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LETTER TO THE EDITOR

Dynamical delocalization for the 1D Bernoulli discrete Dirac operator

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Abstract

A 1D tight-binding version of the Dirac equation is considered; after checking that it recovers the usual discrete Schrödinger equation in the nonrelativistic limit, it is found that for two-valued Bernoulli potentials the zero-mass case presents the absence of dynamical localization for some specific values of the energy, albeit it has no continuous spectrum. For the other energy values (again excluding some very specific ones) the Bernoulli–Dirac system is localized, independently of the mass.

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In one-dimensional quantum systems general random potentials induce localization and no conductance [1, 2], irrespective of the disorder intensity. Exceptions are restricted to random models with local correlations, such as polymer models [3], random palindrome models [4], both including the important precursory random dimers [5, 6] (see [7, 3] for rigorous approaches). In this letter a random discrete model is presented with no local correlation for which delocalization occurs in some situations; to the best of authors' knowledge it is the first tight-binding model with such a property (in [8] dynamical delocalization is shown for a tight-binding Schrödinger model, but the random potential is decaying). Since mathematical proofs will appear elsewhere, it is hoped that the present letter will contact physicists with recent interesting mathematical results on delocalization in one dimension.

The model is in fact very simple. It is a relativistic version of the well-known tight-binding Schrödinger Hamiltonian (with $\hbar = 1$)

$$(H_S\psi)_n = -\frac{1}{2m}(\Delta\psi)_n + V_n\psi_n = \frac{1}{2m}(-\psi_{n+1} - \psi_{n-1} + 2\psi_n) + V_n\psi_n \qquad (1)$$

(recall that it is common to take $+\Delta$ instead of $-\Delta$, and also exclude the constant factor '2' in the kinetic term). For very general random potentials V_n the model (1) is localized, including the Bernoulli potential for which the site energy V_n is assigned one of two values $\pm v$ at random ($-v$ with probability $0 < p < 1$ and $+v$ with probability $1 - p$, say); the spectrum of the corresponding operator has no continuous component [2].

By imposing the strong local correlation that the site energies V_n are assigned for pairs of lattices, i.e, $V_{2n} = V_{2n+1} = \pm v$ for all n, one gets the random dimer model exhibiting delocalized states [5–7, 3]. Despite dynamical delocalization the dimer Schrödinger operator has no continuous component in its spectrum. The first example of a system with dynamical delocalization and pure point spectrum was a peculiar almost periodic operator [9]. Such results clarified the difference between mathematical localization (i.e., pure point spectrum) and dynamical localization (i.e., bounded moments, see the following). In the zero-mass case, the Dirac [13] model discussed here has a pure point spectrum and dynamical delocalization with no added correlation to the Bernoulli potential. A crucial first step for the arguments will be the appropriate way of writing the transfer matrices and their similarity with those of the Schrödinger dimer model.

Previous works have considered the one-dimensional Dirac equation and relativistic effects on conduction in disordered systems [10], localization [11] and comparative studies of relativistic and nonrelativistic Kronig–Penney models with δ-function potentials [11, 12]. Although tight-binding equations for the electronic amplitudes have naturally arisen in some of these studies, the phenomena reported here have not. The interesting question of the comparison of the relativistic and nonrelativistic localization length was numerically investigated [11] in some cases, and it was found that which one is larger depends on the on-site energy and also on the energy particle.

Consider a particle of mass $m \geqslant 0$ in the one-dimensional lattice $\mathbb{Z}$ under the site potential $V = (V_n)$; the Dirac tight-binding version is proposed as

$$H_D(m, c) = H_0(m, c) + V I_2 = \begin{pmatrix} 0 & cd^* \\ cd & 0 \end{pmatrix} + mc^2\,\sigma_3 + V I_2, \tag{2}$$

with $c > 0$ being the speed of light, σ_3 the usual Pauli matrix, I_2 the 2×2 identity matrix and d a finite difference operator (a discrete analogue of the first derivative)

$$(d\psi)_n = \psi_{n+1} - \psi_n.$$

Since d is not Hermitian, its adjoint $(d^*\psi)_n = \psi_{n-1} - \psi_n$ appears in the definition of H_D (the inclusion of the imaginary unit i in front of the difference operators d and d^* is immaterial). In the case that V_n takes a finite number of values, it is clear that H_D is a bounded Hermitian operator acting on $\ell^2(\mathbb{Z}; \mathbb{C}^2)$ and the resulting Dirac equation can be recast in the compact form

$$\mathrm{i}\frac{\partial \Psi_n}{\partial t} = (H_D(m, c)\Psi)_n = \begin{pmatrix} mc^2 + V_n & cd^* \\ cd & -mc^2 + V_n \end{pmatrix} \Psi_n, \tag{3}$$

with the spinor $\Psi = (\Psi_n)$ and $\Psi_n = \binom{\psi_n^+}{\psi_n^-}$.

