Bloch Solutions of Periodic Dirac Equations in SPPS Form

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Abstract
We provide the representation of quasi-periodic solutions of periodic Dirac equations in terms of the spectral parameter power series (SPPS) recently introduced by V.V. Kravchenko \[1, 2, 3\]. We also give the SPPS form of the Dirac Hill discriminant under the Darboux nodeless transformation using the SPPS form of the discriminant and apply the results to one of Razavy’s quasi-exactly solvable periodic potentials.

1 Introduction
The connections between the Dirac equation and the Schrödinger equation are known since a long time ago \[4\] and have been strengthen in the supersymmetric context soon after the advent of supersymmetric quantum mechanics in 1981 \[5, 6, 7, 8\]. There are currently interesting applications of this approach in condensed matter physics \[9, 10, 11\]. In this work, we are interested in the same connection in the case of periodic potentials, see e.g. \[12\]. We here write the Dirac Bloch solutions in Kravchenko form (power series in the spectral parameter) and also the Dirac Hill discriminant in the same form and apply the results to an interesting quasi-exactly solvable periodic potential.

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2 Schrödinger equations of Hill type

The Schrödinger differential equation

\[ L[f(x, \lambda)] = -f''(x, \lambda) + q(x)f(x, \lambda) = \lambda f(x, \lambda) \tag{1} \]

with \( T \)-periodic real-valued potential \( q(x) \) assumed herewith a continuous bounded function and \( \lambda \) a real parameter is known as of Hill type. We begin by recalling some necessary definitions and basic properties associated with the equation \( \text{(1)} \) from the Floquet (Bloch) theory. For more details see, e.g., [13, 14].

For each \( \lambda \) there exists a fundamental system of solutions, i.e., two linearly independent solutions of \( \text{(1)} \), \( f_1(x, \lambda) \) and \( f_2(x, \lambda) \), which satisfy the initial conditions

\[ f_1(0, \lambda) = 1, \quad f_1'(0, \lambda) = 0, \quad f_2(0, \lambda) = 0, \quad f_2'(0, \lambda) = 1. \tag{2} \]

Then the Hill discriminant associated with equation \( \text{(1)} \) is defined as a function of \( \lambda \) as follows

\[ D(\lambda) = f_1(T, \lambda) + f_2'(T, \lambda). \]

The importance of \( D(\lambda) \) stems from the easiness of describing the spectrum of the corresponding equation by its means, namely [13]:

1. sets \( \{ \lambda_i \} \) for which \( |D(\lambda)| \leq 2 \) form the allowed bands or stability intervals,
2. sets \( \{ \lambda_j \} \) for which \( |D(\lambda)| > 2 \) form the forbidden bands or instability intervals,
3. sets \( \{ \lambda_k \} \) for which \( |D(\lambda)| = 2 \) form the band edges and represent the discrete part of the spectrum.

Furthermore, when \( D(\lambda) = 2 \) equation \( \text{(1)} \) has a periodic solution with the period \( T \) and when \( D(\lambda) = -2 \) it has an aperiodic solution, i.e., \( f(x + T) = -f(x) \). The eigenvalues \( \lambda_n, n = 0, 1, 2, ... \) form an infinite sequence \( \lambda_0 < \lambda_1 \leq \lambda_2 < \lambda_3 \leq \lambda_4, ... \), and an important property of the minimal eigenvalue \( \lambda_0 \) is the existence of a corresponding periodic nodeless solution \( u(x, \lambda_0) \) [13]. The solutions of \( \text{(1)} \) are not periodic in general, and one of the important tasks is the construction of quasiperiodic solutions defined by \( f_\pm(x + T) = \beta_\pm(\lambda)f_\pm(x) \).

Here, we use James’ matching procedure [15] that employs the fundamental system of solutions, \( f_1(x, \lambda) \) and \( f_2(x, \lambda) \), in the construction of the quasiperiodic solutions as follows

\[ f_\pm(x, \lambda) = \beta_\pm(\lambda) [f_1(x - nT, \lambda) + \alpha_\pm f_2(x - nT, \lambda)], \quad \begin{cases} nT \leq x < (n + 1)T \\ n = 0, \pm 1, \pm 2, ... \end{cases} \tag{3} \]

where \( \alpha_\pm \) are given by [15]

\[ \alpha_\pm = \frac{f_2'(T, \lambda) - f_1(T, \lambda) + (D^2(\lambda) - 4)^{\frac{1}{2}}}{2f_2(T, \lambda)}. \tag{4} \]
The Bloch factors \( \beta_\pm(\lambda) \) are a measure of the rate of increase (or decrease) in magnitude of the linear combination of the fundamental system when one goes from the left end of the cell to the right end, i.e.,

\[
\beta_\pm(\lambda) = \frac{f_1(T, \lambda) + \alpha_\pm f_2(T, \lambda)}{f_1(0, \lambda) + \alpha_\pm f_2(0, \lambda)}.
\]

