh(z\gamma\delta) + \frac{z^2 - k^2}{2kz} \sin(k\delta) \sinh(z\gamma\delta) \\
&\quad + i\left(-\sin(k\delta) \cosh(z\gamma\delta) + \frac{z^2 - k^2}{2kz} \cos(k\delta) \sinh(z\gamma\delta)\right) \\
M_{12} &= \frac{V}{2kz} \sin(k\delta) \sinh(z\gamma\delta) + i\frac{V}{2kz} \cos(k\delta) \sinh(z\gamma\delta) \\
M_{22} &= M_{11}^* \\
M_{21} &= M_{12}^*,
\end{align*}
$$

(2.15)

where $*$ denotes complex conjugation, and the number $z$ is either real or purely imaginary. It is simple to verify that $\det(M) = 1$.

![Figure 2.2: Profile of the mean density $\phi_n$ for $C = 1$, $D = 0$, $N = 50$, $\gamma = 1$, $L = 10$, and $V = 1$. The different plots refer to the values of energy $E = 0.1 < E_0$ (squares), $E = 0.5 = E_0$ (circles), $E = 0.7 > E_0$ (triangles), and $E = 10.0 \gg E_0$ (diamonds).](image)

We now compute the square modulus of the wave function at the points $\ell_n - \delta/2$:

$$
|\psi_n|^2 := |\psi(\ell_n - \delta/2)|^2 = |C_{n+1}|^2 + |D_{n+1}|^2 + C_{n+1}D_{n+1}^*e^{2ik(\ell_n - \delta/2)} + C_{n+1}^*D_{n+1}e^{-2ik(\ell_n - \delta/2)}
$$

(2.16)

for $n = 0, \ldots, N$. For $n \geq 1$, this quantity is the square modulus of the wave function at the center of the conducting regions $[\ell_{n-1} + \gamma\delta, \ell_n]$. Then, each potential barrier can be
The quantity $\chi_n$ is due to the interference within a conducting region of waves coming from two consecutive barriers. The mean density $\phi_n$ and the interference term $\chi_n$ profiles can be expressed as illustrated in the Appendix A. Since the resulting expressions are rather complex and analytically implicit, we plot the $\phi_n$ profile in Fig. 2.2 as a function of $n$ and the interference term $\chi_n$ in Fig. 2.3 as a function of the energy $E$. Unless otherwise stated, we consider models with $C$ a real positive constant and with $D = 0$, i.e., cases with particles input only at the left boundary of the system of interest. As one may have expected, very large values of $E$ compared to $E_0$, imply that the profile is only little affected by the material inhomogeneity. In particular, it is approximately uniform in space, with $\phi_n$ approximatively constant, indicating that the transport of particles is essentially ballistic, since particles move almost exclusively in the left–to–right direction. Nevertheless, the variety of behaviours shown by Figs. 2.2 and 2.3 indicates that the dependence of our results on the various parameters of the quantum model is rather complex.

In our units the quantum current is defined by $-i/2(\psi^*\psi' - \psi^*\psi')$ [22, equation (3.84)]. Between the consecutive barriers $n$ and $n + 1$, it takes the value $k(|C_{n+1}|^2 - |D_{n+1}|^2)$ which in a stationarity state is uniform in $n$. Because also the plane wave is constant along the
Figure 2.4: The equivalence between the open quantum multi–barrier system (top) and the boundary driven ZRP with independent random walkers (bottom) is obtained choosing the hopping probabilities $p_n, q_n$ and the injection rates $\alpha, \beta$ of the stochastic particle model according to Eqs. (3.32) and (3.34).

multi–barrier system, hence the wave vector $k$ is, the uniformity of the current is expressed by:

$$|C|^2 - |D_1|^2 = |C_2|^2 - |D_2|^2 = \cdots = |C_{N+1}|^2 - |D|^2 \equiv c ,$$

so that $kc$ is the quantum current. Using (2.14) with $n = N$ one can express $C_{N+1}$ in terms of $C$ and the current can be written as:

$$kc = \frac{k}{|(MN)_{11}|^2} [ |C|^2 - |D|^2 - ((MN)_{12}C^*De^{-ik(L-2\delta)} + (MN)^*_{12}CD^*e^{ik(L-2\delta)})] .$$

Finally, taking $D = 0$, it is natural to define the transmission coefficient as:

$$S = \frac{|C_{N+1}|^2}{|C|^2},$$

which is proportional to the current.

