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LETTER TO THE EDITOR

(De)localization in the prime Schrödinger operator**César R de Oliveira and Giancarlo Q Pellegrino**

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Abstract

We report a combined numerical approach to study the localization properties of the one-dimensional tight-binding model with potential modulated along the prime numbers. A localization–delocalization transition was found as a function of the potential intensity; it is also argued that there are delocalized states for any value of the potential intensity.

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Problems related to the distribution of prime numbers are usually interesting and difficult. Perhaps the most challenging open problem in mathematics is the so-called Riemann hypothesis on the distribution of the (nontrivial) zeros of his zeta function, a problem directly related to the distribution of prime numbers and other mathematical issues. Also, the interplay between number theory, with the set of prime numbers playing a major role, and physics has been fruitful; see the short note by Wolf [1] and references therein for recent discussions.

In recent years there has been much interest in spectral properties of discrete Schrödinger operators on $l^2(\mathbb{Z})$

$$(H_V u)_n = u_{n+1} + u_{n-1} + \lambda V_n u_n$$

with nonrandom finite-valued potentials $V = \{V_n\}$ (see [2–7] and references therein); $\lambda > 0$ is the potential intensity. Such one-dimensional models with potentials along almost periodic sequences taking a finite number of values [2–4], like substitution and circle sequences, have been dominated by singular continuous spectra. Recall, however, that for the cases of periodic and random potentials V it is well known that the Hamiltonian H_V has absolutely continuous and point spectra, respectively [8]; these are mathematical characterizations of delocalized and localized (insulator) behaviours, respectively.

There has also been recent work on Schrödinger operators with sparse potentials [9–13]. A characteristic defining a sparse potential is the constancy of its values in a sequence of increasing intervals. In this case one can have point, absolutely continuous and singular continuous spectra, depending on the growing speed of the gaps and how the intensity of the bumps behaves at infinity. There is, in fact, some competition among different properties of the potential, resulting in rich spectral possibilities.

The prime numbers are straightforwardly related to both kinds of potential discussed above, namely nonrandom and sparse. It is well known that the set of prime numbers is not finite

and that there are arbitrarily large gaps between consecutive primes, a property characterizing sparseness. By defining a potential $V_0 = 0$, $V_n = 1$ if $n + 1$ is a prime number and $V_n = 0$ if not, and extending symmetrically to negative values of n , i.e. $V_{-n} = V_n$, one obtains an instance of a finite-valued sparse potential. The non-negative values of the potential V are 01101010001010001...

The main aim of this Letter is to discuss numerically the spectral properties of the corresponding discrete Schrödinger operator, which will be referred to as ‘the prime Schrödinger operator’. The rigorous analytical study of this system, although desirable, seems to be subtle and far from trivial. Since in this Letter we consider this problem from just a numerical point of view, we find it more appropriate to avoid the mathematical spectral terms, and instead shall try to use the physical ones localization (insulator) and delocalization to characterize our results.

By exploring dynamical as well as geometrical quantities related to the spectral properties of the model, we find a (rather smooth) transition from predominantly delocalized states to localized ones, as the potential intensity is increased. Nevertheless, some delocalized states always remain, no matter how large the potential. Also, the combined use of geometrical and dynamical tools, supportive of and to some extent complementary to each other, seems to be applicable to other cases with coexisting spectral components.

Here two different sets of numerical tools are used in such investigations. The *dynamical tools* are the average probability for the system to return to its initial state $u_0 = \delta_{n,n_0}$, concentrated on the site n_0 ,

$$C(t) = \frac{1}{t} \int_0^t |\langle u(s) | u_0 \rangle|^2 ds$$

and the second moment

$$d_2(t) = \sum_n (n - n_0)^2 |u_n(t)|^2$$

$u = (u_n)_{n \in \mathbb{Z}}$. Recall that for large values of t it is expected that $C(t) \sim t^{-D_2}$ and $d_2(t) \sim t^{2\beta}$, with D_2 being the correlation dimension of the spectral measure associated with the initial state [14–16]. Continuous spectra are usually numerically characterized by $0 < D_2, \beta$; although it is possible to have exceptional systems with a point spectrum and with any value $0 \leq \beta < 1$ [17].

