Persistent current and Drude weight in one-dimensional rings with substitution potentials

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Abstract
Persistent currents and Drude weights are investigated using the tight-binding approximation to one-dimensional rings threaded by a magnetic flux and with the potential given by some almost-periodic substitution sequences with different degrees of randomness, and for various potential strengths. The Drude weight D distinguishes correctly conductors and insulators, in accordance with the results indicated by the currents. In the case of insulators the decay of $D(N)$ for large ring lengths N provides an estimate for the localization length of the system. It is shown that a more random sequence does not imply reduced conduction. This discrepancy between the hierarchy of disorder of the sequences and the capacity for conduction of the system is explained by the gaps in the energy spectra.

1. Introduction

The ability of quantum mechanical systems to conduct, and their transport properties in general, have been intensively investigated in recent years in connection with the anomalous transport and localization phenomena that they exhibit [1]. The investigation has also been intensive in the mathematical physics field, where one would like to know the spectral and state properties of Schrödinger operators—even one-dimensionally, as will always be the case here—with potentials lying between the hallmarks set by periodic potentials with absolutely continuous spectra and Bloch states at one extreme, and random potentials with pure point spectra and localized states at the other [2]. In between there appear a variety of behaviours which seem to be dictated in great measure by the randomness of the potential. To cite just two properties, it is accepted that the mean square displacement $d(t)$ and the quantum probability of return $C(t)$ for an initial delta-function state are algebraic functions of time ruled by certain exponents, $d(t) \sim t^{2\beta}$ and $C(t) \sim t^{-\alpha}$. These exponents just by themselves reflect how random the potential is: ballistic motion in periodic potentials is characterized by $\beta = \alpha = 1$, localization

in random potentials by $\beta = \alpha = 0$, while anomalous diffusion in non-periodic potentials shows $0 < \alpha, \beta < 1$. On the mathematical side, a considerable amount of effort has been devoted to relating these dynamical exponents to the dimensions of the spectral measure [2]. However, up to now these relations have been very difficult to apply in practical calculations: on the one hand, the information dimension D_1 provides only lower bounds for the exponent β ruling the algebraic decay of the mean square displacement; on the other hand, in the case of the return probability $C(t)$ the associated correlation dimension D_2 is not in general attainable by means of analytical calculations, and its numerical computation is extremely difficult due mainly to the limiting process involved.

In this scenario, one-dimensional non-periodic potentials generated as substitution sequences have emerged as a convenient theoretical 'laboratory', since the sequences are neither completely random nor periodic, even though they are formed by following well defined rules. In addition, they can be classified by their autocorrelation measures, revealing a hierarchy with respect to disorder. These two aspects of the substitution sequences—a sort of correlated disorder—allow us to investigate transport properties, as well as mathematical ones, in a more controlled way. In this way the counter-intuitive result that a more random potential can give rise to better transport properties than a less random one was derived recently [3]. From another point of view, with the recent development of techniques for growing superlattices, one could consider the experimental and technological exploitation of systems characterized by these non-periodic substitution potentials [4].

It therefore seems desirable to have results for concrete physical situations, in order to test theoretical predictions concerning not only disordered systems and localization phenomena, but also the almost-periodic substitution potentials themselves. Towards this end, we investigate here the tight-binding approximation to the problem of mesoscopic rings threaded by a time-independent magnetic flux, and calculate the persistent current and Drude weight in cases where the on-site potential is given by some substitution sequences with different degrees of randomness. The system is described by the Hamiltonian for a one-dimensional ring with spinless fermions:

$$H = -\sum_{k=1}^{N} \left[\exp\left(i\frac{2\pi}{N}\phi \right) c_k^+ c_{k+1} + \exp\left(-i\frac{2\pi}{N}\phi \right) c_{k+1}^+ c_k \right] + \sum_{k=1}^{N} W_k c_k^+ c_k. \quad (1)$$

In this expression N is the number of sites in a ring with lattice spacing equal to one, the magnetic flux ϕ is measured in units of the quantum of flux $\phi_0 = hc/e$, W_k is the potential energy at site k, and the hopping constant is set equal to one. This model is particularly convenient for our purposes for two reasons: first, it admits non-periodic substitution sequences in a simple way; second, the association of the wave vector in the one-dimensional lattice with the parameter ϕ allows us to easily explore the transport properties as functions of the sensitivity of the energy bands to variations in the magnetic flux. In this way the Drude weight, shown by Kohn to be useful for a quantitative characterization of the insulating state [5], and also the persistent current, predicted by Büttiker, Imry, and Landauer [6], can both be calculated as derivatives of the ground-state energy with respect to the flux.