3. Boundary driven heterogeneous Zero Range Process

In this section, we show how the parameters of the quantum model illustrated in Section 2 can be tuned so that the stationary $\phi_n$ profile coincides with the stationary density profile.
of a Zero Range Process (ZRP) [4–6, 15, 19, 20] on a 1D lattice. As we shall see at the end of Section 4, the recipe that we give here also works for a disordered system, although such a case is not easily treatable in analytical terms. The ZRP considered hereafter consists of independent random walkers that jump to nearest neighboring sites with site–dependent hopping probabilities. The lattice is coupled, at its horizontal boundaries, to two external (infinite) particle reservoirs characterized by fixed injection rates, cf. Fig. 2.

More precisely, let us denote by \( \Lambda = \{1, \ldots, N\} \) a lattice with \( N \geq 1 \) sites, and let the corresponding finite state or configuration space be denoted by \( \Omega_N = \mathbb{N}^\Lambda \), which consists of the configurations \( \eta = (\eta_1, \ldots, \eta_N) \), where the non–negative integer \( \eta_n \) represents the number of particles at site \( n \). Given \( \eta \in \Omega_N \) such that \( \eta_n > 0 \) for some \( n = 1, \ldots, N \), we let \( \eta^{n,n\pm 1} \) be the configuration obtained by moving a particle from the site \( n \) to the site \( n \pm 1 \). We understand \( \eta^{1,0} \) and \( \eta^{N,N+1} \) to be the configurations obtained by removing a particle, respectively, from the sites 1 and \( N \). Similarly, \( \eta^{0,1} \) and \( \eta^{N+1,N} \) denote the configurations obtained by adding a particle to the sites 1 and \( N \), respectively. The intensity function is chosen to be \( u(k) = k \), for \( k \in \mathbb{N} \), so that the ZRP is equivalent to a superposition of independent random walkers.

Let \( p_n, q_n > 0 \), with \( q_n = 1 - p_n \) denote the hopping probabilities on \( \Lambda \), and let \( \alpha, \beta > 0 \) be the injection rates from the left and the right reservoirs, respectively. The ZRP is then defined as the continuous time Markov jump process \( \eta(t) \in \Omega_N, t \geq 0 \), with rates

\[
\begin{align*}
  r(\eta, \eta^{0,1}) &= \alpha \quad \text{and} \quad r(\eta, \eta^{N+1,N}) = \beta \\
  r(\eta, \eta^{n,n-1}) &= q_n u(\eta_n) \quad \text{for } n = 1, \ldots, N \quad (3.24) \\
  r(\eta, \eta^{n,n+1}) &= p_n u(\eta_n) \quad \text{for } n = 1, \ldots, N \quad (3.25)
\end{align*}
\]

for particles injection at the boundaries,

\[
(L_N f)(n) = \alpha (f(\eta^{0,1}) - f(\eta)) + \beta (f(\eta^{N+1,N}) - f(\eta)) + \sum_{n=1}^{N} [q_n u(\eta_n)(f(\eta^{n,n-1}) - f(\eta)) + p_n u(\eta_n)(f(\eta^{n,n+1}) - f(\eta))]
\]

for any real function \( f \) on \( \Omega_N \). This means that particles hop on the lattice to the neighboring sites to the left and to the right with rates, respectively, \( q_n u(\eta_n) \) and \( p_n u(\eta_n) \). The system
is “open” in the sense that a particle hopping from the site 1 or \( N \) can leave the system via, respectively, a left or a right jump, with rates \( q_1 u(\eta_n) \) and \( p_N u(\eta_N) \). Finally, particles are injected in the system at the left and right boundaries with rates, respectively, \( \alpha \) and \( \beta \).