Due to the rather irregular distribution of prime numbers [1], we suspect the quantum dynamics generated by H_V can strongly depend on the initial wavefunction, at least for small times; therefore, the initial condition was always concentrated on $n_0 = 0$. These dynamical tools were restricted to $0.5 \leq \lambda$, since for small λ it is not possible to neglect logarithmic corrections to the algebraic behaviours of $C(t)$ and $d_2(t)$ [6].

The other kind of tool, *geometrical tools*, are the direct inspection of eigenfunctions and the *Lyapunov exponent* (LE) γ , also called *inverse localization length*, calculated for each eigenfunction of the finite-basis approximation. The typical basis size used here is 10^4 ; the robustness of the numerical calculations with respect to the basis size was verified in each case. Localization, i.e. a point spectrum, is characterized by nonvanishing γ .

From the Thouless formula [8, 18], in particular from its proof, one sees that the LE at energy E can be estimated as

$$\gamma(E) \approx \frac{1}{N} \sum_{j=1}^N \ln |E - E_j|$$

with E_j running over all eigenvalues (distinct from E) of the finite-basis approximation of size N .

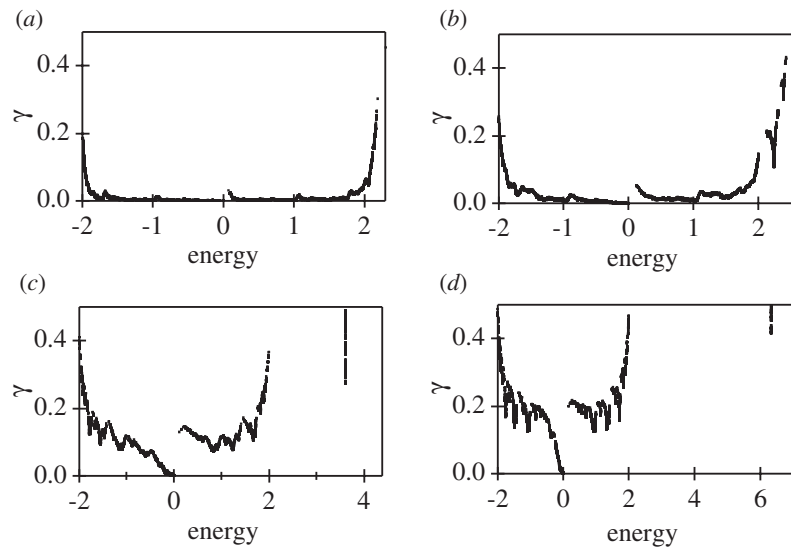


Figure 1. LE γ versus energy for the prime Schrödinger operator. (a) $\lambda = 0.5$; (b) $\lambda = 1.0$; (c) $\lambda = 3.0$; (d) $\lambda = 6.0$.

In figure 1 the LE γ is shown as a function of the energy for some values of the potential intensity λ . For $\lambda = 0.5$ the vanishing of the LE for most energies E indicates the predominancy of delocalized states; by increasing the potential intensity the LE becomes different from zero, except in a left neighbourhood of $E = 0$. This phenomenon was verified for all values of potential intensity considered (up to $\lambda = 40.0$), i.e. the LE vanishes just below $E = 0$. This strongly indicates a transition from delocalization to localization with a remaining set of delocalized states near $E = 0$.

The above conclusions were also supported by numerical solutions of the Schrödinger equation and computation of dynamical quantities (also with lattice size up to 10^4). In figure 2 $d_2(t)$ is shown for two values of λ ; $d_2(t)$ saturates for $\lambda = 6.0$ (as well as $C(t)$; not shown), indicating the presence of localized states; while for $\lambda = 0.5$ the values of $d_2(t)$ increase until a critical probability density value is reached at the basis border ($|u|^2 < 10^{-6}$ was used), indicating the presence of delocalized states. Notice that, due to the presence of both localized and delocalized states for the prime Schrödinger operator, it can be difficult to retrieve information on its spectral type only from dynamical quantities. This justifies the choices of potential intensity values in figure 2, used to exemplify the spectral transition: for $\lambda = 0.5$ most states are delocalized, while for $\lambda = 6.0$ the energy band corresponding to delocalized states is very narrow.