The values of \( \beta_\pm(\lambda) \) are directly related to the Hill discriminant, \( \beta_\pm(\lambda) = \frac{1}{2}(D(\lambda) \mp \sqrt{D^2(\lambda) - 4}) \), and obviously at the band edges \( \beta_+ = \beta_- = \pm 1 \) for \( D(\lambda) = \pm 2 \), respectively.

### 3 SPPS representation for solutions of the one-dimensional Dirac equation

We consider the following Dirac equation

\[
L[W] = [-i\sigma_y d_x + \sigma_x \Phi(x)] W = \omega W, \tag{5}
\]

where the scalar potential \( \Phi(x) \) is periodic function with period \( T \), \( W \) is the spinor \( W = \begin{pmatrix} f \\ g \end{pmatrix} \) and \( \sigma_x, \sigma_y \) are the Pauli matrices \( \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \) and \( \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \).

The uncoupled Schrödinger equations derived from equation (5) are

\[
(-d_x + \Phi)(d_x + \Phi)f = \lambda f, \tag{6}
\]
\[
(d_x + \Phi)(-d_x + \Phi)g = \lambda g, \tag{7}
\]

where \( \lambda = \omega^2 \) is the spectral parameter. It is clear that the solutions \( f \) and \( g \) are related by the following relationship

\[
(d_x + \Phi)f = \omega g, \tag{8}
\]

therefore with the solution \( f \) at hand, we can construct the solution \( g \) immediately.

We start with equation (8). Notice that the solution \( u \) of the equation (6) for \( \lambda = 0 \) can be obtained as follows \( u(x) = e^{-\int \Phi(x)dx} \) and \( u(x) \) is a nodeless periodic function with the period \( T \) if \( \Phi(x) \in \mathbb{C}^1 \) and \( \int_0^T \Phi(x)dx = 0 \).

Once having the function \( u(x) \) the solutions \( f_1(x, \lambda) \) and \( f_2(x, \lambda) \) of (6), (2) for all values of the parameter \( \lambda \) can be given using the SPPS method [1].

\[
f_1(x, \lambda) = \frac{u(x)}{u(0)} \hat{\Sigma}_0(x, \lambda) + u'(0)u(x)\Sigma_1(x, \lambda),
\]
\[
f_2(x, \lambda) = -u(0)u(x)\Sigma_1(x, \lambda). \tag{9}
\]
The functions $\tilde{\Sigma}_0$ and $\Sigma_1$ are the spectral parameter power series

$$
\tilde{\Sigma}_0(x, \lambda) = \sum_{n=0}^{\infty} \tilde{X}^{2n}(x) \lambda^n, \quad \Sigma_1(x, \lambda) = \sum_{n=1}^{\infty} X^{2n-1}(x) \lambda^{n-1},
$$

where the coefficients $\tilde{X}^{(n)}(x), X^{(n)}(x)$ are given by the following recursive relations

$$
\tilde{X}^{(0)}(x) \equiv 1, \quad X^{(0)}(x) \equiv 1,
$$

$$
\tilde{X}^{(n)}(x) = \begin{cases} 
\int_0^x \tilde{X}^{(n-1)}(\xi) u^2(\xi) d\xi & \text{for an odd } n \\
- \int_0^x \tilde{X}^{(n-1)}(\xi) \frac{d\xi}{u^2(\xi)} & \text{for an even } n
\end{cases} \quad (10)
$$

$$
X^{(n)}(x) = \begin{cases} 
- \int_0^x X^{(n-1)}(\xi) \frac{d\xi}{u^2(\xi)} & \text{for an odd } n \\
\int_0^x X^{(n-1)}(\xi) u^2(\xi) d\xi & \text{for an even } n
\end{cases} \quad (11)
$$