The stationary measure for this process [15] is the product measure on the space \( \Omega_N \)

\[
\mu_N(\eta) = \prod_{n=1}^{N} \nu_n(\eta_n) \quad \text{with} \quad \nu_n(\eta_n) = e^{-z_n \frac{\eta_n}{\eta_n!}}
\] (3.27)

where the real numbers \( z_1, \ldots, z_N \), called fugacities, satisfy the equations [15,20]

\[
\begin{align*}
z_1 &= \alpha + q_2 z_2 \\
z_n &= p_{n-1} z_{n-1} + q_{n+1} z_{n+1} \quad \text{for} \quad n = 2, \ldots, N-1 \\
z_N &= p_{N-1} z_{N-1} + \beta
\end{align*}
\] (3.28)

which, recalling that \( p_n + q_n = 1 \) for any \( n \), can be rewritten as

\[
\alpha - q_1 z_1 = p_1 z_1 - q_2 z_2 = \cdots = p_n z_n - q_{n+1} z_{n+1} = \cdots = p_{N-1} z_{N-1} - q_N z_N = p_N z_N - \beta \quad (3.29)
\]

The main quantities of interest, in our study, are the stationary occupation number profiles

\[
\rho_n = \mathbb{E}_{\mu_N}[\eta_n] = e^{-z_n} \sum_{k=0}^{\infty} k \frac{z_n^k}{k!} = z_n
\] (3.30)

where \( \mathbb{E}_{\mu_N} \) denotes the mean computed with respect to the measure \( \mu_N \), and the stationary current

\[
J_n = \mathbb{E}_{\mu_N}[u(\eta_n)p_n - u(\eta_{n+1})q_{n+1}] = \mathbb{E}_{\mu_N}[\eta_n p_n - \eta_{n+1} q_{n+1}] = p_n z_n - q_{n+1} z_{n+1}
\] (3.31)

for \( n = 1, \ldots, N \). The stationary current represents the difference between the average number of particles crossing a bond between two adjacent sites on the lattice from the left to the right and the corresponding number hopping in the opposite direction. From (3.28) it easily follows that the stationary current does not depend on the site \( n \), as required for stationary states, therefore we shall simply write \( J \equiv J_n = p_N z_N - \beta \).

The equivalence of the stationary profiles of the stochastic ZRP and of the quantum Kronig–Penney model is now obtained tuning the parameters as follows. First, introduce

\[
I_n = |C_{n+1}|^2 + S_{n+1} + |D_n|^2 + S_n, \quad n = 1, \ldots, N
\] (3.32)

with \( S_n \) defined by Eq. (2.19). Then, in order to match the density profiles of the quantum process with those of the ZRP, when the parameters of the quantum process are given, we take

\[
p_n = \frac{|C_{n+1}|^2 + S_{n+1}}{I_n} \quad \text{and} \quad q_n = \frac{|D_n|^2 + S_n}{I_n}, \quad n = 1, \ldots, N
\] (3.33)
as hopping probabilities, and

\[ \alpha = |C|^2 + S_1 \quad \text{and} \quad \beta = |D|^2 + S_{N+1}, \tag{3.34} \]

as the left and right injection rates of the ZRP. The idea underlying this identification is that \(|\psi_n|^2\), namely the square modulus of the wave function evaluated at the center of the conducting region on the right of the \(n\)-th barrier (i.e. at \(\ell_n - \delta/2\)) yields two contributions: one, corresponding to \(|C_{n+1}|^2 + S_{n+1}\), associated with the average rate of the right jump of a particle from the \(n\)-th site and another, given by \(|D_{n+1}|^2 + S_{n+1}\), associated with the average rate of the left jump from the \((n+1)\)-th site. It is important to note that, the rules \((3.33)\) and \((3.34)\) give non-negative hopping probabilities that sum to 1 when \(|C_n|^2 + S_n > 0\) and \(|D_n|^2 + S_n > 0\) for all \(n = 0, 1, \ldots, N + 1\). As explained in the Appendix \(A\), this is the case...
in the $\gamma, L$-continuum limit \[10\] with $D = 0$, namely, for $N$ large enough when all the other parameters are kept fixed.