Of course, a numerical vanishing LE is not exactly zero. The LE γ_p for a periodic case was computed with the above method; since it should be zero in the spectrum of the corresponding Schrödinger operator, any $\gamma \leq \gamma_p$ was in practice considered to indicate the presence of delocalized states for the prime case. This was used to estimate the length of the interval $[-b(\lambda), 0]$ of the ‘delocalized band’ as a function of λ . As another check for such a transition, the dynamical quantities $d_2(t)$ and $C(t)$ were computed for short times taking into account two different sets of eigenvectors: those whose eigenvalues were in the delocalized band $[-b(\lambda), 0]$, and those in intervals with positive LE. The distinctions in their qualitative behaviours are evident. For example, in figure 3 the value $\lambda = 1.0$ was fixed and d_2

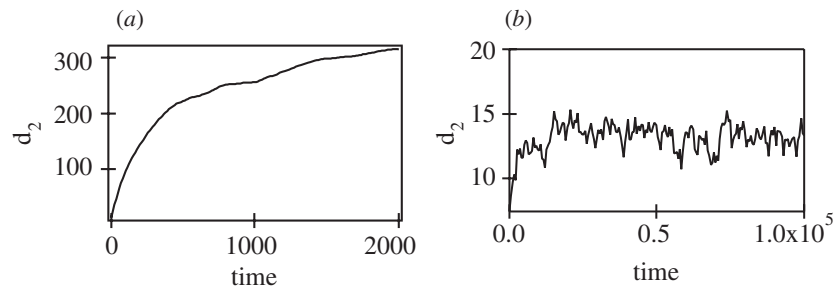


Figure 2. The second moment d_2 as a function of time for (a) $\lambda = 0.5$ and (b) $\lambda = 6.0$. Notice the different scales (for $\lambda = 6.0$ the time evolution did not reach the basis border).

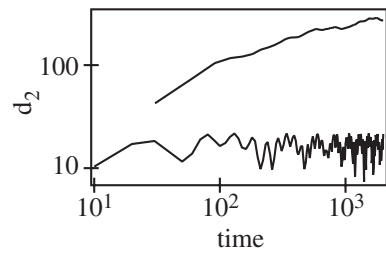


Figure 3. The second moment d_2 as a function of time for $\lambda = 1.0$ (base 10 log–log scale). The upper curve was obtained taking into account only the eigenvectors whose eigenvalues were in the range $[-0.6, 0.0]$. The lower curve is similar, but with eigenvalues in the range $[1.6, 2.0]$ (see also figure 1(b)).

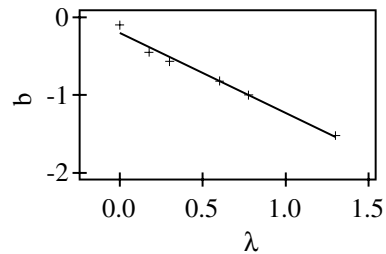


Figure 4. Delocalized band length b as a function of the potential intensity λ (base 10 log–log scale). The best fitting line is also shown.

was computed by restricting the dynamics to eigenvalues in the range $[-0.6, 0.0]$ (a subset of $[-b(1), 0]$) and also to eigenvalues in the range $[1.6, 2.0]$ (corresponding to positive LE). In the former case $d_2(t)$ grows with time, while in the latter case it is clearly bounded; such results also support the presence of mobility edges in the spectrum of the prime Schrödinger operator.

Figure 4 shows some values of $b(\lambda)$; the best fitting line is also shown and its slope is equal to -1 . Therefore, it is numerically found that $b(\lambda) \sim \lambda^{-1}$, at least for large λ , so it does not vanish and the spectrum of the prime Schrödinger operator should have a set of delocalized states for any potential intensity. Notice that the eigenfunctions corresponding to eigenvalues in the range $[-b(\lambda), 0]$ are extended over the finite bases, while they are exponentially localized if the corresponding LE is greater than zero (not shown here).

In summary, a delocalization–localization transition, with mobility edges, was found numerically for the one-dimensional prime Schrödinger operator, a transition as the intensity of the potential is increased; however, there remains a band of delocalized states whose length scales as $\sim\lambda^{-1}$, assuring the presence of delocalized states for any value of λ . These results, and the calculations presented, suggest that the same approach could be applied to cases with other aperiodic potentials, for which one suspects simultaneous continuous and point spectral components.

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