A Dirac-type variant of the xp-model and the Riemann zeros

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Abstract – We propose a Dirac-type modification of the xp-model to a \( x \sigma \cdot \mathbf{p} \) model on a semi-infinite cylinder. This model is inspired by recent work of Sierra et al. on the xp-model on the half-line. Our model realizes the Berry-Keating conjecture on the Riemann zeros. We indicate the connection of our model to that of gapped graphene with a supercritical Coulomb charge, which might provide a physical system for the study of the zeros of the Riemann Zeta function.

There have been an increasing interest in physical models that might shed light on the Riemann hypothesis regarding the zeros of the Riemann Zeta functions. This program aims at a possible realization of a conjecture by Polya and Hilbert on the zeros of the Riemann Zeta function [1,2]. The Polya-Hilbert conjecture [2] states that the complex zeros of the Riemann Zeta function on the critical line are described by the eigenvalues of a self-adjoint operator. One of the original proposals for such an operator arose from the work of Berry [3,4], followed by Connes [5] and Sierra [6–11] with their collaborators. The attempts towards the construction of such an operator are guided by various properties that are ascribed to it [3,4], including the requirements that it should exhibit a chaotic classical dynamics with isolated periodic trajectories and that it should break the time-reversal invariance.

Guided by these requirements, Berry and Keating [4] suggested that the operator \( \mathcal{H}_0 = xp \) is a good candidate for the realization of the Polya-Hilbert conjecture. The Berry-Keating operator \( xp \) breaks the time-reversal invariance. However, it does not lead by itself to closed trajectories, which requires various additional identifications in the classical phase space. There are distinct identifications or regularizations leading to similar realizations of the Polya-Hilbert conjecture. However, each of such identifications also suggests distinct interpretations of the model at the level of a semi-classical analysis. There were two main distinct regularizations. One was proposed by Berry and Keating, which leads to a discrete spectrum for the model. Another regularization was proposed by Connes [5], which leads to a continuum spectrum with a missing discrete set of eigenvalues. The spectrum counting in the case of Berry and Keating and the missing spectral line counting in the case of Connes are though similar. Both pictures were later seen to be equivalent by Sierra [8,9] in a quantum model displaying a discrete spectrum inside a continuum.

An interesting physical realization of the Berry-Keating operator was given by Sierra and Townsend [7], who observed that the xp-operator appears as the Hamiltonian of the quantum Hall effect when restricted to the lowest Landau level [12]. They further argued that from this perspective, the Berry-Keating Hamiltonian has a quantum description consistent with the Polya-Hilbert conjecture. The relationship of Riemann zeros to other quantum systems such as the inverted harmonic oscillator [13] and the Morse potential [14] have also been discussed in the literature.

Recently, Sierra and Rodriguez-Laguna [10] have proposed a new operator \( \mathcal{H}_1 = xp + \ell^2_p / p \) where the particle is restricted to the (regularized) half-line \( l_x \leq x \leq \infty \), with \( \ell^2_p / p \) a constant. The operator \( \mathcal{H}_1 \) satisfies the essential properties of the Berry-Keating model and in addition gives rise to closed classical trajectories. In the quantum theory, the appearance of the \( 1/p \) term in \( \mathcal{H}_1 \) leads to a non-local boundary condition. With an appropriate choice of the kernel of \( 1/p \), \( \mathcal{H}_1 \) was shown to admit a 1-parameter family of self-adjoint extensions with a spectrum that is bounded from below and is thus a legitimate quantum Hamiltonian operator. For certain choices of the self-adjoint extension parameter, this model seems to be consistent with the Polya-Hilbert conjecture.

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The smooth part of eq. (1) can be written as
\[ N(E) = \langle N(E) \rangle + S(E), \quad (1) \]
where \( N(E) \) is the number of complex zeros of the Riemann Zeta function with positive imaginary part less than \( E \), \( \langle N(E) \rangle \) is the smooth part of \( N(E) \) and \( S(E) \) denotes a fluctuation in the counting (also known as error function) given by
\[ S(E) = \frac{1}{\pi} \arg \zeta \left( \frac{1}{2} + iE \right) = \mathcal{O}(\log(E)). \quad (2) \]
The smooth part of eq. (1) can be written as
\[ \langle N(E) \rangle = \frac{\vartheta(E)}{\pi} + 1, \quad (3) \]
where the phase \( \vartheta(E) \) of the Riemann Zeta function on the critical line (also known as Riemann-Siegel function \([2]\)) is given by
\[ \vartheta(E) = \arg \Gamma \left( \frac{1}{4} + \frac{iE}{2} \right) = -\frac{1}{2} E \log \pi. \quad (4) \]
Recall that by the use of Stirling’s formula — valid for large \( E \) — the above Riemann-Siegel function may be written as
\[ \vartheta(E) \sim \frac{E}{2} \log \frac{E}{2} - \frac{E}{2} + \mathcal{O}(1). \quad (5) \]
The Hamiltonian operators introduced in \([3–5,7,10,11]\) provide an estimate for the phase \( \vartheta(E) \) of the Riemann Zeta function, which can be used in the Riemann-van Mangoldt formula \((1)\) to make inferences about the zeros of the Riemann Zeta function.