One can check by a straightforward calculation that the solutions $f_1$ and $f_2$ fulfill the initial conditions (2), for this the following relations are useful

$$
\frac{d}{dx} \left( \tilde{\Sigma}_0(x, \lambda) \right) = -\frac{\tilde{\Sigma}_1(x, \lambda)}{u^2(x)}, \quad \text{where} \quad \tilde{\Sigma}_1(x, \lambda) = \sum_{n=1}^{\infty} \tilde{X}^{2n-1}(x) \lambda^n \quad (12)
$$

and

$$
\frac{d}{dx} \left( \Sigma_1(x, \lambda) \right) = -\frac{\Sigma_0(x, \lambda)}{u^2(x)}, \quad \text{where} \quad \Sigma_0(x, \lambda) = \sum_{n=0}^{\infty} X^{2n}(x) \lambda^n. \quad (13)
$$

The pair of linearly independent solutions $g_1(x, \lambda)$ and $g_2(x, \lambda)$ of (7) can be obtained directly from the solutions (9) by means of (8). We additionally take the linear combinations in order that the solutions $g_1(0, \lambda)$ and $g_2(0, \lambda)$ satisfy the initial conditions $g_1(0, \lambda) = g_2'(0, \lambda) = 1$ and $g_1'(0, \lambda) = g_2(0, \lambda) = 0$

$$
g_1(x, \lambda) = \frac{u(0)}{u(x)} \tilde{\Sigma}_0(x, \lambda) - \frac{\Phi(0)}{\lambda u(0) u(x)} \Sigma_1(x, \lambda),
$$

$$
g_2(x, \lambda) = \frac{1}{\lambda u(0) u(x)} \tilde{\Sigma}_1(x, \lambda). \quad (14)
$$

Thus, the two spinor solutions of the Dirac equation (5) are given by

$$
W_1 = \begin{pmatrix} f_1 \\ g_1 \end{pmatrix}, \quad \text{and} \quad W_2 = \begin{pmatrix} f_2 \\ g_2 \end{pmatrix}
$$

and these solutions satisfy the following initial conditions

$$
W_1(0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \text{and} \quad W_2(0) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.
$$
3.1 Bloch solutions and Hill’s discriminant

The second order differential equations (6) and (7) have periodic potentials $V_{1,2} = \Phi' \pm \Phi''$, correspondingly. The important tasks for this case are the construction of the Bloch solutions which are subject to the Bloch condition $f(x + T) = e^{ikT}f(x)$ ($k$, a wave number) and the description of the spectrum.

In [16] the SPPS representations of Hill discriminants $D_f(\lambda)$ and $D_g(\lambda)$ associated with the equations (6) and (7) were obtained in the form

$$D_f(\lambda) = \frac{u(T)}{u(0)}\Sigma_0(T, \lambda) + \frac{u(0)}{u(T)}\Sigma_0(T, \lambda) + (u'(0)u(T) - u(0)u'(T))\Sigma_1(T, \lambda),$$

$$D_g(\lambda) = \frac{u(0)}{u(T)}\Sigma_0(T, \lambda) + \frac{u(T)}{u(0)}\Sigma_0(T, \lambda) + \frac{1}{(\Delta \lambda)u^2(0)u^2(T)}(u'(0)u(T) - u(T)u'(0))\Sigma_1(T, \lambda).$$

It is clear that since $u(x)$ is a $T$-periodic function ($u(0) = u(T)$) the expression in brackets in the above formulae vanishes. Now writing the explicit expressions for $\Sigma_0(T, \lambda, \lambda_0)$ and $\Sigma_0(T, \lambda, \lambda_0)$, a representation for Hill’s discriminant associated with (6) and (7) is the following

$$D_f(\lambda) = D_g(\lambda) = \sum_{n=0}^{\infty} \left(\tilde{X}^{(2n)}(T) + X^{(2n)}(T)\right)\lambda^n. \quad (15)$$

Equations (6) and (7) are isospectral and we obtain the Hill discriminant associated with the Dirac equation (5). We formulate this result as the following theorem:

**Theorem.** Let $\Phi(x) \in C^1$ be a $T$-periodic function which satisfies the condition $\int_0^T \Phi(x)dx = 0$. Then the Hill discriminant for (5) has the form

$$D_W(\omega) = \sum_{n=0}^{\infty} \left(\tilde{X}^{(2n)}(T) + X^{(2n)}(T)\right)\omega^{2n},$$

where $\tilde{X}^{(2n)}$ and $X^{(2n)}$ are calculated according to (11) and (17), $u = e^{-\int \Phi(x)dx}$ and the series converges uniformly on any compact set of values of $\omega$.