It is evident from the model that we assume non-interacting electrons and zero temperature. Although electron–electron interactions and average effects give important contributions to the transport properties—and to the amplitude of persistent currents, as we briefly recall below and in section 3—with these approximations one can still obtain a quite successful description of the qualitative features of the model [7]. They are justifiable in the present case since we attempt mainly to characterize how the randomness of the potential affects the motion of the particles; in so doing we would like therefore to avoid the contributions from other effects.

The aim of this paper is to report and discuss the results, obtained for Hamiltonian (1), for the persistent current and Drude weight as functions of the degree of randomness of the potential and for various potential strengths. Many related works have been published concerning different aspects of the problem. Persistent currents, Drude weight, and also optical conductivity, in mesoscopic rings, have been investigated predominantly in Hubbard models, where the on-site interaction between particles with spin plays a major role. This was done in a series of papers ending up with criteria for determining whether a state is metallic, insulating, or superconducting [8]. Interaction between spinless particles together with on-site potentials have been considered, mostly with disordered potentials [9–12] but also with the Aubry–André potential [13]. Recently, particles with spin interacting over finite open chains modulated by the almost-periodic Fibonacci potential have been considered as well [14]. The general picture emerging from these works is not yet completely clear and points to a competition between the effects caused by interaction, potential, and charge and spin degrees of freedom; it has been shown, moreover, that the results are sensitive to whether one averages over realizations of the potential [10, 11] or whether one considers individual samples [12]. As regards solely the effects of the potential, however, the ring with non-periodic substitution potentials has been much less fully considered; the Fibonacci potential was treated by Jin *et al* [15]. The properties of systems with substitution potentials have been otherwise intensively studied in open chains, although mainly in the cases of Fibonacci, Thue–Morse, and Rudin–Shapiro sequences [16].

The Fibonacci potential is by far the most thoroughly studied among these substitution potentials. It is generally considered to be the most ordered one either in the sense of its autocorrelation measure—a pure point, as for periodic potentials—or in the sense of its dynamical exponents [3]. In this paper, however, Fibonacci potentials will be absent, since we would like to compare the results obtained for the different potentials in half- and quarter-filled rings; recall that the lengths of the potential sequences in that case are given by the Fibonacci numbers.

In what follows, section 2 presents the definitions and some properties of the potentials given by the Thue–Morse, Rudin–Shapiro, paper-folding, and period-doubling sequences. In section 3.1 persistent currents are calculated for the various potentials (with different amplitudes) as functions of the magnetic flux. A more quantitative characterization of the conducting properties for the various systems is presented in section 3.2, where the Drude weight is calculated and where some attempt is made to fit its behaviour as a function of the length of the ring. Also, in section 3.3 the cases indicated by the Drude weight to be insulators are analysed in terms of the gaps in the energy spectra. Section 4 finishes the article with a discussion of the results obtained.

2. Non-periodic substitution potentials

In the following sections, Hamiltonian (1) will be considered with on-site potential energies W_k given by some sequences which in turn are constructed using well defined substitution rules. We will be interested mainly in almost-periodic sequences which are convenient in the context of disordered systems because we have not only non-periodicity but also non-perfect correlation [17].

The sequences that we will use are constructed using an alphabet of two letters $\{a, b\}$ and a specific substitution rule for each sequence:

$$a \rightarrow ab \quad b \rightarrow ba \qquad \text{Thue–Morse (TM)}$$
$$a \rightarrow ab \quad b \rightarrow aa \qquad \text{period doubling (PD)}.$$

Starting with one of the letters and applying successively the substitution rules, we generate

almost-periodic sequences—for example, the PD sequence

$$abaaababababaaabaa \cdots.$$

The Rudin–Shapiro (RS) and paper-folding (PF) cases are worked out using an alphabet of four letters $\{a', b', c', d'\}$, with the rules

$$a' \to a'b' \quad b' \to a'c' \quad c' \to d'b' \quad d' \to d'c' \qquad \text{Rudin–Shapiro (RS)}$$
$$a' \to a'b' \quad b' \to c'b' \quad c' \to a'd' \quad d' \to c'd' \qquad \text{paper folding (PF)}$$

and the identifications $a', b' \to a$ and $c', d' \to b$ in both cases. The first elements of the sequence RS are

$$aaabaabaaaabbb \cdots.$$

At each step these sequences have length $N = 2^m$ at the mth iteration. We then define the potential on site k, taking $W_k = 0$ if the kth letter in the sequence is a, and $W_k = \lambda$ in the case where it is b; in such a way the strength λ of a given potential can also be varied.