One can easily verify that the nonrelativistic limit of (3) is the equation associated with the Schrödinger operator (1); this is an important support for the Dirac model just introduced. Following the traditional prescription for the nonrelativistic limit of the Dirac equation [13], first one removes the rest energy by inserting $\Psi = \mathrm{e}^{-\mathrm{i}mc^2 t}\Phi = \mathrm{e}^{-\mathrm{i}mc^2 t}\binom{\phi^+}{\phi^-}$ into (3) so that

$$\mathrm{i}\frac{\partial \Phi}{\partial t} = c\begin{pmatrix} d^*\phi^- \\ d\phi^+ \end{pmatrix} - 2mc^2 \begin{pmatrix} 0 \\ \phi^- \end{pmatrix} + V\Phi.$$

For large values of c, the equation in the second row above can be solved approximately as $\phi^- = d\phi^+/2mc$, and inserting this into the first equation results in

$$\mathrm{i}\frac{\partial \phi^+}{\partial t} = \frac{1}{2m} d^* d\phi^+ + V\phi^+. \tag{4}$$

Similarly, by considering $\Psi = \mathrm{e}^{\mathrm{i}mc^2 t}\Phi$ one finds

$$\mathrm{i}\frac{\partial \phi^-}{\partial t} = -\frac{1}{2m} dd^*\phi^- + V\phi^-. \tag{5}$$

Since $d^*d = dd^* = -\Delta$, then (4) and (5) correspond to the one-dimensional tight-binding Schrödinger equation associated with (1) with positive and negative free energies, respectively.

Another point directly related to the continuous Dirac equation is the presence of the so-called zitterbewegung [13] phenomenon for (3); here the particular case of free particle and small mass m will be explicitly considered. Following section 69 of Dirac's book [14], let $\hat{n}$ denote the position operator $(\hat{n}\Psi)_n = n\Psi_n$, so that its time evolution under the free operator $H_0(m, c)$ is $\hat{n}(t) = \mathrm{e}^{\mathrm{i}H_0 t}\hat{n}\,\mathrm{e}^{-\mathrm{i}H_0 t}$; the velocity operator is then

$$\frac{\mathrm{d}\hat{n}(t)}{\mathrm{d}t} = \mathrm{i}[H_0, \hat{n}(t)] = \mathrm{e}^{\mathrm{i}H_0 t} cA(0)\,\mathrm{e}^{-\mathrm{i}H_0 t} = cA(t),$$

with $A = A(0) = \mathrm{i}\begin{pmatrix} 0 & -d^*-1 \\ d+1 & 0 \end{pmatrix}$. Note that A is Hermitian, $A^2 = I_2$, so that its spectrum is ± 1 and then the spectrum of cA is $\pm c$. Since $\mathrm{e}^{-\mathrm{i}H_0 t}$ is unitary, it follows that the spectrum of the above velocity operator is $\pm c$ for all t. Hence, it indicates that the possible speed measurements would result only in $\pm c$. Now, for small mass m the time derivative of the velocity operator is given by

$$\frac{\mathrm{d}(cA(t))}{\mathrm{d}t} = \mathrm{i}[H_0, cA(t)] = 2\mathrm{i}H_0 F(t), \tag{6}$$

with

$$F(t) = \frac{\mathrm{i}c^2}{2} H_0^{-1}\,\mathrm{e}^{\mathrm{i}H_0 t}\begin{pmatrix} dd^* & 0 \\ 0 & -d^*d \end{pmatrix}\mathrm{e}^{-\mathrm{i}H_0 t}.$$

The operator $F = F(0)$ anticommutes with H_0; thus $\mathrm{d}F(t)/\mathrm{d}t = 2\mathrm{i}H_0 F(t)$ and it is found that $F(t) = \mathrm{e}^{2\mathrm{i}H_0 t}F$, which is fast oscillating. Inserting this into (6) one finds $\mathrm{d}(cA(t))/\mathrm{d}t = \mathrm{d}F(t)/\mathrm{d}t$; after integrating from 0 to t one gets $\mathrm{d}\hat{n}(t)/\mathrm{d}t = cA - F + \mathrm{e}^{2\mathrm{i}H_0 t}F$ and the velocity quickly oscillates around an average value; this is a version of zitterbewegung.