In order to construct the Bloch solutions for the Dirac equation (5) we use the solutions (9) and (14) and apply the procedure of James [15]. Notice that because the Hill discriminants for the equations (6) and (7) are identical the Bloch factors for both equations are equal. The so-called self-matching solutions for the equations (6) and (7), are correspondingly

$$F_{\pm}(x, \lambda) = f_1(x, \lambda) + a_{\pm}f_2(x, \lambda) \quad \text{and} \quad G_{\pm}(x, \lambda) = g_1(x, \lambda) + b_{\pm}g_2(x, \lambda),$$
where \(a_{\pm}\) and \(b_{\pm}\) are calculated by the formula (4) with the corresponding fundamental system of solutions (9) and (14). By means of \(F_{\pm}\) and \(G_{\pm}\) we write the self-matching spinor solution of the equation (5)

\[
w_{\pm}(x, \lambda) = \begin{pmatrix} F_{\pm}(x, \lambda) \\ G_{\pm}(x, \lambda) \end{pmatrix}.
\]

Finally, the Bloch solutions of the equation (5) take the form

\[
W_{\pm}(x, \lambda) = \beta_{\pm}(\lambda) \left( w_{\pm}(x - nT, \lambda) \right), \quad \left\{ \begin{array}{l} nT \leq x < (n + 1)T \\ n = 0, \pm 1, \pm 2, \ldots \end{array} \right.
\]

4 Numerical calculation of eigenvalues based on the SPPS form of Hill’s discriminant

As is well known [13], the zeros of the functions \(D(\lambda) \mp 2\) represent eigenvalues of the corresponding Hill operator with periodic and aperiodic boundary conditions, respectively. In this section, we show that besides other possible applications the representation (15) gives us an efficient tool for the calculation of the discrete spectrum of a periodic Dirac operator.

The first step of the numerical realization of the method consists in calculation of the functions \(\tilde{X}(n)\) and \(X(n)\) given by (10) and (11), respectively. This construction is based on the eigenfunction \(u(x)\). Next, by truncating the infinite series for \(D(\lambda)\) (15) we obtain a polynomial in \(\lambda\)

\[
D_N(\lambda) = \sum_{n=0}^{N} \left( \tilde{X}^{(2n)}(T) + X^{(2n)}(T) \right) \lambda^n
\]

\[
= 2 + \sum_{n=1}^{N} \left( \tilde{X}^{(2n)}(T) + X^{(2n)}(T) \right) \lambda^n.
\]

The roots of the polynomials \(D_N(\lambda) \mp 2\) give us the eigenvalues corresponding to equation (1) with periodic and aperiodic boundary conditions, respectively.

As an example we consider the Dirac equation (5) with the scalar potential

\[
\Phi(x) = \sin 2x \left[ \frac{\xi}{2} - \frac{2A(\xi)}{\xi - A(\xi) \cos 2x} \right],
\]

with \(A(\xi) = \left( 1 - \sqrt{1 + \xi^2} \right)\) and \(\xi\) a real positive parameter. This scalar potential satisfies the conditions of theorem 3.1. The corresponding second order differential equations are

\[
-d_x^2 f + V_1 f = \lambda f,
\]

\[
-d_x^2 g + V_2 g = \lambda g,
\]
where the Schrödinger potential

\[ V_1(x) = \frac{\xi^2}{8} (1 - \cos 4x) - 3\xi \cos 2x, \]  

is the case \( m = 2 \) in the quasi-exactly solvable family of the so-called trigonometric Razavy potentials \[17\], \( V_R = \frac{\xi^2}{8} (1 - \cos 4x) - (m + 1)\xi \cos 2x \). For a given integer \( m \), if \( \xi < 2(m + 1) \) the potentials \( V_R(x) \) are of single-well periodic type and if \( \xi > 2(m + 1) \) they are of double-well periodic type.

\[ V_2(x) = V_1(x) + 4 \cos 2x \left( \frac{\xi}{2} - \frac{2A(\xi)}{\xi - A(\xi) \cos 2x} \right) + \frac{8A(\xi) \sin^2 2x}{(\xi - A(\xi) \cos 2x)^2} \]  

is the supersymmetric partner potential and therefore it is also quasi-exactly solvable. The Schrödinger equations with these potentials can be used for the description of torsional oscillations of certain molecules \[17\]. Plots of the potentials \( V_1(x) \) and \( V_2(x) \) are displayed in Fig. 1 for two values of \( \xi \).