The values of the hopping probabilities $p_n$ for several different values of the energy are plotted in Fig. 3.5. Note that in the various panels the thick black dashed lines indicate the behavior of the probability in the $\gamma, L$-continuum limit considered in the Appendix A, see Eq. (A.40).

The top left panel of this figure shows that, for $E < E_0$, such probabilities are practically constant and smaller than $1/2$ in most of the space. As the energy grows, the hopping probabilities develop oscillations till they settle about the value 1.

Equations (3.33) and (3.34) imply

\[
\alpha - I_n q_n = |C|^2 - |D|^2, \quad I_N p_N - \beta = |C_{N+1}|^2 - |D|^2
\]

(3.35)

and

\[
p_n I_n - q_{n+1} I_{n+1} = |C_{n+1}|^2 - |D_{n+1}|^2
\]

(3.36)

for $n = 1, \ldots, N - 1$. Using the conservation of the quantum current, Eq. (2.20), in Eqs. (3.35) and (3.36), and by comparing with Eq. (3.29), one thus obtains $z_n = I_n$ for $n = 1, \ldots, N$, and the equivalence between the quantum current and the current (3.31) of the stochastic model is established. Moreover, since Eq. (2.20) yields $|C_n|^2 + |D_{n+1}|^2 = |C_{n+1}|^2 + |D_n|^2$, one realizes that equations (2.17) and (3.30) imply $\phi_n = \rho_n$ for every $n$, which is the equivalence of the quantum mean density profile and the stationary occupation profile of the stochastic particle system.

We conclude this section recalling that, as also noted at the end of Section 2, the quantum current (2.20) reduces to the transmission coefficient in (2.22), when $D = 0$ and $C = 1$. Thus, the recipe given in Section 3 allows us to interpret the transport properties of the quantum model in terms of the stationary current of a boundary driven random walk on a 1D lattice \[15\].

4. Discussion of profiles in stationary states

In this section we compare the exact expression (2.17) of $\phi_n$ and $\rho_n$ with the profile obtained from Monte Carlo simulations of the ZRP model. We also compare the current $J$ of the stochastic process, obtained from Monte Carlo simulations, with the $c$ of (2.20), that is the quantum current divided by $k$. To do that, we take the parameters values prescribed by equations (3.33) and (3.34). We further take $C = 5$, $D = 0$, $N = 50$, $\gamma = 1$, $L = 10$, and $V = 1$, which yields $E_0 = 0.5$, cf. (2.4). Because $D = 0$, given an energy $E > 0$, $N$ must be correspondingly large, cf. comment below (3.34) and the Appendix A.
Figure 4.6: **Left panel:** Profile of particles density $\phi_n$ of the quantum multi–barrier system given by (2.17) (dashed line), and occupation number profile of the ZRP process, with hopping probabilities (3.33), obtained via MC simulations, by measuring the stationary site occupation (open circles) as well as the ratio of the stationary hopping rate to the left to the corresponding hopping probability $q_n$ (filled squares), for $C = 5, D = 0, N = 50, \gamma = 1, L = 10, V = 1, E = 0.1$. **Right panel:** MC measure of the current in the ZRP model as a function of time $t$ (empty circles) compared to the theoretical value of the quantum transmission coefficient multiplied by $|C|^2$, see Eqs. (2.21) and (2.22) (dashed line).