These non-periodic sequences have a classification with respect to their degree of randomness, which is based on their autocorrelation measure [17]. As is the case for periodic sequences, PF and PD sequences have pure point autocorrelation measures; while RS sequences have absolutely continuous autocorrelation measures, as independent random sequences do. The TM case lies in an intermediate position, since it has a singular continuous autocorrelation measure. One would expect the differences in degree of randomness of the potentials to produce different spectral types for the energy levels, and in this way explain the variation in how difficult it is for the particles to move. In other words, one would expect more random potentials to lead to more limited transport properties. The point is that all the rigorously studied cases produce singular continuous spectra [18] (the RS and PF cases being open problems [19]); yet their dynamical properties are very different and, so it seems, do not respect the hierarchy of disorder indicated by the autocorrelation measures [3]. In order to obtain a clearer picture of the situation, we would like to map the role of the potential as a function of its degree of randomness in physical quantities, such as persistent currents and conductivity via the Drude weight.

In what follows, the N eigenvalues E and corresponding eigenfunctions $\psi_E(k)$ are obtained for Hamiltonian (1) using exact diagonalization for ring lengths from $N = 16$ up to $N = 256$. A gauge transformation can eliminate the flux in the Hamiltonian by transforming the usual periodic boundary conditions into $\psi_E(k + N) = e^{i2\pi\phi}\psi_E(k)$. In this way it was shown that the energy bands associated with the lattice vector $q = -2\pi\phi/N$ are periodic functions of the flux ϕ [20]. The effects of the potential on the transport properties are thus seen as the energy bands being flattened out to various extents.

3. Results

3.1. Persistent currents

Since their discovery in 1983, persistent currents have come to constitute an important subject, both theoretically and experimentally, which is still open as regards the amplitudes of the currents. The roles of the various contributions to the amplitudes have proved particularly difficult to treat: electron–electron interactions, disorder of the potential, statistical effects. Many of these issues have been reviewed in reference [21] (see also reference [10]). As predicted by Büttiker, Imry, and Landauer [6], in the presence of a non-vanishing magnetic flux ϕ, even if it is time independent, each energy band $E_n(\phi)$ carries a persistent current

proportional to its derivative with respect to the flux. At zero temperature, the contributions of the M occupied levels below the Fermi energy sum up to

$$I(\phi) = \sum_{n=1}^{M} \frac{\partial E_n}{\partial \phi}. \tag{2}$$

Figure 1 shows typical curves for the currents for half- and quarter-filled rings with the various substitution potentials at strength $\lambda = 0.2$. One can note that the order of increasing amplitudes is preserved along the entire flux axis; consequently, in order to estimate a sequence of increasing currents with respect to the potential disorder, we plot in figure 2 the mean currents
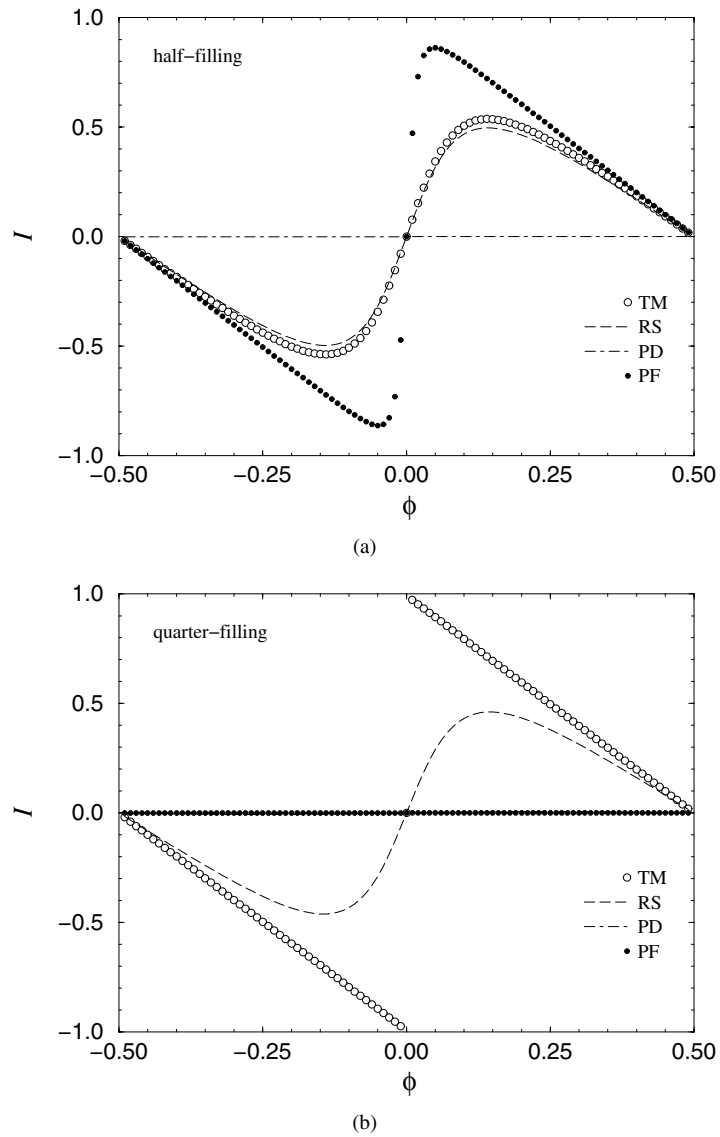