In this letter, following the spirit of the work of Sierra et al. \([10,11]\), we propose a variant of the \( xp \)-model on the half-line where the operator \( p \) is replaced by a suitable two-dimensional Dirac-type operator \( \hat{p} \). The aim is to obtain a proper self-adjoint \( xp \)-operator on the half-line.

Let us consider the Dirac operator
\[ \hat{p} \equiv \sigma \cdot p = \sigma_x p_x + \sigma_y p_y, \quad (6) \]
where \( p_a = -i\partial_a \), with \( a = x, y \), and \( \sigma_x, \sigma_y \) are Pauli matrices. Thus,
\[ \hat{p} = -i \begin{pmatrix} 0 & \partial_x - i\partial_y \\ \partial_x + i\partial_y & 0 \end{pmatrix}. \quad (7) \]
We assume that this operator acts on two-component column-vectors valued on a Hilbert space defined on a semi-infinite cylinder. The semi-infinite cylinder is described by \( 0 \leq x < \infty \) and the \( y \)-direction is a circle of radius \( R \). There are a \( U(1) \) worth of possible boundary conditions that guarantees the conservation of probability. This statement is equivalent to say that there is a \( U(1) \) family of self-adjoint operators \( \hat{p} \) on the semi-infinite cylinder.

The above considerations on the operator \( \hat{p} \) should be contrasted with the fact that there is no self-adjoint operator \( p \) on the half-line. This statement can be checked by computing the deficiency indexes \( n_\pm \) and then use the criteria discovered by von Neumann \([15,16]\). The deficiency indexes \( n_\pm \) are defined as the dimension of the space of square-integrable solutions of the equations \( p\psi_\pm = \pm i\psi_\pm \). For the operator \( p \) on the half-line, we have \( n_+ = 1 \) and \( n_- = 0 \). Thus, by the von Neumann theorem, there is no self-adjoint operator \( p \) on the half-line. Equivalently, there is no boundary condition on the half-line that guarantees the conservation of probability.

We now consider the Hamiltonian \( H = xp \). This is our proposed modified version of the \( xp \)-model. This Hamiltonian acts on a suitable domain of the Hilbert space of square-integrable functions on the cylinder. Let us consider the normal ordered operator
\[ H = \sqrt{x} \hat{p} \sqrt{x}. \quad (8) \]
Similar to the operator \( \hat{p} \), there is a \( U(1) \) family of self-adjoint operators \( H \) on the semi-infinite cylinder. Indeed, \( H \) inherits the same possible self-adjoint domains from \( \hat{p} \). We observe that a different choice of the normal ordering in the definition of \( H \), like, for instance, \( H = (1/2)(xp + px) \) does not change the conclusions of the following analysis.

Observe that the Hamiltonian \((8)\) is time-reversal odd. In the present case, time-reversal transformations are performed by \( \Theta = \exp(i\pi/2)K \), with \( K \) being a complex conjugate operator, such that it is an anti-unitary transformation \( \Theta^2 = -1 \). It is straightforward to see that \( \Theta H \Theta^{-1} = -H \). This fact means that for appropriate boundary conditions the spectrum of the quantized Hamiltonian contains time conjugate pairs, that is, eigenfunctions with energy \( E \) are mapped to eigenfunctions with energy \( -E \) under \( \Theta \). This will play a crucial role later in our analysis.