The numerical simulations are performed as follows: the process starts with zero particles, but the injection of particles at the left boundary quickly makes the lattice populated. After a sufficiently large time, the particles distribution reaches a stationary state. At stationarity, the occupation number profile is measured with two different methods, that are mathematically equivalent, but numerically independent: i) the number of particles at each site is averaged collecting its values at time intervals larger than the decorrelation time, that is of the order of the number $N$ of sites; ii) the total number of particles jumping from a generic site $n$ to the left is computed and, at the end of the simulation, is divided by the total time, that is given by the sum of exponentially distributed time intervals between two consecutive jumps, and by the probability $q_n$ to perform the left jump. Using (3.31) also this ratio should yield $z_n = \rho_n$.

The match between these two independent calculations demonstrates the good accuracy of our numerical simulations, which is important, since in the sequel we shall discuss the disordered case, for which no analytical results are currently available.

We shall now distinguish the regimes with energy $E < E_0$, and cases with energy $E > E_0$, as suggested in [10, Remark 4.4]. In our study $E_0 = 1/2$.

Case $E = 0.1 < E_0$, **monotonic decay:** The top left panel of Fig. 2.3 shows that the
Figure 4.7: As in Fig. 4.6 for $E = 0.5$.

Figure 4.8: As in Fig. 4.6 for $E = 0.7$.

Figure 4.9: As in Fig. 4.6 for $E = 10$. 
Figure 4.10: Profile of $\phi_n$ for a single realization of the quantum disordered multi–barrier system given by (2.17) (dashed line), and occupation number profile of the ZRP process with hopping probabilities (3.33) obtained via MC simulations, by measuring the stationary site occupation (open circles) as well as the ratio of the stationary hopping rate to the left to the corresponding hopping probability $q_n$ (filled squares), for $C = 5$, $D = 0$, $N = 50$, $\gamma = 1$, $L = 10$, $V = 1$ and with different values of energy: $E = 0.1$ (top left panel), $E = 0.5$ (top right panel), $E = 0.7$ (bottom left panel) and $E = 10$ (bottom right panel).

$p_n$ is constant in most of the system positions, and smaller than $1/2$. At the right end of the system a sudden increase takes place. The occupation number profile is, instead, monotonically decreasing, see Fig. 4.6, and convex.

Case $E = E_0 = 0.5$, transition behavior: The $p_n$ profile in this case is shown in the top right panel of Fig. 2.3, and it turns out to be monotonically increasing. The occupation number profile, plotted in Fig. 4.7, is monotonically decreasing, but the total mass on the lattice is larger with respect to the previous case. This can be ascribed to the fact that in that case the injection rate $\alpha$ from the left reservoir has increased with respect to the case with $E = 0.1$. 
Case $E = 0.7 > E_0$, oscillatory behavior: The probability profile $p_n$ is shown in the bottom left panel of Fig. 2.3 and it is an oscillatory function. As a consequence, the occupation number profile shown in in Fig. 4.8 is also an oscillating function.

Case $E = 10 \gg E_0$, ballistic behavior: The transition probability profile $p_n$ is shown in the bottom panel of Fig. 2.3 and it is very close to 1. Therefore, the stochastic model is made of particles undergoing a strongly asymmetric random walk on the lattice. Fig. 4.9 shows the occupation number profile which is, indeed, almost uniform.

Finally, we investigate numerically the equivalence between a disordered version of the Kronig–Penney model introduced in [21] and a boundary driven ZRP with random hopping probabilities, cf. e.g. [16, 17]. The quantum disordered model is constructed by drawing, first, the random variables $\lambda_n, \delta_n$ from a uniform distribution, and then by rescaling them, in order to fulfill the two constraints

$$\sum_{n=1}^{N} (\lambda_n - \gamma \delta_n) = 0 \quad \text{and} \quad \sum_{n=1}^{N} (\lambda_n + \delta_n) = L$$

with $\gamma, L$ fixed. Remarkably, the correspondence method developed in Section 3 still holds here, as long as the parameters $p_n$ and $q_n$ defined by Eq. (3.33) are positive and smaller than one. This result is established via numerical simulations; in fact we can not guarantee it in the random case, since the corresponding product of random matrices does not lead to an expression like (A.39).