(a)

(b)

Figure 1. Persistent currents for the various substitution potentials at strength $\lambda = 0.2$ and ring length $N = 256$: (a) half-filling; (b) quarter-filling.
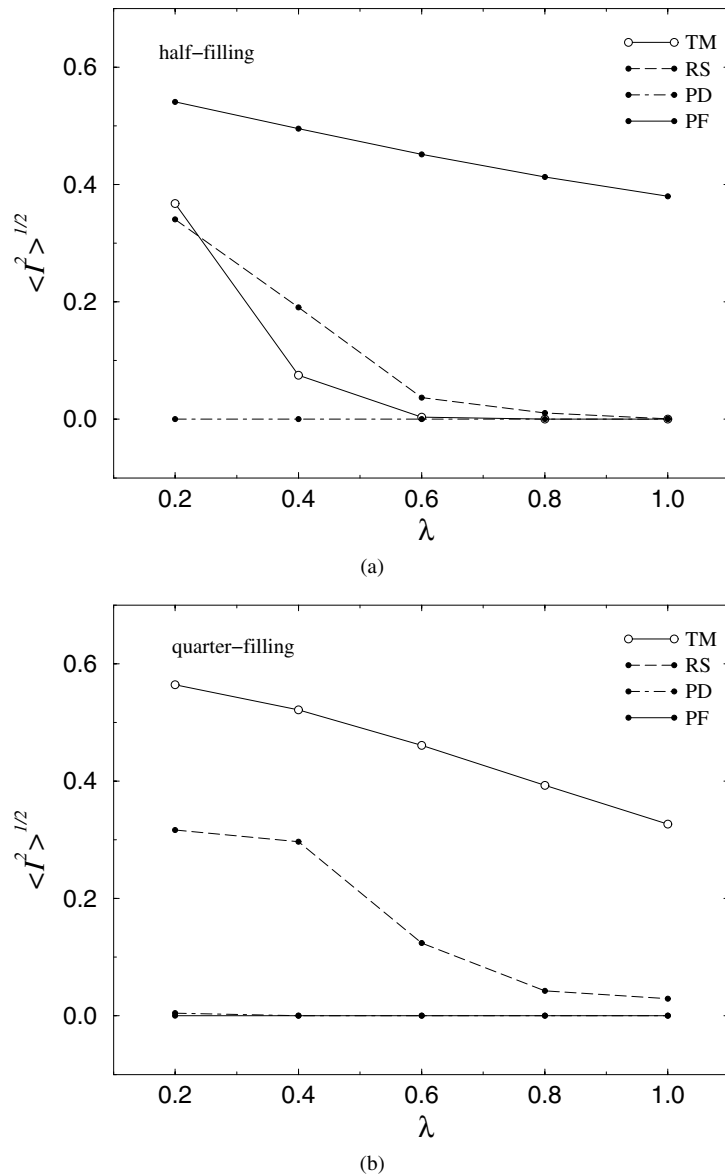
Figure 2. Mean current amplitudes as functions of the potential strength: (a) half-filling; (b) quarter-filling.

$\langle I^2 \rangle^{1/2}$, averaged over the flux period, for the interval of potential strength $0.2 \leqslant \lambda \leqslant 1.0$. In these figures the unit of current is the maximum amplitude obtained for a null potential.

It is interesting to note that this hierarchy of amplitudes does not follow the order that would be expected if one was guided solely by a measure of the potential disorder. On the basis of the results given by the autocorrelation measure, one could predict the sequence (PD, PF)/TM/RS for the decreasing current amplitudes carried by the different potentials. However, we see that the results obtained for half-filling suggest otherwise: PF/RS/TM/PD; while for quarter-filling, the results indicate TM/RS/(PF, PD).

3.2. Drude weight

In order to give a more quantitative description of the above observations, we calculate in what follows the Drude weight for the various situations. As prescribed originally by Kohn [5], this quantity—useful in the characterization of conducting properties, as we will see bellow—can be obtained as the second derivative of the ground-state energy level with respect to the lattice vector $q = -2\pi\phi/N$, which in our case reduces to

$$D = N \sum_{n=1}^{M} \frac{\partial^2 E_n}{\partial \phi^2}\bigg|_{\phi=\phi_{min}}. \tag{3}$$

This expression is equivalent to that obtained using Kubo linear response formulae [8]. In the first works following Kohn, D was calculated at $\phi = 0$ and it was realized that its signal depends on whether the number of occupied levels M is even or odd. In this way, the diamagnetic responses of various systems were discussed in the literature, as well as the less common paramagnetic one for $M = 4p$ (see the 1991 work by Fye *et al* in reference [8]). However, as was implemented by Bouzerar, Poilblanc, and Montambaux [10] and clearly explained by Giamarchi and Shastry [11], D describes a situation of equilibrium between the charge carriers and should be calculated at the value of ϕ where the ground-state energy has a minimum (ϕ_{min} in the expression above). Due to the characteristic lengths of our sequences, we adopt here the latter point of view and take $M = 4p$ for either half- or quarter-fillings, with $M = N/2$ and $M = N/4$ respectively. In this way $\phi_{min} = 1/2$ in all cases and we avoid different kinds of response, thus comparing all systems in the same situation.