The computer algorithm was implemented in Matlab 2006. The recursive integration required for the construction of \( \tilde{X}_0(n), X_0(n), \tilde{X}(n) \) and \( X(n) \) was done by representing the integrand through a cubic spline using the \texttt{spapi} routine with a division of the interval \([0, \pi]\) into 5000 subintervals and integrating using the \texttt{fnint} routine. Next, the zeros of \( D_N(\lambda) \pm 2 \) were calculated by means of the \texttt{fnzeros} routine.

In the following tables, the eigenvalues were calculated employing the SPPS representation \[15\] for four different values of the parameter \( \xi \). The first two values are below the threshold value \( \xi_{thr} = \frac{1}{6} \) for \( m = 2 \) from single-well to
double-well types of Razavy’s potentials while the last two values are above this threshold value. For comparison, we use the eigenvalues given analytically by Razavy in terms of the parameter \( \xi \) as follows \[^\text{(17)}\]

\[
\lambda_0 = 2 \left( 1 - \sqrt{1 + \xi^2} \right), \quad \lambda_3 = 4, \quad \lambda_4 = 2 \left( 1 + \sqrt{1 + \xi^2} \right).
\]

| \( n \) | \( \xi = 1 \) (SPPS) | \( \lambda_n \) (Ref. \[^\text{(17)}\]) |
|-------|----------------|----------------|
| 0     | -0.828427124746190 | -0.828427124746190 |
| 1     | -0.628906956748252 |                               |
| 2     | 2.315132548422588  |                               |
| 3     | 3.999991462865745  | 4                           |
| 4     | 4.828420096225068  | 4.828427124746190           |
| 5     | 9.238264469324272  |                               |
| 6     | 9.294265517212145  |                               |

| \( n \) | \( \xi = 2 \) (SPPS) | \( \lambda_n \) (Ref. \[^\text{(17)}\]) |
|-------|----------------|----------------|
| 0     | -2.472135954999580 | -2.472135954999580 |
| 1     | -2.428136886851045 |                               |
| 2     | 3.184130151531468  |                               |
| 3     | 4.000004180961838  | 4                           |
| 4     | 6.472138385406806  | 6.472135954999580           |
| 5     | 9.864117523158974  |                               |
| 6     | 10.253256926576858 |                               |

| \( n \) | \( \xi = 11 \) (SPPS) | \( \lambda_n \) (Ref. \[^\text{(17)}\]) |
|-------|----------------|----------------|
| 0     | -20.09072203437452 | -20.09072203437452 |
| 1     | -20.090721031408926 |                               |
| 2     | 3.999728397824670  |                               |
| 3     | 4.000000543012631  | 4                           |
| 4     | 24.092379855485746 | 24.090722034374522           |
| 5     | 24.125593160436161 |                               |
| 6     | 36.212102534969766 |                               |

| \( n \) | \( \xi = 20 \) (SPPS) | \( \lambda_n \) (Ref. \[^\text{(17)}\]) |
|-------|----------------|----------------|
| 0     | -38.049968789001575 | -38.049968789001575 |
| 1     | -38.049968789002322 |                               |
| 2     | 3.999999942823312  |                               |
| 3     | 3.999999999630503  | 4                           |
| 4     | 42.050313148383374 | 42.049968789001575           |
| 5     | 42.050347742353317 |                               |
| 6     | 74.691604620863302 |                               |

In Fig. 2, we display the plots of the Hill discriminants for the values of the Razavy parameter \( \xi = 1, \xi = 2, \) and \( \xi = 3, \) respectively. In general, these
plots contain damped oscillations with higher amplitudes at higher $\xi$. On the other hand, getting the spectrum in $\lambda$ is equivalent with having the eigenvalues $\omega_n = \pm \sqrt{\lambda_n}$ of the Dirac system under consideration.

Fig. 2: The polynomial $D_N(\lambda)$ for the Hill equations with Razavy’s partner potentials for three values of the parameter $\xi$ calculated by means of formula (16) for $N = 100$. The first minimum of the discriminant in this plot, i.e., for $\xi = 3$, goes down to -260.9 at $\lambda = -2.469$.

5 Conclusions

In summary, in this work we presented the SPPS form of the quasi-periodic (Bloch) solutions of periodic one-dimensional Dirac operators as well as of the Hill discriminant. We applied the obtained results to the Dirac system with the periodic scalar potential that leads to one of Razavy’s quasi-exactly solvable periodic potentials.

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