The results of the MC simulations are reported for a single realization of the disordered quantum system in Fig. 4.10, which shows a striking equivalence between the quantum and the stochastic processes here investigated. The black dashed line displayed in the various panels of Fig. 4.10 corresponds to the exact quantum profile $\phi_n$ in Eq. (2.17), obtained by using the transfer matrix formalism discussed in Section 2, whereas the filled and empty symbols denote the results of the MC simulations based on the two alternative methods outlined before.

Lastly, we tested the connection between the regular quantum model and the quenched average of its disordered versions, constructed by drawing the random barrier widths under the constraints given in (4.37). To this aim, we considered a set of $10^2$ disordered realizations of the multi–barrier system with positive $p_n$ and $q_n$, cf. (3.33). In particular, we numerically computed both the quenched average of $\phi_n$, coming from a straight implementation of the transfer matrix technique, and the quenched average of $\rho_n$, obtained via MC simulations by averaging over the stationary occupation profiles of the ZRP. Results for the quenched averages, for different values of $E$ and $N$, are displayed in Fig. 4.11. As expected, the quenched average of $\rho_n$ perfectly agrees with the quenched average of $\phi_n$ for all the considered energies and numbers of barriers. We further observe that the quenched disordered averages
Figure 4.11: Profile of $\phi_n$ (2.17) for the regular Kronig–Penney model (solid line), numerical quenched average of $\phi_n$ for the quantum disordered multi–barrier system (black symbols), numerical quenched average of $\rho_n$ (3.30) for the ZRP model (open symbols). The quenched average has been taken over $10^2$ random realizations of the multi–barrier system such that the parameters $p_n$ and $q_n$ are in the interval $(0, 1)$, to let the ZRP model be well defined. The values of the parameters are $C = 5$, $D = 0$, $\gamma = 1$, $L = 10$, $V = 1$, for energies $E = 0.1$ (squares), $E = 0.5$ (circles), $E = 0.7$ (triangles), and $E = 10$ (diamonds). Shown are the cases with $N = 50$ (left panel), $N = 200$ (central panel) and $N = 1000$ (right panel).

and the behavior of the regular Kronig–Penney models also converge to each other for growing $N$. This reinforces the results of Refs. [11,12,25], showing convergence with growing $N$ of the transmission coefficients of the random systems to the regular case values.

The correspondence highlighted in Figs. 4.10 and 4.11 can be used to investigate, or to interpret, some of the peculiar properties of the random Kronig–Penney model [14] with the techniques developed in the study of the ZRP, and viceversa. In particular, the disordered version of the quantum multi–barrier model, with the random variables $\lambda_n$, $\gamma_n$ scaled as in Eq. (4.37), can be studied as an instance of a random walk in a random environment (with site randomness), for which a rich theory has been developed [23,24,26,27]. On the other hand, phenomena such as Sinai’s localization [3], which is observed in random walks in random environments, can be investigated in terms of our random Kronig–Penney model.

5. Conclusions
In this paper we have shown that the quantum multi–barrier finite Kronig–Penney model and the ZRP are equivalent if the hopping probabilities of the stochastic process are properly tuned with the the parameters of the quantum system. In particular, we have evidenced that, for the finite Kronig–Penney model with unitary input only from the left boundary, the transmission coefficient corresponds to the stationary current in a boundary driven heterogeneous ZRP [15], realized by independent particles performing a random walk on a lattice with site–dependent hopping probabilities.
If \( p_n \) and \( q_n \) are taken as prescribed by equation (3.33) and \( \alpha \) and \( \beta \) as prescribed by equation (3.34), the stationary profile \( \phi_n \) and the current of the quantum model are correctly recovered from the ZRP, for any value of the energy \( E \).

To see how the choice of parameters is essential, let us drop the dependence of \( p_n \) and \( q_n \) on \( S_n \) and \( S_{n+1} \), in (3.33). In this case, one may still recover the correct value of the stationary current but not the stationary profile for an arbitrary value of the energy.