The behaviour of D as a function of N gives a criterion for distinguishing between conductors and insulators [5]. We restrict our remarks to our one-dimensional case. For metallic conductors, D tends to a finite non-zero value as $N \to \infty$; whereas for insulators, D vanishes in that limit. This criterion has a more intuitive interpretation if one realizes that D is inversely proportional to the effective-mass tensor, which in one dimension is simply the second derivative written out above. We present in figure 3 the $D(N)$ results for the sequences considered in section 2. It is seen that the overall aspects of $D(N)$ and its rates of decay in the various situations confirm the conduction ordering suggested by the persistent currents shown in figure 2—that is, PF/RS/TM/PD for half-filling and TM/RS/(PF, PD) for quarter-filling.

It has been proposed in the context of Hubbard models [5, 9, 10] that, in general, insulators show an exponential decay, $D(N) \propto \exp(-N/\xi)$, governed by the localization length ξ. The behaviours here vary from well defined insulator (as, for example, in the PD case) to conductor (as the quarter-filling TM sequence manifests itself), with transitions between these states in some cases. We attempted therefore a more general fit:

$$D(N) = A + BN^\gamma e^{-N/\xi} \tag{4}$$

where the parameters A, B, γ, and ξ passed a χ^2-test, and $D(N)$ is measured in units of the value D_0 attained for each filling in the largest ring with null potential. Some justifications for the fitting procedure are in order here. As regards the sizes of the system, we avoided filling the range between $N = 16$ and $N = 256$ with more points because this would mean taking incomplete sequences, since each iteration in their construction has a definite size (a power of 2). On the other hand, going to greater sizes does not alter the results. As regards the number of fitting parameters, formula (4) was chosen to take into account all possible behaviours, and also to check for meaningless fitting results. We think that this strategy was successful, since there was no situation in which the fitting curve could show dependence on all parameters. In fact, whenever it showed an exponential decay, the free-constant parameter A was absent. The results are detailed in table 1. We see that most of the cases showed no dependence on parameter A, except for the PF half-filling case for which $D = A + BN^\gamma$, with the exponent
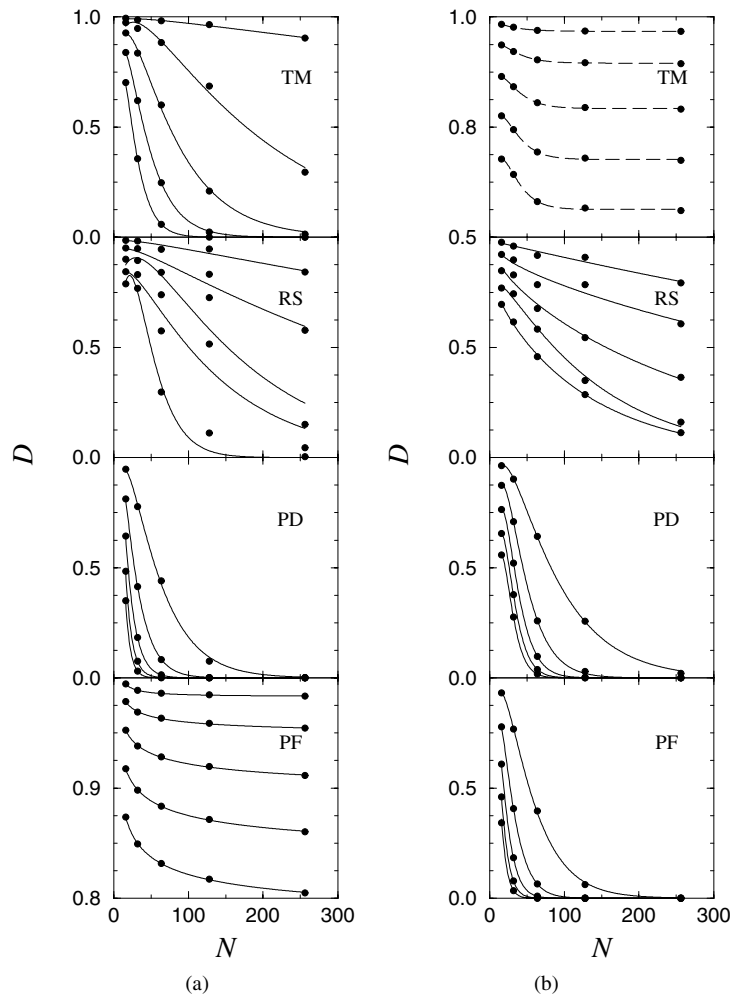
Figure 3. Drude weight as a function of the number of sites in the ring (filled circles): (a) half-filling; (b) quarter-filling. Fitting curves are shown as solid lines.