For a two-component column-vector
\[ \Psi(x, y) = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}, \quad (9) \]
the eigenvalue equation \( H\Psi = E\Psi \) leads to
\[ \sqrt{x}(\partial_x - i\partial_y)\sqrt{x}\psi_2 = iE\psi_1, \quad (10) \]
\[ \sqrt{x}(\partial_x + i\partial_y)\sqrt{x}\psi_1 = iE\psi_2. \quad (11) \]
This system of equations is equivalent to a second-order differential equation for one of the components, let us say \( \psi_1(x, y) \). From the topology of the \( y \)-direction, we may
consider the Ansätze
\begin{equation}
\psi_1(x, y) = \frac{1}{\sqrt{2\pi}} \frac{\varphi(x)}{x} e^{i\frac{1}{2}x^2y}, \quad (12)
\end{equation}
\begin{equation}
\psi_2(x, y) = \frac{1}{\sqrt{2\pi}} \frac{\chi(x)}{x} e^{i\frac{1}{2}x^2y}, \quad (13)
\end{equation}
with \( n \in \mathbb{Z} \) and \( \alpha \in [0, 1) \). The integer \( n \) is associated with the winding number due to the compactification of the \( y \)-direction.

The analysis presented below is valid for each value of \( n \) and we assume it to be fixed to some arbitrary value without loss of generality. The parameter \( \alpha \) is associated with the phase of the quasi-periodic boundary conditions along the \( y \)-direction. It parameterizes the family of self-adjoint domains in the domain of self-adjointness of the momentum operator. 

The time-reversal invariance aspects of the present model are the following. The Dirac operators in eqs. (10) and (11) transform correctly under time reversal. Observe that time-reversal transformation flips the two components of the spinor and changes the sign of the energy. However, the Ansätze (12) and (13) violate the time-reversal symmetry. The reason for this is the following. Note, first, that the parameter \( \alpha \) which characterizes the domain of self-adjointness of the momentum operator supported on the compact \( y \)-direction has the physical interpretation of a magnetic flux passing through the circle. The magnetic field automatically breaks the time-reversal invariance. Now, even if \( \alpha = 0 \), the axis of the cylinder is semi-infinite and the corresponding coordinate can always be taken as positive. Thus, even for \( \alpha = 0 \), the quantity \( x = u \) in eq. (14) must be taken as positive. This means that \( n \) is a positive integer. In turn, implies that the winding modes are chiral. Hence the time-reversal invariance is broken.

In order to set up the allowed boundary conditions, we first regularize the semi-infinite line \( 0 \leq x < \infty \) to \( x_0 \leq x < \infty \), for a positive \( x_0 \). Equivalently we can say that
\begin{equation}
 u_0 = \frac{2}{R} (n + \alpha)x_0. \quad (16)
\end{equation}
At \( x = x_0 \) or, equivalently, at \( u = u_0 \), we consider the boundary condition
\begin{equation}
\varphi(u_0) = 0. \quad (17)
\end{equation}
Note that if both \( n = 0 \) and \( \alpha = 0 \), then \( u_0 = 0 \) even if \( x_0 \neq 0 \). In what follows, we shall assume that values of \( n \) and \( \alpha \) are such that \( (n + \alpha) \neq 0 \). Later we discuss the case for small but finite \( u_0 \).

The analysis of boundary conditions presented below can be cast in a more formal language of self-adjoint domains and the von Neumann theorem [15,16]. The boundary condition on the wave functions for the singular attractive inverse-square potential following from the self-adjoint extension has been discussed in [18,19]. The close relation between the boundary conditions following from the introduction of a cut-off to that obtained from self-adjoint extension has also been discussed in the literature [16,19,20]. Here we prefer to report on this route of regularization and renormalization, since it is more familiar among physicists.

The general solution of the Whittaker equation with boundary condition (17) is (apart from an overall multiplicative constant)
\begin{equation}
\varphi(u) = [M_{\frac{1}{2}, -iE_0}(u_0) M_{\frac{1}{2}, +iE_0}(u)] - [M_{\frac{1}{2}, +iE_0}(u_0) M_{\frac{1}{2}, -iE_0}(u)], \quad (18)
\end{equation}
where \( M_{\alpha, \beta}(x) \) is the Whittaker function (see eq. (13.1.32) of [17]),
\begin{equation}
M_{\alpha, \beta}(u) = e^{-\frac{u}{2}} u^{\alpha + \frac{1}{2}} M\left(\frac{m - k + \frac{1}{2} + 2m; u}\right), \quad (19)
\end{equation}
with \( M(a, b; u) \) being Kummer’s confluent hypergeometric functions [17].

We observe, before proceeding to the analysis of the spectrum itself, that the solution \( \varphi(u) \) in (18) is odd under time reversal. Indeed, by mapping \( E_0 \) to \( -E_0 \), \( \varphi(u) \) goes to \( -\varphi(u) \), as it should.