It is reasonable to expect that our correspondence method produces the equivalence of the two models considered in this paper also in other situations. After all, everything in the ZRP depends on the hopping probabilities and on the boundary conditions, like they depend on the boundary conditions and on the potential barriers in the quantum model. This may allow us to treat rigorously the large \( N \) limit of mesoscopic disordered systems numerically investigated in Refs. \[11,12,25]\, for which no general ergodic–like results seem to have been so far developed.

We have also shown that a random walk in a random environment correctly reproduces the transport properties of the quantum disordered model. Thanks to this equivalence, one concludes for the stochastic process that the stationary profiles may vary from monotonically decreasing to oscillating because of the variation of the energy of an incoming plane wave, of the associated quantum multi–barrier model. When this energy exceeds a critical value, the stationary states turn from monotonically decaying to oscillating.

Finally, we also numerically observed the convergence, for \( N \) large, of the quenched averages of the mean density \( \phi_n \) and the stationary occupation \( \rho_n \), for the disordered multi-barrier systems, to the corresponding value measured with the regular Kronig–Penney model. This implies that the quantum model has no localization for growing \( N \). After all, this is natural in small systems, and reveals the different nature of our large \( N \) limit, compared to the standard hydrodynamic limit.

The equivalence of quantum multi–barrier models and stochastic particle systems now suggests various avenues for future research, such as the investigation of \textit{uphill currents} in the quantum models. These kinds of currents, indeed, have been recently found in interacting particle (or spin) systems on lattices \[1,4,7,9]\.

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\textbf{A. The} \( \gamma, L \)–continuum limit of the hopping probabilities
In this appendix we consider the Kronig–Penney model introduced in the Section 2 in the case $D = 0$ (see the comment below (2.6)). As mentioned below the equation (2.4), see also [10], the $\gamma, L$–continuum limit is realized by keeping fixed all the parameters of the Kronig–Penney model but the number of barriers $N$, which tends to infinity. Recalling the matrix $M$ defined in (2.15), following [10], we let

$$
\Phi = \text{Re}(M_{11}) = \cos(k\delta) \cosh(z\gamma\delta) + \frac{z^2 - k^2}{2kz} \sin(k\delta) \sinh(z\gamma\delta) .
$$

Denoting the eigenvalues of $M$ by $\mu_1$ and $\mu_2 = \mu_1^{-1}$, one finds

$$
\mu_1 = \Phi - \sqrt{\Phi^2 - 1} \quad \text{and} \quad \mu_2 = \Phi + \sqrt{\Phi^2 - 1}
$$

which can be real or complex–valued, depending on the value of $\Phi$. It is important to remark that $\mu_1 \neq \mu_2$, indeed, by expanding $\Phi$ in Taylor series with respect to $\delta$ in a neighborhood of $\delta = 0$, one has

$$
\Phi(\delta) = 1 - \frac{1}{2}L^2(E - E_0)\delta^2 + \frac{1}{24}L^4 \left[ E^2 - 2EE_0 + E_0^2 \gamma(2 + \gamma) \right] \delta^4 + o(\delta^4) ,
$$

which proves that, for $\delta$ small, $\Phi(\delta) < 1$ (resp. $\Phi(\delta) > 1$) for $E > E_0$ (resp. $E < E_0$). Moreover, for $E = E_0$ the above expansion becomes $\Phi(\delta) = 1 - L^4E_0^2\delta^4/[24(1 + \gamma)^2] + o(\delta^4)$ which proves that, for $\delta$ small, $\Phi(\delta) < 1$ even for $E = E_0$.