γ varying from -0.29 to -0.95. In this situation, therefore, D shows no dependence on ξ, presenting instead a polynomial decay. On the other hand, the TM quarter-filling case did not admit the fitting described above.

The fitting curves $D(N)$ appear in figure 3 as solid lines, together with the numerical results obtained from equation (3) (filled circles). Dashed lines are for the cases where the fitting expression given by equation (4) does not work. We see excellent agreement in the PD and PF cases, and in the TM case at half-filling; good agreement in the RS case; and none in the TM quarter-filling case. The fitting procedure is interesting at this point because it provides information—via the localization length ξ, when it arises—concerning the link between the insulating property and disorder under the action of the various substitution potentials. In figure 4, ξ is plotted as a function of the potential strength λ. As expected, the localization length diminishes with the increase of the potential strength, thus meaning more localized wave functions. Obviously if $\xi > N$ for a given length N, the corresponding wave functions will cover the whole ring and the system can conduct. The finite value of ξ suggests, however,

Table 1. Fitting parameters as in equation (4) for the various substitution potentials. The indices h and q refer to half-filling and quarter-filling, respectively. The localization length ξ is given in units of the (nearest integer) number of sites. The symbol '—' indicates no dependence of the curve on the corresponding parameter, whereas the symbol '- -' indicates non-applicability of the fitting expression.

Potential	A_h	B_h	γ_h	ξ_h	A_q	B_q	γ_q	ξ_q
TM 0.2	—	0.96	0.01	1935	- -	- -	- -	- -
TM 0.4	—	0.65	0.17	150	- -	- -	- -	- -
TM 0.6	—	0.51	0.31	53	- -	- -	- -	- -
TM 0.8	—	0.42	0.47	25	- -	- -	- -	- -
TM 1.0	—	0.34	0.66	14	- -	- -	- -	- -
RS 0.2	—	0.96	0.01	1308	—	0.98	0.00	1205
RS 0.4	—	0.89	0.03	427	—	1.02	−0.03	773
RS 0.6	—	0.51	0.23	125	—	1.02	−0.04	316
RS 0.8	—	0.64	0.15	105	—	0.73	−0.06	125
RS 1.0	—	0.09	1.03	20	—	0.88	−0.04	139
PD 0.2	—	0.51	0.37	36	—	0.51	0.32	55
PD 0.4	—	0.74	0.36	17	—	0.19	0.82	20
PD 0.6	—	1.07	0.13	11	—	0.07	1.31	12
PD 0.8	—	4.88	−0.21	9	—	0.03	1.68	9
PD 1.0	—	6.47	−0.23	7	—	0.01	1.97	7
PF 0.2	0.98	0.16	−0.95	—	—	0.43	0.45	31
PF 0.4	0.94	0.11	−0.43	—	—	0.29	0.78	13
PF 0.6	0.88	0.16	−0.30	—	—	0.33	0.86	8
PF 0.8	0.81	0.22	−0.29	—	—	0.48	0.81	6
PF 1.0	0.76	0.29	−0.35	—	—	0.62	0.81	5

that if N is sufficiently large the system will show itself to be an insulator. This is the case for TM and RS sequences at half-filling, and also for the RS sequence at quarter-filling, for potential strengths $\lambda < 0.4$.