We would like to have a solution \( \varphi(u) \) that is square integrable. For that we first note that as \( u \to \infty \) [17],
\begin{equation}
M(a, b; u) \approx \frac{e^{\pi a} \Gamma(b)}{\Gamma(b - a)} u^{-a} + \frac{\Gamma(b)}{\Gamma(a)} e^u u^{a - b} + O\left(\frac{1}{u}\right). \quad (20)
\end{equation}
Therefore, as \( u \to \infty \),
\begin{equation}
\varphi(u) \to \frac{A e^{\frac{u}{2}}}{\sqrt{u}} \left[ M_{\frac{1}{2}, -iE_0}(u_0) \frac{\Gamma(1 + 2iE_0)}{\Gamma(1 + iE_0)} - M_{\frac{1}{2}, +iE_0}(u_0) \frac{\Gamma(1 - 2iE_0)}{\Gamma(1 - iE_0)} \right]. \quad (21)
\end{equation}
Thus, the requirement of square integrability implies the condition
\begin{equation}
\frac{M_{\frac{1}{2}, -iE_0}(u_0)}{M_{\frac{1}{2}, +iE_0}(u_0)} = \frac{\Gamma(1 - 2iE_0)\Gamma(1 + iE_0)}{\Gamma(1 + 2iE_0)\Gamma(-iE_0)}. \quad (21)
\end{equation}
We now analyze condition (21) in the limit \( u_0 \to 0 \), but finite, which corresponds to a small but finite cut-off. Observe that ideally one would like to take \( u_0 \) equal zero. However, due to quantum instability associated with
a strongly attractive inverse-square potential, we cannot really remove it. Equivalently, if \( u_0 \) were zero, there would be a continuous spectrum of energy. Yet, it is sensible to consider an expansion for small \( u_0 \). In this case, by using certain properties of the Gamma function (see eq. (6.1.32) of [17]) and of the Whittaker function (19), we obtain

\[
\frac{\Gamma \left( \frac{1}{4} + \frac{iE_n}{2} \right)^2}{\Gamma \left( \frac{1}{4} - \frac{iE_n}{2} \right)^2} \left( \frac{u_0}{8} \right)^{-2iE_n} = \cot \left( \frac{\pi}{4} + \frac{iE_n}{2} \right).
\]

(22)

We now consider the limit of asymptotically large values of \( E_n \). In this asymptotic limit, using eqs. (22) and (4), we obtain

\[
e^{i4\theta(E_n)} \left( \frac{u_0}{8\pi} \right)^{-i2E_n} e^{-ix} = 1.
\]

(23)

This condition (23) is comparable to (but not the same), and indeed has the same spirit as, eq. (22) of [7] (instead of the dimensionless parameter \( L^2/\ell^2 \) there, here we have the parameter \( u_0 \)).

After we take the logarithm of both sides of eq. (23) and use (3), we obtain

\[
2 \frac{E_n}{2\pi} \log \left( \frac{u_0}{8\pi} \right) + \frac{9}{8} - 2(N(E_n)) = N_{E_n},
\]

(24)

where \( N_{E_n} \) is an integer, which, following [7], can be interpreted as counting the number of states whose energy is less than some fixed \( E_n \). Note that the factor of 2 on the l.h.s. of eq. (24) indicates that in this model the number of missing spectral lines is twice as much as in the usual \( xp \)-model. Equation (24) is almost identical to eq. (23) of [7].

It may be noted that the total energy of the system has a degeneracy arising from the quantity \( n \). However, as pointed out before, the above analysis is valid for each fixed value of \( n \). In addition, the interesting results arise from the analysis of the equation in the semi-infinite direction of the cylinder. Thus, the degeneracy arising from the appearance of the quantity \( n \) can be removed by fixing it to some arbitrary value, without loss of generality.

We have thus far shown that the \( xp \)-model together with the boundary condition (17) leads to an algebraic equation for the spectrum given by (22). On the one hand, this algebraic condition contains the phase of the Riemann Zeta function (4) which is part of the Riemann-van Mangoldt counting formula (1). On the other hand, apart from the ratios of certain Gamma functions, it contains an undetermined parameter, namely the cut-off \( u_0 \).

The appearance of the cut-off \( u_0 \) in (17) deserves some comments. As mentioned earlier, the cut-off \( u_0 \) is related to the self-adjoint extension parameter of the strongly attractive inverse-square potential on the half-line [18,19]. Similar to the discussions in [16,20] of a conformal quantum mechanics, this cut-off implies a breaking of the scale symmetry by quantization. That means that a scale anomaly emerges in this problem. Indeed, from a classical perspective, the \( xp \)-model, and also the \( xp \) one, is scale invariant. Also from another perspective, the Hamiltonian associated with eq. (15) in the short-distance limit is singular and scale invariant. But the boundary condition (17) breaks this scale invariance. The analysis of such singular behavior for equations like eq. (15) is given in [19]. The works [21–23] also contain important discussions for the emergence of a scale anomaly in a similar context.