In the sequel we shall often use the $n$–th power $M^n$ of $M$ for $n = 1, \ldots, N$. By slightly abusing the notation, we shall denote its elements by $M^n_{ij}$. One can use the equation (2.14) to express the coefficients $C_{n+1}$ and $D_{n+1}$ in terms of the boundary condition $C$ (recall that we assumed $D_{N+1} = D = 0$). One first writes (2.14) for $n = N$ and finds $D_1 = CM^N_{21}e^{-ik\delta}/M^n_{11}$, then, using again (2.14) for a general $n$, one gets

$$
C_{n+1} = C \frac{e^{-ik\ell_n}}{M^n_{11}}(M^n_{11}M^n_{22} - M^n_{21}M^n_{12}) \quad \text{and} \quad D_{n+1} = C \frac{e^{ik(\ell_n - 2k)}}{M^n_{11}}(M^n_{21}M^n_{11} - M^n_{11}M^n_{21}) \quad (A.38)
$$

which for $n = N$ reproduce $C_{N+1}$ and $D$, while for $n = 0$ they yield $C$ and $D_1$.

Recalling the definition of hopping probabilities (3.33), we wish to express in terms of the boundary condition $C$ the two quantities $|D_n|^2 + S_n$ and $|C_{n+1}|^2 + S_{n+1}$, respectively the average hopping rates to the left and to the right from the $n$–th site of the ZRP model. Using (A.38) we find

$$
\frac{|D_{n+1}|^2 + S_{n+1}}{|C|^2} = \frac{|M^n_{21}M^n_{11} - M^n_{11}M^n_{21}|^2 + \text{Re}[(M^n_{11}M^n_{22} - M^n_{21}M^n_{12})(M^n_{12}M^n_{22} - M^n_{22}M^n_{12})e^{ik\delta}]}{|M^n_{11}|^2}
$$

for $n = 0, \ldots, N - 1$ and

$$
\frac{|C_{n+1}|^2 + S_{n+1}}{|C|^2} = \frac{|M^n_{11}M^n_{22} - M^n_{21}M^n_{12}|^2 + \text{Re}[(M^n_{11}M^n_{22} - M^n_{21}M^n_{12})(M^n_{12}M^n_{22} - M^n_{22}M^n_{12})e^{ik\delta}]}{|M^n_{11}|^2}
$$
for \( n = 1, \ldots, N \).

To compute the \( N \) large limit of the quantities above express the \( n \)-th power of the matrix \( M \) as in [10, Eq. (3.15)]:

\[
M^n = \left( \frac{\mu_1^n - \mu_2^n}{\mu_1 - \mu_2} \right) M - \frac{\mu_2 \mu_1^n - \mu_1 \mu_2^n}{\mu_1 - \mu_2} I ,
\]

where \( I \) is the identity matrix.

Recalling the definition (3.33) of right hopping probability \( p_n \), we let \( x = n/N \in (0,1] \) and, in the limit \( N \to \infty \), we find

\[
p(x) = \begin{cases} 
\frac{1}{2} + \frac{E_0 - E}{E_0(1+\cosh(2L\sqrt{E_0-E}(1-x)))} & E < E_0 \\
\frac{1}{2} + \frac{1}{2+2E_0 L^2(1-x)^2} & E = E_0 \\
\frac{1}{2} + \frac{E-E_0}{2E-E_0(1+\cos(2L\sqrt{E-E_0}(1-x)))} & E > E_0 
\end{cases}
\]

(A.40)

One readily notes that \( p(x) \in [0,1] \), as illustrated in Fig. 3.5 (see, also, the comment at the end of the paragraph below (3.34)).

Finally, the \( \gamma, L \)-continuum limit of the stationary current (3.31), takes the form:

\[
J = \lim_{N \to \infty} \left( |C_{n+1}|^2 - |D_{n+1}|^2 \right) = \begin{cases} 
\frac{8E_0(E-E_0)}{8E_0(E-E_0)+E_0^2(1-\cos(2L\sqrt{E_0-E}))} & E < E_0 \\
\frac{4}{4+2E_0L^2} & E = E_0 \\
\frac{8E_0(E-E_0)}{8E_0(E-E_0)+E_0^2(1-\cos(2L\sqrt{E-E_0}))} & E > E_0 
\end{cases}
\]

(A.41)

For \( C = 1 \), the expression \( \text{(A.41)} \) yields the asymptotic value of the transmission coefficient \( S \) obtained in [10, Eq. (4.3)].

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