3.3. Spectral gaps

The characteristics seen in the Drude weights for insulators can be explained in terms of the widths of the gaps in the energy spectra. In fact, systems with singular continuous spectra, which are commonly encountered under almost-periodic potentials, show spectra which are Cantor sets; therefore gaps appear with different widths at different energy values. The question of where (large) gaps will appear has not yet received a definite answer, but some clues have been provided by gap-labelling procedures [22]. For the cases investigated here, gaps open in accordance with the results shown by the calculations related to the Drude weight. This finding is presented in figure 5 where the difference between the last filled energy level and the next one, $\Delta = E_{M+1} - E_M$, was computed at $\phi = \phi_{min}$ for the largest ring considered ($N = 256$) and is plotted as a function of the potential strength λ. We see two distinct types of gap. The cases which are clearly insulators, since they meet the criterion of showing exponential decay of the Drude weight D, have gaps increasing with λ and much larger than the gaps shown by those cases which are conductors for the values of N considered. Also, for the systems which present greater gaps in figure 5, we have checked the linear relation $\Delta(\lambda) \sim \xi^{-1}(\lambda)$, not shown
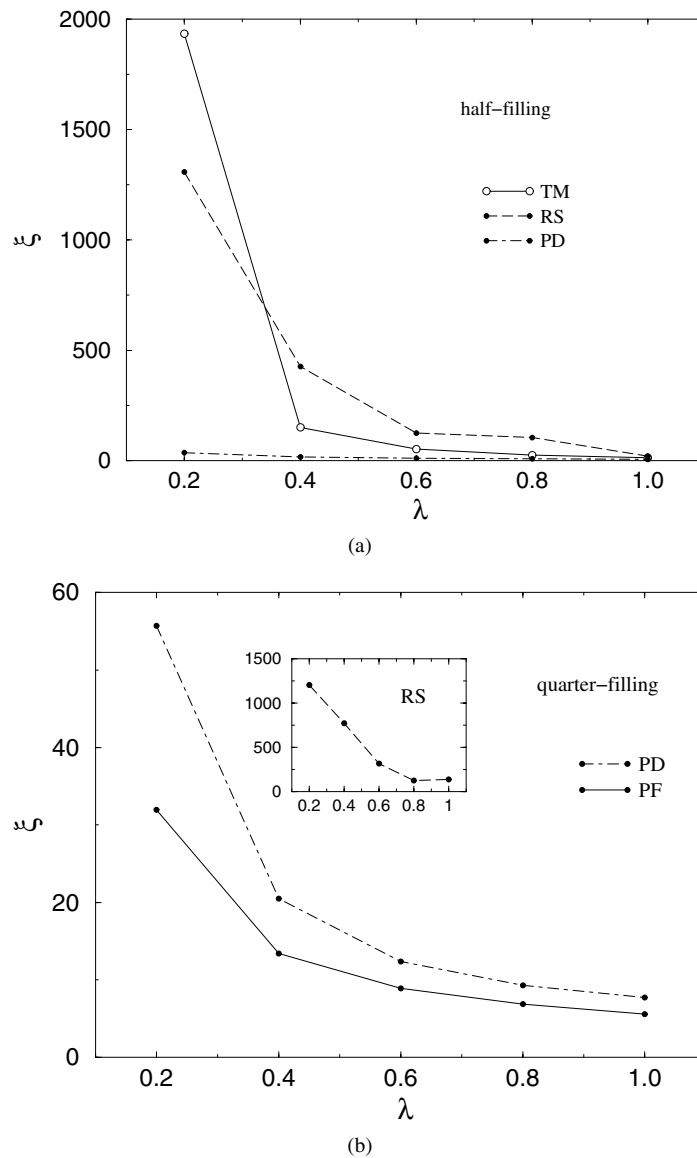
Figure 4. Localization length ξ as a function of strength of the potential λ: (a) half-filling; (b) quarter-filling. The results for the RS case are shown in the inset for clarity.

here (see the 1991 article by Fye *et al* in reference [8]). There is very good agreement for TM and PD cases at half-filling and also for PD and PF cases at quarter-filling. The exception is the RS case, which appears as an insulator but for which the results concerning the gaps are commonly intractable.

This relation between the Drude weight and the gaps in the spectra can be pursued further. On the one hand, Fye *et al* [8] obtained results pointing to the Drude weight being independent of whether the boundary conditions are periodic or open. On the other hand, gap-labelling procedures have shown that for open chains the integrated density of states (IDS) for the TM potential has an open gap at IDS = 1/2 and a closed gap at IDS = 1/4; the PD case presents
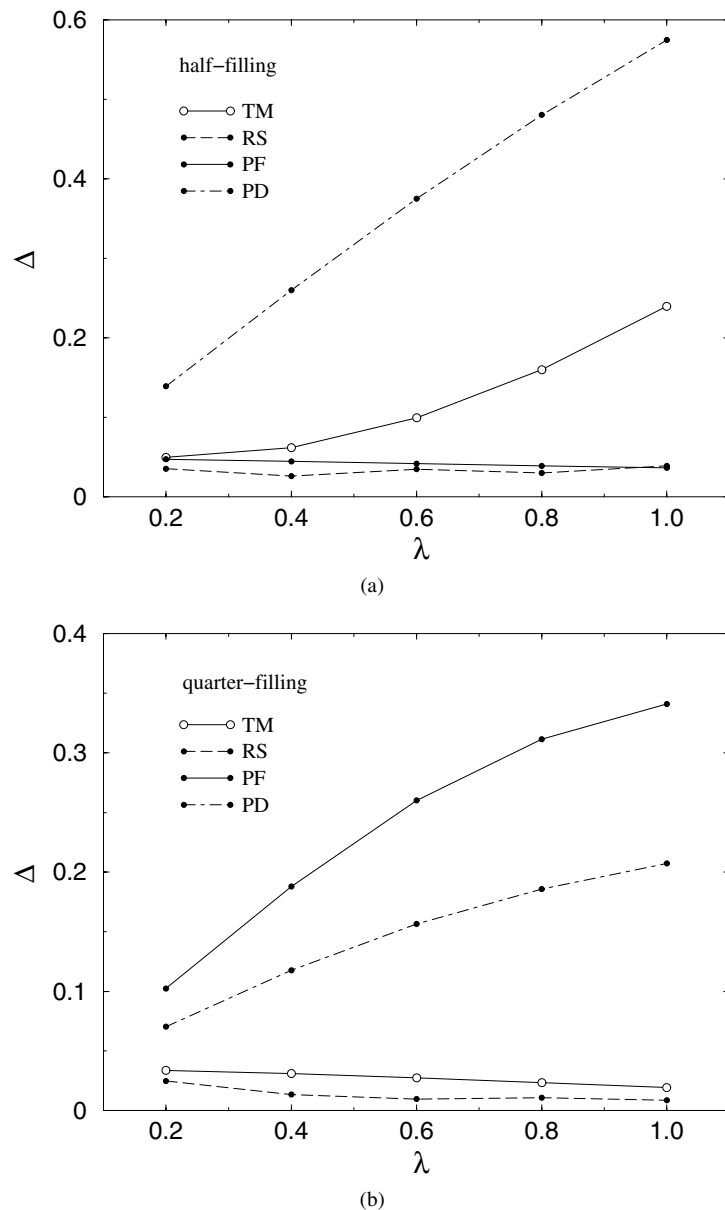
Figure 5. Gaps in the energy spectra (symbols) at (a) half-filling and (b) quarter-filling for the flux value $\phi = \phi_{min}$.