The restoration of the scale anomaly at the quantum level is relevant for the problem of the Riemann Zeta function. Indeed, that allows us to enforce some of the requirements of Berry and Keating at the quantum level. One mechanism for the restoration of an otherwise anomalous symmetry is by the use of an appropriate mixed state [24]. This restoration mechanism with respect to the present problem is under current investigation and will be reported elsewhere.

Another objective of this letter is to present, following the spirit of the work of Sierra and Townsend [7], a possible physical realizations for the \( H = xp \) model. To this end, let us first consider the Calogero model, whose solutions can be classified using the degree \( k \) of a polynomial that appears in the analysis [25]. It was shown in [26] that for \( k = 0 \), the Calogero model with a complex coupling has real eigenvalues. The corresponding differential equation (see eq. (12) of [26]) has exactly the same form as eq. (15), although the parameters appearing in the equations in these two cases have different interpretations. The main similarity between the two lies in the fact that they both describe a system of strongly coupled inverse-square interaction. Such a system was first discussed by Landau, who observed that the strongly attractive inverse-square coupling leads to a quantum instability that was characterized by a “fall to the centre” [27]. Subsequently, a more complete quantum treatment was given by Case [19] who found that the spectrum is unbounded from below and is characterized by a one-parameter family of an undetermined constant. In technical terms, this unknown constant is nothing but the self-adjoint extension parameter, which encodes in itself the combined effects of the short-distance physics. In this work, as well as in [26], the same role is played by the cut-off \( u_0 \). Hence, the essential physics described here is that of a Calogero-type system with a strongly attractive inverse-square interaction.

This naturally leads to the question if there is indeed a physical system which realizes such a potential. If a physical system exists whose eigenvalue equation is exactly governed by eq. (15), then the spectrum of that physical system would provide a concrete realization of the Polya-Hilbert conjecture. While we do not have an exact answer to this question, we notice that there is a graphene system
whose equations are again very similar to what has been described above.

It is now well known that the dynamics of low-energy excitations in graphene is governed by a Dirac equation [28]. For our purpose, we consider the case of gapped graphene [29,30]. In the presence of an external supercritical Coulomb impurity [30–33], the effective radial equation for gapped graphene [34] has the same formal structure as that of eq. (15), although again with a different interpretation of the parameters. In addition, the solutions of a gapped-graphene system with supercritical Coulomb charge [34] have the same form as eq. (15) described above. When the external Coulomb charge in graphene is strongly attractive or equivalently in the supercritical region, the system again exhibits a quantum instability and a “fall to the centre” [31–36], whose qualitative behaviour is similar to what we find here. In a graphene system, such an instability manifests itself through characteristic features in the local density of states (LDOS), which, in principle, can be measured using a scanning tunneling microscope (STM) [31–33]. With a suitable reinterpretation of the system parameters, the STM measurements of the LDOS in gapped graphene with a supercritical Coulomb charge may yield valuable information regarding the spectrum of our model considered here.

It may also be mentioned that the same equation obtained in [26], appears in the analysis of non-relativistic AdS/CFT correspondence [37]. Typically, such strongly attractive inverse-square operators arise also in the analysis of the near-horizon conformal structure of black holes [38,39]. While none of these problems are identical to what has been considered here, the structural similarity of the equations and the corresponding solutions perhaps indicates a deeper relationship between these systems.

The systems described above share the common feature that they all correspond to a strongly attractive inverse-square potential characterized by quantum instability. In such systems, it is possible to employ a renormalization group scheme to address the issue of the instability [40]. The instability indicates an incomplete understanding of the short-distance physics. Typically such a system can be analyzed by first introducing a cut-off and then by studying the renormalization group flow of the relevant parameters of the system, given by the corresponding $\beta$-function. It would be interesting to study the consequences of the RG flow for the system described here.

In summary, in this letter, we have proposed a Dirac-type variant of the $H = xp$ given in eq. (8). We then analysed its spectrum and related it with the Riemann-van Mangoldt counting formula for the complex zeros of the Zeta function [2]. An important observation is that in order to find this quantum spectrum the scale invariance of the classical $xp$-model is necessarily broken. Based on this fact, we believe that the restoration of the scale invariance at the quantum level will have crucial implications to the Hilbert-Polya conjecture. Finally we suggested a physical realization of the present model in terms of the dynamics of the low-energy excitations of graphene in the presence of an external supercritical Coulomb impurity.

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