Now the localization results will be discussed. Consider model (2) with V_n taking the values $\pm v$, $v > 0$ randomly. Denote by $\delta_n^{\pm}$ the elements of the canonical position basis of $\ell^2(\mathbb{Z}; \mathbb{C}^2)$, for which all entries are $\binom{0}{0}$ except at the nth entry, which is given by $\binom{1}{0}$ and $\binom{0}{1}$ for the superscript indices + and −, respectively. If $\Psi_n = \binom{\psi_n^+}{\psi_n^-}$ is a solution of the eigenvalue equation

$$(H_D(m, c) - E)\Psi = 0,$$

then it is simple to check that

$$\begin{pmatrix} \psi_{n+1}^+ \\ \psi_n^- \end{pmatrix} = T_{V_n}^E \begin{pmatrix} \psi_n^+ \\ \psi_{n-1}^- \end{pmatrix}, \qquad \text{with} \quad T_{V_n}^E = \begin{pmatrix} 1 + \frac{m^2c^4-(E-V_n)^2}{c^2} & \frac{mc^2+E-V_n}{c} \\ \frac{mc^2-E+V_n}{c} & 1 \end{pmatrix}.$$

$T_{V_n}^E$ is the transfer matrix at the nth step. Recall that the Lyapunov exponent $\gamma(E)$ represents the average rate of exponential growing of the norm of transfer matrices

$$\left\| T_{V_n}^E \cdots T_{V_2}^E T_{V_1}^E \right\| \approx \mathrm{e}^{\gamma(E)\,n};$$

where $1/\gamma(E)$ is called the localization length. A vanishing Lyapunov exponent is an indication of delocalization, so the next task is to find possible energies $\tilde{E}$ with $\gamma(\tilde{E}) = 0$. In order to get vanishing Lyapunov exponents and diffusion, the arguments will follow those in [3, 7]; detailed mathematical proofs will appear elsewhere [15].

Given an initial spinor Ψ with only one nonzero component (i.e., well localized in space), the dynamical delocalization will be probed by the time average of the mean-squared displacement (also called second dynamical moment)

$$M_\Psi^m(t) = \frac{1}{t}\int_0^t \sum_n n^2\left(\left|\left\langle \delta_n^+, \mathrm{e}^{-\mathrm{i}H_D(m,c)s}\Psi\right\rangle\right|^2 + \left|\left\langle \delta_n^-, \mathrm{e}^{-\mathrm{i}H_D(m,c)s}\Psi\right\rangle\right|^2\right)\mathrm{d}s;$$

dynamical localization is characterized by a bounded $M_\Psi^m(t) \leqslant$ constant, for all t; otherwise the system is said to present dynamical delocalization.

First, the spectral questions will be faced. By adapting the multiscale analysis [2, 16] to the Dirac operator (2) it is possible to show that, due to the random character of the Bernoulli potential, for typical realizations the spectrum of $H_D(m, c)$ has no continuous component for any $m \geqslant 0$, and with exponentially localized eigenfunctions. In other words, mathematical localization holds for H_D.

By using the Furstenberg theorem as the main tool [17], for $m > 0$ it is shown that $\gamma(\tilde{E}) = 0$ if, and only if, $\tilde{E} = 0$ (for $v = c\sqrt{2+m^2c^2}$) and the four possibilities $\tilde{E} = \pm c/\sqrt{2} \pm c\sqrt{2+m^2c^2}$ (for $v = c/\sqrt{2}$); so, for other values of energies dynamical localization can be shown. For such $\tilde{E}$ values with $\gamma(\tilde{E}) = 0$, it was not yet possible to give an answer about dynamical localization.

Nevertheless, restricted to the massless ($m = 0$) case, if $0 < v \leqslant c$ the Lyapunov exponent vanishes for $\tilde{E} = \pm v$ and $v \neq c/\sqrt{2}$, and following [3] it is possible to show that

$$M_\Psi^0(t) \geqslant \text{constant}\, t^{3/2},$$

i.e., there is no dynamical localization despite the absence of a continuous component in the spectrum of the random operator $H_D(0, c)$. Due to its importance here, it is worth including the main argument for the vanishing of $\gamma(E = v)$ (the case $E = -v$ being similar). In this case, the possible transfer matrices are

$$T_{-v}^v = \begin{pmatrix} 1 - \left(\frac{2v}{c}\right)^2 & \frac{2v}{c} \\ -\frac{2v}{c} & 1 \end{pmatrix}, \qquad T_v^v = I_2.$$

Note that T_{-v}^v and T_v^v are commuting matrices and both have spectral radius equal to 1 (for such v). If n_- denotes the average number of times that the potential $-v$ occurs in n trials, then $n - n_-$ is the average number of times that the transfer matrix is the identity. Thus, if p is the probability for the potential value $-v$,

$$\gamma(v) = \lim_{n\to\infty} \frac{1}{n} \ln\left\| T_{V_n}^E \cdots T_{V_2}^E T_{V_1}^E \right\| = \lim_{n\to\infty} \frac{n_-}{n} \ln\left\| \left(T_{-v}^v\right)^{n_-} \right\|^{1/n_-} = p \ln 1 = 0.$$

The heuristics for the dynamical delocalization in this case can be found in the paper by Dunlap, Wu and Phillips in [6]. The main concern for the proof is the uniform boundedness of the product of transfer matrices [3, 15]. It is very important to stress that here delocalization is not synonymous of zero Lyapunov exponent, as some people have considered.