open gaps at both IDS $= 1/2$ and IDS $= 1/4$; and for the RS and PF cases there are no conclusive results [22]. Accepting that these results for open chains are valid for sufficiently large rings, and noting that the IDS is directly translated into our filling factor, we see that the results shown in figures 1–4 are consistent with gap-labelling predictions. In particular, these predictions would explain why the current is maximal for TM quarter-filling, since there would be a closed gap at IDS $= 1/4$. On the other hand, the vanishing currents for the PF case at quarter-filling could suggest a closed gap at IDS $= 1/4$.

Although this relation clearly needs more investigation, the observations above may provide a more intuitive understanding of the relation between the transport properties of the system and its spectral type, as recalled in the introduction.

4. Discussion and conclusions

The results of the previous sections show that the behaviour of $D(N)$ distinguishes correctly the conductors and insulators as suggested by the relative amplitudes of the persistent currents. Indeed, the exponential decay of $D(N)$ in the case of insulators, and the resulting localization length ξ, are reinforced by the structure of gaps in the energy spectra. The other cases, where that decay is slower than exponential, clearly need more investigation before they can be modelled by the behaviour of $D(N)$. Chaves and Satija [13] have recently conjectured the existence of a new phase state between insulator and conductor for deterministic aperiodic systems, with a polynomial decay of D as a function of the system size N. Our results, seen in the figures and in the fitting output, point in the same direction, although suggesting a richer behaviour, perhaps with mixtures of and transitions between the above possibilities.

Some care must be exercised in comparing the results presented in this paper and other results available in the literature dealing with the relations between transport properties or diffusion exponents and the degree of randomness of the potential [1–3]. The latter mostly deal with a single particle moving in an open chain, with an initial delta-function state at a given position. In that case, all the energy eigenstates contribute to the quantum state of the system, contrary to the situation seen here where only the lowest levels, up to the filling, are present. Whether the result of Fye *et al* [8] that the Drude weight does not depend on the boundary conditions is applicable here needs to be investigated more systematically.

We have thus investigated in this work how different degrees of randomness in the potential affect the persistent currents and the conducting properties—via the Drude weight—of half- and quarter-filled rings threaded by a magnetic flux. This was done in the tight-binding approximation with the potential being given by some almost-periodic substitution sequences (Thue–Morse, Rudin–Shapiro, paper-folding, and period-doubling). The results show that it is by no means obvious which potential allows better conducting properties, if one is guided solely by a measure of its degree of randomness—for example, the autocorrelation measure of the sequence itself. More specifically, that measure predicts the following hierarchy of disorder: (PD, PF)/TM/RS, while the persistent-current amplitudes follow the orders PF/RS/TM/PD for half-filling and TM/RS/(PF, PD) for quarter-filling. A more quantitative estimate, given by the decay of the Drude weight as a function of the ring length, shows that, for half-filling, TM and PD systems are indeed insulators and PF ones can conduct, whereas, for quarter-filling, PD and PF systems are insulators and TM ones are conductors (RS systems do not have so simple a classification). This discrepancy is, moreover, confirmed and explained by the gaps opened in the energy spectra as functions of the potential strength for the various sequences.

Acknowledgments

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