For small but nonzero mass, it is expected that the dynamics follow closely the massless case, at least for a small period of time. The final result to be reported is an inequality confirming such expectation; by using the Duhamel formula, it can be shown that, given an initial Ψ, there exists $C > 0$ so that, for all $t > 0$,

$$\left| M_\Psi^0(t) - M_\Psi^m(t) \right| \leqslant Cmc^2t^4. \tag{7}$$

Therefore, if the time t is not too large and/or the mass m is sufficiently small, the mean squared displacement follows rather closely the delocalized massless case, so that inattentive numerical simulations could give a wrong insight.

It is natural that this model would be applied to any case where the one-dimensional tight-binding Schrödinger operator was used; it would be the first step for their relativistic versions. Since the Dirac operator in the massless case presents dynamical delocalization, this becomes a potential source for explaining some observed effects (at least for small m) as details in the theory of mesoscopic systems [18].

Summing up, a natural one-dimensional Dirac tight-binding model was proposed which was supported by its nonrelativistic limit (it recovers the discrete Schrödinger model) and the presence of zitterbewegung. Then results about mathematical and dynamical localization were reported for such an operator with random Bernoulli potentials: for all values of $c > 0$ and mass $m \geqslant 0$, there is mathematical localization, but in the massless case and potential intensity $v \leqslant c$, particular values of the energy imply the absence of dynamical localization, although no potential correlation was imposed. It is possible that this model is the simplest one with such delocalization. Finally, relation (7) gives quantitatively an estimate of how, for small time t, the dynamics of the localized regime follows the delocalized one.

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References

[1] Anderson P W 1958 *Phys. Rev.* **109** 1492
Ramakrishnan T V and Lee P A 1985 *Rev. Mod. Phys.* **57** 287
[2] Carmona R, Klein A and Martinelli F 1987 *Commun. Math. Phys.* **108** 41
Shubin C, Vakilian R and Wolff T 1998 *Geom. Funct. Anal.* **8** 932
[3] Jitomirskaya S, Schulz-Baldes H and Stolz G 2003 *Commun. Math. Phys.* **233** 27
[4] Carvalho T O and de Oliveira C R 2003 *J. Math. Phys.* **44** 945
[5] Flores J C 1989 *J. Phys.: Condens. Matter* **1** 8471
[6] Dunlap D H, Wu H-L and Phillips P W 1990 *Phys. Rev. Lett.* **65** 88
Phillips P W and Wu H-L 1991 *Science* **252** 1805
Wu H L, Goff W and Phillips P W 1992 *Phys. Rev.* B **45** 1623
[7] De Bièvre S and Germinet F 2000 *J. Stat. Phys.* **98** 1135
[8] Germinet F, Kiselev A and Tcheremchantsev S 2004 *Ann. Inst. Fourier* **54** 787
[9] del Rio R, Jitomirskaya S, Last Y and Simon S 1996 *J. Anal. Math.* **69** 153
[10] Roy C L 1989 *J. Phys. Chem. Solids* **50** 111
Roy C L and Basu C 1992 *Phys. Rev.* B **45** 14293
[11] Basu C, Roy C L, Maciá E, Domínguez-Adame F and Sánchez S 1994 *J. Phys. A: Math. Gen.* **27** 3285
[12] Domínguez-Adame F, Maciá E, Khan A and Roy C L 1995 *Physica* B **212** 67
[13] Bjorken S D and Drell J D 1965 *Relativistic Quantum Mechanics* (New York: McGraw-Hill)
Itzykson C and Zuber J B 1985 *Quantum Field Theory* (New York: McGraw-Hill)
Thaller B 1991 *The Dirac Equation* (Berlin: Springer)
[14] Dirac P A M 1987 *The Principles of Quantum Mechanics* 4th edn (Oxford: Oxford University Press)
[15] de Oliveira C R and Prado R A *Spectral and Localization Properties for the One-Dimensional Bernoulli Discrete Dirac Operator* in preparation
[16] Germinet F and De Bièvre S 1998 *Commun. Math. Phys.* **194** 323
[17] Furstenberg H 1963 *Trans. Am. Math. Soc.* **108** 377
Bougerol P and Lacroix J 1985 *Products of Random Matrices with Applications to Schrödinger Operators* (Boston, MA: Birkhäuser)
[18] Imry Y 2002 *Introduction to Mesoscopic Physics* 2nd edn (Oxford: Oxford University Press)